PREFACE

The Greek Association of Computational Mechanics (GRACM), founded in 1991, represents a small but active scientific community in Greece. Being affiliated with the International Association for Computational Mechanics (IACM) and the European Community on Computational Methods in Applied Sciences (ECCOMAS), GRACM has been from the very beginning oriented towards international scientific interaction and cooperation. The GRACM Conferences aim at bringing together the members of the Greek computational mechanics community, domestic and of the diaspora, and colleagues from abroad, mainly from academia.

A main target of this 7th GRACM Congress was the participation of young researchers, with particular consideration of the adverse circumstances in the country. This was promoted by offering reduced fees and by encouraging the organization by them of special sessions on state-of-the-art topics. The coexistence, for the first time in GRACM conferences, of stand-alone sessions on computational biomechanics and systems biology with traditional ones, such as on earthquake engineering and fluid mechanics, is a major success of the Congress.

The 7th GRACM Congress hosts the 1st ECCOMAS PhD Olympiad 2011, a newly launched forum for the presentation of the best PhD theses completed in the last year within the affiliated Societies of ECCOMAS.

The Congress CD-proceedings include the program, abstracts and full papers as well as the abstracts of the 1st ECCOMAS PhD Olympiad. This Book of Abstracts contains all abstracts of the two events.

We thank the authors and speakers for their contribution and participation, the invited speakers for their inspiring presentations, the paper reviewers and the members of the Scientific Committee for their help in securing the scientific quality of the Congress, and the members of the Organizing Committee for their hard work in getting everything right and on time. We are also thankful to our technical and financial sponsors: the National Technical University of Athens, the Technical University of Crete, the National Center for Scientific Research “Demokritos”, the Mentor Hellas Scientific Engineering Software, the BETA CAE Systems SA, and the NIKI Information Technologies & Digital Engineering.

Athens, June 2011

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A DEVICE FOR MULTIPLE INDENTATION TESTS OF CARTILAGE DISKS


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Keywords: cartilage, degeneration, high-throughput, indentation

ABSTRACT

Cartilage degeneration is undoubtedly severe for patients with osteoarthritis (OA), one of the most common diseases of articular cartilage with great social impact. Thus, mechanical properties of articular cartilage are of great importance concerning the ability of the tissue to carry loads and therefore fulfilling its purpose. It is also well proven that, OA results in a dramatic degradation of the tissue mechanical properties, thus causing severe pain due to bone-to-bone contact.

In order to determine whether a cartilage disk is osteoarthritic or normal, there are various biological and biomechanical indicators. Our endeavour is to understand the intracellular mechanisms that lead to cartilage degeneration and develop novel treatments that block the degenerative mechanisms. Concentrating on the biomechanical aspect, indentation tests of cartilage disks is the most common way to measure the tissue’s mechanical properties, of which Young’s Modulus is the most widely used. Practically, observing the progress of the tissue’s Young’s Modulus over time when treated with specific degeneration-causing stimuli and disease-modifying compounds (i.e. inhibitors), could provide us with useful data on whether the cartilage degeneration evolves or not and at what degree. To date these indentation tests of single disk explants last over a week per disk which, taking into account the complexity of cells and the amount of the disks that must be tested, makes the screening of compounds intractable.

In this paper, we propose a 24-parallel measurement device which could apply creep indentation tests on cartilage disks. Our device consists of a well plate head guide that positions 24 indenters in the center of 24 wells of a standard 24-well plate, which allows all biomechanical researchers to use it. The motion of the indenters is monitored every 4 minutes, by a LASER displacement sensor (μ-ε ILD1402) that allows accuracy ±2μm. The necessary movement of the plate, in order to use only one sensor, is carried out by a two-axes stage, driven by software. Different media and drugs can be used and the media can be replaced via a custom designed liquid-handling system, during the experiment. In each well, a 3mm cartilage disk (1 to 2mm in thickness) is centered by a conical part and compressed under the constant weight of the 20gr indenter. The dimensions of the device allow the usage of incubator to succeed suitable conditions for the experiments. To analyze the data, a finite elements model that simulates the indentation test has been employed.

Mechanical properties are determined by replicating the creep test in-silico and by cross-referencing the simulation results with the experimental response curves. A biphasic model of articular cartilage is constructed within the ABAQUS (FEM software) framework and Young's modulus is incorporated as a free parameter. By fitting the model to measured stress-strain curves, an estimation of Young's modulus is evaluated.

Major applications of this device are in the area of tissue engineering and soft tissue biomechanics. In this paper we would like to quantify the efficacy of multiple potential drugs for arthritis. In each plate, 24 cartilage disk explants treated with different compounds together with degeneration-causing stimuli are monitored over time, and their Young’s modulus is recorded real time. Moreover, being able to measure the progress of Young’s Modulus during the whole process and not at certain time intervals gives us the ability to compare normal and osteoarthritic as well as the efficacy of the compounds to modify the progress of cartilage degeneration.

For the purpose of this paper we conducted creep indentation tests, as described above, on bovine cartilage disks: normal disks, disks treated with human interleukin (IL-1a) -a stimuli proven to cause cartilage degeneration-and disks treated with collagenase –an enzyme proven to cause rapid matrix degradation. Finally, we compare the results between them and with those taken from similar single disk indentation tests. In that way, we accelerated the whole process three times and we acquired the progress of the disks’ Young’s Modulus in a real time basis.
TACKLING CARTILAGE DEGENERATION VIA A COMBINATION OF SYSTEMS BIOLOGY AND BIOMECHANICS APPROACH

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Keywords: Biomechanics, Systems Biology, Biphasic Theory, Proteomics, Signaling Pathways.

1. ABSTRACT

Arthritis is the leading cause of disability in Europe affecting one of every six people and resulting in a significant burden for our economy and our society. The most common type of arthritis is osteoarthritis (OA), a painful disease, in which cartilage is degenerated and loses its mechanical integrity. It is now evident that OA is not just a natural cause of aging but an imbalance of signaling mechanisms that leads to cartilage degeneration.

Two different approaches are proposed to study OA: Systems Biology and Biomechanics. The systems biology approach uses ground-breaking experimental assays and an optimization formulation to identify the intracellular signaling mechanisms that are responsible for cartilage degeneration. The biomechanics approach uses biphasic theory to quantify the degeneration of the tissue. The combination of those approaches can shed a light into possible treatments of osteoarthritis.

2. METHODS

Systems Biology approach: Cartilage cells known as chondrocytes are isolated from human femoral heads following standard isolation procedures, stimulated by 90 different cytokines and then incubated for up to 24 hours. 18 intracellular and 60 extracellular signals are measured using a high throughput method of bead-based fluorescent readings (Luminex xMAP assay, Austin, TX). Data are normalized and plotted using custom software based on DATARAIL, and subsequent analysis is performed using PLSR, PCA, clustering algorithm, and integer linear programming (ILP) formulation.

Biomechanics approach: Two types of models are used to quantify tissue degeneration: an analytical, linear elastic model and a biphasic model. The presence of fluid-phase is used to model the viscoelastic behavior of cartilage explants (via the hydraulic permeability, k).

3. RESULTS

The biomechanics approach is able to quantify the mechanical degeneration of the tissue whereas the Systems Biology approach is able to identify proteins in the body that are responsible for cartilage degeneration such as the known IL1a, IL1b, and TNFα but also the less known TLR stimuli. Closer look into the pathways constructed by the ILP formulation identify possible ways of reversing the loss of mechanical properties via targeting of the NFκB and possibly the p38 pathway. Follow up experiment using selective p38 and IKK inhibitors proved the pro-catabolic response of chondrocytes triggered by TLR agonists is NFκB dependant.

4. CONCLUSIONS

The combination of Systems Biology and Biomechanics was able to identify new players of OA but also revealed new ways of inhibiting cartilage degeneration by selected drug targets. Our approach sheds a light into possible treatments of osteoarthritis and suggests novel therapeutic interventions of a disease with incredible medical, economic, and social impact.
NON-EQUILIBRIUM MOLECULAR DYNAMICS SIMULATION OF THE STRETCHING BEHAVIOR OF ADHESIVE POLYMERS

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Keywords: Stretching deformation, Non-Equilibrium Molecular Dynamics Simulations, Adhesives

ABSTRACT

Based on principles of statistical mechanics [1], we have developed a generalized non-equilibrium molecular dynamics (NEMD) algorithm for the molecular simulation of the stretching deformation [2] of adhesive polymers adsorbed on solid substrates. The simulations are carried out in the \( NP_{xx}P_{yy}P_{zz}T \) statistical ensemble [3-4], where \( N \) denotes the number of interacting atomistic units in the system, \( P_i \) the normal pressure in the \( i \)-direction, and \( T \) the temperature. In the present work, we focus on the deformation of a polymeric system under conditions of uniaxial deformation [5]. This refers to a sample confined between two parallel substrates that are being pulled apart with a constant rate. The simulations in this case are conducted in the \( NP_{xx}L_yP_{zz}T \) statistical ensemble implying that one has full control on the box dimension \( L_y \) along the stretching (\( y \)-) direction.

To test the code we first employed it in exploratory simulations with three linear polyethylene (PE) melts (a 240-chain \( C_{50}H_{102} \) system at density \( \rho = 0.74 \) g/cm\(^3\), a 216-chain \( C_{178}H_{358} \) system at density \( \rho = 0.75 \) g/cm\(^3\), and a 216-chain \( C_{400}H_{802} \) system at density \( \rho = 0.76 \) g/cm\(^3\)) [6], all of them confined between two graphitic surfaces. The three systems were subjected to uniaxial elongation along the \( y \)-direction at \( T = 450 \) K in the \( NP_{xx}L_yP_{zz}T \) statistical ensemble by pulling the sample along the \( y \)-direction at constant velocity. The lateral values of the pressure (i.e., along the \( x \)- and \( z \)- directions) were both set equal to 1 atm. At \( T = 450 \) K, the system longest relaxation time is \( \sim 0.56 \) ns for the \( C_{50}H_{102} \) PE, \( \sim 15.6 \) ns for the \( C_{178}H_{358} \) PE, and \( \sim 220 \) ns for the \( C_{400}H_{802} \) PE melt. As an example of the quality of the results that can be obtained by such a simulation experiment, we mention that for the \( C_{178}H_{358} \) PE system subjected to a stretching rate that corresponds to a Weissenberg number (\( Wi \)) equal to 1000, several cavities formed inside the system after approximately 14 ps, which eventually led to crazing and fracture of the material.

Results will also be presented from corresponding deformation simulations not with PE but with model acrylic adhesives, such as random copolymers of n-butyl acrylate with a short side-chain acrylic like methyl acrylate and acrylic acid.

IMPLEMENTATION OF A CYCLIC SOIL PLASTICITY MODEL IN A FINITE-DIFFERENCE SOLUTION ALGORITHM

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Keywords: Bounding surface plasticity, critical state models, liquefaction, explicit integration, automatic substepping, finite-difference code, lateral spreading

ABSTRACT

The numerical procedure followed for the implementation of the NTUA-SAND model in a Finite Difference solution algorithm is presented herein. The NTUA-SAND model is a bounding surface plasticity model developed for the simulation of monotonic and cyclic loading of non-cohesive soils, while special attention is given to liquefaction related phenomena. It uses the framework of Critical State Soil Mechanics, while it incorporates three open cone-type surfaces with apex at the origin of stress space: (i) the critical surface at which deviatoric deformation develops for fixed stresses and no volume change (constant void ratio e), (ii) the bounding surface which locates the peak deviatoric stress ratios states and (iii) the dilatancy surface which dictates the sign of the plastic volumetric strain increment during loading. A vanished elastic region is also adopted so that the response in every step is elasto-plastic. The NTUA-SAND model was implemented in the commercially available finite-difference code FLAC using its UDM capability. Stress-integration was accomplished with the aid of a sub-stepping technique with automatic error control. The algorithm belongs to the family of explicit stress-integration techniques and divides automatically the applied strain increment into sub-increments. An appropriate size of each substep is found through the use of a modified second-order Euler scheme. The overall accuracy of this scheme is evaluated at element level by simulating cyclic loading along complex stress paths. The performance of the numerical algorithm in complex boundary value problems is evaluated in terms of accuracy and computational cost, via a number of parametric analyses studying the lateral spreading response of an inclined liquefied sand layer.
MOLECULAR DYNAMICS SIMULATION OF IMIDAZOLIUM-BASED [Tf2N-]
IONIC LIQUIDS

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Keywords: ionic liquids, molecular simulation, molecular dynamics

ABSTRACT

Ionic Liquids (ILs) are organic salts with melting points usually near room temperature. Their most remarkable property is that their vapor pressure is negligibly small, so that ILs are non-volatile, non-flammable and odorless. Other characteristics of ILs include high thermal and electrochemical stability, high ionic conductivity and good solvency properties. In principle, ILs can be tailored for a specific application by the right choice of cation and anion and are potential candidates for use in a wide range of applications as environmentally benign reaction and separation media. Especially, the imidazolium based ILs family has received significant attention in terms of experimental investigation and molecular modeling of their structural, thermodynamic and transport properties.

In the present work, the behavior of [Cₙmim][Tf₂N⁻], n = 4, 8, 12 ILs at a wide range of thermodynamic points is examined by means of molecular dynamics (MD) simulation. This type of cations is consisted of an imidazolium ring and one alkyl chain with n carbon atoms. A previously developed methodology for the calculation of the charge distribution which incorporates ab initio quantum mechanical calculations based on density functional theory (DFT) was used to accurately parameterize the atomistic force field to be used in the classical molecular simulations. Long molecular dynamics simulations of several tens of nanoseconds, were performed in order to extract the thermodynamic (density, thermal expansion, isothermal compressibility), structural (conformational analysis, radial distribution functions between the centers of mass of ions and between individual sites) and dynamical (relaxation times of the reorientation of the bonds and the torsion angles, self-diffusion coefficients) properties. The influence of the temperature and the cation’s alkyl chain length on the above mentioned properties was thoroughly investigated. The calculated thermodynamic, structural and derivative properties are in good agreement with the experimental data. ILs under study were found to have extremely slow dynamics as indicated also by the wide range of relaxation times calculated, a fact that makes the calculation of their diffusivity a very challenging task, especially at low temperatures.
CFD MODELLING OF VERTICAL ELECTRICAL FURNACE FOR PERLITE EXPANSION – STUDY OF AIR TEMPERATURE AND VELOCITY PROFILES

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Keywords: Industrial mineral, Perlite, Expansion, CFD.

ABSTRACT

Expanded perlite is widely used in Construction and Manufacturing industry mainly due to its good thermal and acoustical insulating properties. Although expanded perlite has a number of favourable properties, it is also characterised by some unfavourable properties, like low mechanical properties and unacceptably high “open” porosity, limiting the range of its applications. These unfavourable properties are the result of the applied expansion technology. Generally, perlite expansion is performed by feeding raw perlite grains into a vertical furnace heated by direct gas flame at its bottom end and directing a forced air flow upwardly. The ore particles are typically introduced to the hottest region of the expansion chamber near the flame, at a temperature of about 1450 °C. At these conditions raw perlite expands 10 to 15 times its original volume producing a material of bulk density in the range of 60 – 120 kg/m³ that is 20 – 40 times lower than the bulk density of crude perlite. The main problems of this process include the violent and poorly controlled heating of perlite, resulting in sponge-like, soft, porous particles and the large heat losses due to the hot off-gasses stream, leading to high energy consumption.

The objective of the thermal processing of perlite in a vertical electrical furnace is to produce expanded material characterized by low density, spherical shape and non porous external surface. The electrically heated vertical furnace provides fully controlled operational conditions, such as heating rate and retention time, and can lead to the production of expanded perlite particles with enhanced mechanical, insulating and physical properties. In this furnace, the continuous feeding of raw perlite takes place from the top, and heating is properly controlled throughout the whole area of the furnace and the temperature is gradually increased from 800 °C at the top of the furnace to 1200 °C at its bottom.

The aim of this work is the application of a computational fluid dynamics (CFD) approach to study the field of temperature and air velocity profiles inside the vertical electrical expansion furnace in order to understand and optimise the system thermal behaviour. In this frame the effect of various operational parameters including the temperature and flow rate of the feed air and the temperature of the furnace wall on the air velocity and temperature profile has been investigated. A continuous monitoring system consisting of 7 thermocouples was placed in equal distances from top to the bottom inside the furnace to measure the temperature of air inside the heating chamber and validate the CFD output. The results of both the experimental and CFD study were compared and discussed.
DISPERSION OF TOXIC CONTAMINANTS FROM LARGE TANK FIRES AND PARAMETRIC ANALYSIS FOR VARIOUS SIZES OF TANKS

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Keywords: Tank fire, Pollutant dispersion, Smoke plume, Turbulence, CFD, Field model.

ABSTRACT

Significant tank fire accidents, such as the December 11th, the 2005 Buncefield Oil Storage Depots (B.O.S.D) disaster and the recent massive tank fire of October 23rd, 2009 at Caribbean Petroleum Refining, demonstrate the large scale of destruction in the surroundings, but also the implication of potential environmental issues from these types of accidents.

The purpose of the present work is the numerical simulation of toxic contaminants dispersion, as well as the parametric analysis for three different diameters of storage tanks, 85, 70 and 50m, respectively. A methodology is presented to calculate the ground-level concentration of the toxic pollutants and the height of the plume rise. Then, the relationship is examined of the phenomenon for two fuels (crude and diesel oil), and three different wind velocities 8, 10 and 12 m/s, respectively. Moreover, the repercussions for the environmental and human health from the toxic pollutants are investigated and a nomograph of dimensionless ground-level concentrations vs. dimensionless height from the origin of the tank is developed. The nomograph is very important for the practicing engineers and especially for safety engineers, because it may assist the bad effects from toxic pollutants dispersion.

Numerical simulations were performed with the use of CFD techniques for a physical domain of 34521 m length, 2400 m width and 3000 m height. The mathematical model is expressed by the continuity equation, the three momentum equations, chemical species concentration equations, energy equation, kinetic energy and dissipation rate equation of turbulence. The above mentioned set of equations, along with the appropriate auxiliary relations and boundary conditions has been solved by means of the Finite Volume Method. The modified RNG k–ε model was employed, in order to account for turbulent flow with strong buoyancy forces and a hybrid scheme was employed to discretize the equations. The CFD code PHOENICS with an iterative algorithm, namely SIMPLEST was used for the numerical simulation.

Parametric analysis is performed for 18 different scenarios. According to the results, the highest plume rise at 2003 m appears for the scenario with diesel oil, wind velocity 8 m/s and tank diameter 85 m, whilst the lowest value, of plume height at 625 m, appears for the scenario with crude oil, wind velocity 12 m/s and tank diameter 50 m. Moreover, 18 different values of dimensionless buoyancy flux number, F/U1/2L, were examined, in order to derive the nomograph. For all scenarios the ground-level concentrations of toxic pollutants do not exceed the safety limits of IDLH and there are no death zones due to the pollutants concentrations.
SHAPE OPTIMIZATION USING THE ONE-SHOT ADJOINT TECHNIQUE ON GRAPHICS PROCESSING UNITS


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Keywords: Graphics Processing Units, Computational Fluid Dynamics, Optimization / Adjoint methods.

ABSTRACT

This paper presents the implementation of the one-shot continuous adjoint technique [1], for incompressible flows, on NVIDIA Graphics Processing Units (GPUs) for design/shape optimization problems. Instead of separately and successively solving the state (flow) and the co-state (adjoint) equations, prior to computing the gradient of the objective function and correcting the designed shape (as in any optimization loop based on the steepest-descent algorithm), the one-shot technique [2] copes with all three of them (i.e. the state, co-state and shape correction equations) simultaneously or in an one-shot fashion. The one-shot adjoint approach may reduce the overall computational cost of the optimization compared to the standard adjoint technique.

On the other hand, during the last two years, our research group has successfully ported the in-house CFD software on NVIDIA GPUs, using the CUDA architecture, [3]. The GPU-enabled solvers achieved parallel speed-up values which, depending on the case, may exceed 50. In this paper, the adjoint solver is also ported on the GPUs, this time in the one-shot fashion. By doing so, the reduction of the CPU cost from the use of the one-shot approach and the parallel speed-up due to the use of GPUs can be superimposed, leading to noticeably small optimization turnaround times. A distinguishing feature of the direct/adjoint solvers, that this paper is based on, is the use of the vertex-centered finite volume technique (VCFVT) for the integration of the equations in unstructured grids. VCFVT calls for very delicate memory handling in order to maximize the parallel efficiency of the GPU-enabled software, in contrast to the use of either the cell-centered finite volume technique (CCFVT) on unstructured grids or the use of VCFVT or CCFVT on structured grids, where memory access is fully organized. The extra difficulty of the VCFVT is that the number of nodes linked with any grid node may vary a lot. Since a GPU executes the same code (kernel) in parallel (several threads are executed at the same time), the variable number of adjacent nodes per node reduces the parallel efficiency of the GPU-enabled software. To minimize this loss in performance, special memory handling along with appropriate rearrangement (renumbering) of the grid nodes based on the number of their adjacent nodes are necessary.

The gradient of the objective function is computed using the adjoint method for incompressible flows with heat transfer, while dynamic meshes have been employed in order to avoid grid regeneration upon completion of the computation of the sensitivities.

This paper focuses on the computational gain achieved by the one-shot technique on GPUs, compared to the same technique employed on CPUs. Two cases will be shown: (a) the shape optimization of a heat exchanger tubes for maximum heat transfer and minimum total pressure losses and (b) the design of a 2D turbomachinery cascade for minimum total pressure losses. The continuous adjoint method will be presented for incompressible flows, by considering variations of the turbulence model variables, as originally proposed in [4].

A FAST-CONVERGENT SPECTRAL METHOD FOR WAVE PROPAGATION AND SCATTERING IN NON-UNIFORM WAVEGUIDES

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Keywords: non-uniform waveguides, coupled modes, local-mode series

ABSTRACT

We consider the problem of wave propagation and scattering in non-uniform waveguide (Fig.1) governed by the a general second-order, strongly elliptic equation with variable coefficients

\[ L \ u = \frac{\partial}{\partial x_1} \left( a_{ij} \frac{\partial u}{\partial x_j} \right) + ku = 0, \]

where \( a_{ij} \) and \( k \) are real functions of \( x_1 \) and \( x_2 \) (\( a_{ij} > 0 \) and symmetric satisfying condition of uniform ellipticity in the domain \( D \)); see, e.g., [1]. For simplicity we focus here on two-dimensional waveguide, limited above by a Dirichlet boundary and below by an irregular Robin boundary,

\[ u = 0, \ \text{on} \ x_2 = h_1(x_1), \ \text{and} \ \frac{\partial u}{\partial n_1} + \sigma u = 0, \ \text{on} \ x_2 = h_1(x_1), \]

where \( \frac{\partial u}{\partial n_1} = a_{ij} \left( \frac{\partial u}{\partial x_j} \right) \), and \( n_1 \) denotes the outer normal on \( \partial D \). The waveguide is excited by incident plane waves propagating in the positive \( x_1 \) direction.

The above problem finds important applications to wave propagation in an inhomogeneous standing or moving medium, as, e.g., underwater acoustic propagation and scattering in shallow water and seismoacoustics [2,3], atmospheric acoustics [4]. Similar problems are also encountered in variable cross-section electromagnetic waveguides [5].

In the present work an improved coupled-mode method is established, based on an enhanced local-mode series for the representation of the wave field, which includes an additional mode accounting for the effects of the boundary slope. The additional mode provides an implicit summation of the slowly convergent part of the local-mode series, rendering the remaining part to converge much faster, like \( O(n^{-4}) \), where \( n \) is the mode order.

Using the enhanced representation, in conjunction with an appropriate variational principle, a new system coupled-mode equations is derived for the determination of the modal-amplitude functions. Numerical applications including comparisons with other solutions illustrate the role and significance of the additional mode and the efficiency of the present coupled-mode theory, which can be naturally extended to treat propagation and scattering problems in three-dimensional multi-layered waveguides.

References
HEART VALVE TISSUE ENGINEERING

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ABSTRACT

Tissue engineered heart valves appear promising as autologous valvular substitutes that may have the ability to grow and remodel. From a mechanical point of view, the \textit{in vivo} functionality and durability of the heart valve relies on the strength and anisotropic properties of the valve leaflets. In a mature heart valve, a distinct anisotropic collagen architecture is observed that enables flexibility of the valve leaflets in the radial direction, and that creates the required strength in the circumferential direction. One of the challenges in heart valve tissue engineering is to mimic this anisotropic collagen structure in terms of collagen amount, collagen orientation and intrinsic properties of the collagen fibers. Mechanical stimulation has been shown to influence collagen synthesis, accumulation and organization. In a sequence of experiments the effect of mechanical loading on the synthesis and orientation of collagen as well as the structural properties of the collagen is investigated (1), (2), (3), (4), (5). This has resulted in a new bioreactor culture paradigm that yields heart valves with sufficient strength for implantation at the aortic position(6). Preclinical experiments in a sheep model, using a minimally invasive transapical approach, yields promising results(7).

Yet, the precise mechanism of collagen orientation, as well as contractile force development when subject to static and dynamic loads is not fully understood. To further understanding of this mechanism microtissues may be applied that can be visualized using multiphoton confocal microscopy. In addition, computational models are developed to analyse the development of cytoskeletal orientation and cellular traction forces in three-dimensional tissues. Comparisons with experimental results are made.

DYNAMIC ANALYSIS OF THIN VISCOELASTIC PLATES OF VARIABLE THICKNESS MODELED WITH FRACTIONAL DERIVATIVES

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Keywords: thin plates, variable thickness, viscoelastic, fractional derivative models, boundary element method, analog equation method.

ABSTRACT

Thin plates made of modern viscoelastic materials combine light weight and increase damping effects and are used very often in engineering practice in order to reduce the weight and the vibrations when subjected to dynamic loads. Various linear and nonlinear models have been proposed to predict the response of the viscoelastic materials using differential or integral constitutive equations. The differential constitutive equations are generalized by replacing the integer order derivatives with fractional order ones, since many researchers have shown recently that fractional derivative models describe accurately the response of many viscoelastic materials with much less parameters than integer order derivative models.

Due to the great interest of the subject, many researchers have studied the dynamic response of viscoelastic plates modeled with hereditary integral or integer order differential models. In most cases the Laplace or Fourier transform was used to convert the viscoelastic problem to an equivalent elastic one, which is solved with approximate or numerical methods, like FEM and FDM. Other researchers used FEM or BEM for the spatial plate problem with direct time integration of semi-discretized evolution equations. The literature is rather limited on viscoelastic bodies modeled with fractional derivative models due to the difficulty to solve the resulting fractional order differential constitutive equations [1-2].

In this paper we study the linear vibrations of thin plates of arbitrary geometry and variable thickness made of linear viscoelastic material modeled with multi-parameter fractional derivative models. The plate is subjected to any type of boundary conditions under interior and edge transverse loads. The governing equation and the boundary conditions are derived first in terms of the stress resultants using the principle of virtual work and then they are differentiated to apply the fractional derivative constitutive equations. Thus an initial boundary value problem with fractional order derivatives with respect to time describes the response of the plate in terms of the transverse displacement. The order of the time derivatives depends on the order of the viscoelastic constitutive equation which in general is of order greater than two, thus additional initial conditions are required for the well-posedness of the problem. A method is presented to establish the redundant initial conditions in terms of the physical ones, displacement and velocity. The Analog Equation Method AEM [3] is applied to convert the original equation into a thin plate equation of constant thickness (biharmonic) under a fictitious time dependent load, unknown in the first instance. Application of the BEM with domain discretization to approximate the domain integrals yields an initial value problem for the fictitious load, which is a system of linear ordinary fractional differential equations generally of order greater than two. The system is solved using the numerical method presented recently by Katsikadelis [4]. The proposed analysis is illustrated with the fractional Kelvin-Voigt model and Standard solid (three parameter) model.

References
COMPUTATIONAL METHODS TO STUDY THE TRANSPORT PROPERTIES OF THE Na/Ca EXCHANGER

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Keywords: Percolation, Finite difference method, Ion channels and concentrations, Current clamp, Voltage clamp

ABSTRACT

The plasma membrane constitutes a selective barrier between the inside and the outside of a cell. It controls the entry and the exit of various molecules and ions between the two compartments. All cells develop a potential difference (PD) between the two faces of the membrane. This PD is responsible for the electric activity of excitable cells, which appears in the form of oscillations of the membrane potential. These oscillations take place in many physiological processes, in particular in neuronal, cardiac and pancreatic cells \cite{1}.

The aim of this work was to evaluate the role of a membrane protein, the Na/Ca exchanger (NCX) in the regulation of the oscillations of the membrane potential. NCX allows Ca\textsuperscript{2+} extrusion from the cell and entry of Na\textsuperscript{+} along its electrochemical gradient without energy consumption. In addition, because NCX is electrogenic and voltage dependent, it can reverse during cellular activation and contributes to Ca\textsuperscript{2+} entry into the cell \cite{2}.

We used the percolation concept introduced in 1953 by Hammersley in order to describe statistical systems made up of a great number of objects which can be connected between them \cite{3}. Our goal was to study the diffusion of ions through the membrane. For that, we have to use the Fick’s laws, which treat partial derivative equations. Analytically, the solution of these equations is very difficult and sometimes impossible. We used a very simple numerical method – the finite difference method (FDM) \cite{4}.

By a simple electric model of the plasma membrane, we detected the presence of an inward current, which is proportional to the intracellular Na\textsuperscript{+} concentration and an outward tail current due to the exit of K\textsuperscript{+} ions, which causes the hyperpolarization of the plasma membrane (Figure 1). Temporal fractal structures of the active channel distributions enabled us to follow the diffusion of the Ca\textsuperscript{2+} intracellular ions (Figure 2).

Reference :

\begin{itemize}
\item \cite{3} Stauffer D., Aharony A. (1991): « Introduction to Percolation Theory ». \textit{Taylor and Francis, London}
\end{itemize}

![Figure 1: Comportment of the current membrane for $C_{Na} = 10$ mmol/l and $C_{Na} = 20$ mmol/l.](image1)

![Figure 2: Temporal distribution of the active channels for a network $100 \times 100$ with various ion concentrations.](image2)
BRIDGING LENGTH SCALE IN FLUID PHASE EQUILIBRIUM VIA HISTOGRAM REWEIGHTING OF GIBBS ENSEMBLE MONTE CARLO SIMULATIONS

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Keywords: Monte Carlo, Phase equilibrium, Multi scale modeling.

ABSTRACT

Over the last decades molecular simulation has contributed significantly in the accurate and efficient prediction of fluid phase equilibria. In this work we combine two of the most powerful methods that have greatly enhanced our ability to simulate accurately fluid phase equilibria: (a) the “Gibbs ensemble” method (A. Z. Panagiotopoulos Molecular Physics, 61 (1987) 813-826) and (b) the multiple histogram method (A.M. Ferrenberg, R. H. Swendsen, Physical Review Letters, 61 (1988), 2635-2638). The result of such combination is a simple and very accurate method of predicting fluid phase equilibrium close to and away from the critical point. Furthermore by performing a number of discrete GEMC simulations over the range of interest, multiple histogram is able to provide a continuous function that can be used as an input in computational fluid dynamics.

In this work we derive the combination of the multiple histogram reweighting method with the Gibbs ensemble method in the case of a pure fluid. Extension of the approach to mixtures is straightforward. From now on we will refer to the total number of particles as Ntot and to the total volume of the system as Vtot. Unlike other cases where the multiple histogram may be applied, in this specific application one should always keep in mind that the total number of particles and the total volume of the system have to be kept constant, at the same values, along all the different simulations that will be linked in the histogram.

We have examined the vapor liquid equilibrium of two systems: (a) pure CO2 and (b) pure n-pentane. For the simulation of the CO2 molecule we have used the model has three Lennard-Jones sites with charges centered at each atom. The carbon-oxygen bonds are rigid and 1.1638 Å long. Furthermore, the model uses point charges centered at atom sites that result in a quadrupole moment of 4.3 esu, close to the experimental value. The long range electrostatics were treated using Ewald summation.

For the simulation of n-pentane we have used the TraPPE united atom mode, which represents each molecule as a set of five charge-free Lennard-Jones sites centered at each carbon atom. The carbon-oxygen bonds are rigid and 1.1638 Å long. Furthermore, the model uses point charges centered at atom sites that result in a quadrupole moment of 4.3 esu, close to the experimental value. The long range electrostatics were treated using Ewald summation.

For the simulation of n-pentane we have used the TraPPE united atom mode, which represents each molecule as a set of five charge-free Lennard-Jones sites centered at each carbon atom. In all simulations we have generated our samples using the Sclenomics MAPS 3.2 platform. Initially, we generated random molecular configurations for the two boxes, with each box containing half of the total number of molecules and occupying half of the total volume, using the Amorphous Builder plugin. The Gibbs ensemble Monte Carlo simulations have been performed using the Towhee engine plugin. We have combined the use of Gibbs Ensemble Monte Carlo simulations with the multiple histogram reweighting method in order to reproduce the phase envelope of pure CO2 and n-pentane using realistic molecular force fields. The proposed approach enables one to use the Gibbs ensemble in combination with histogram reweighting, and therefore reap all the benefits that come with this. We are able to predict, from a discrete set of simulations of the coexisting phases, any other pair of points on the phase envelope, in the vicinity of the original simulations.

Financial support from the European Commission through project "Quantitative Failure Consequence Hazard Assessment for Next Generation CO2 Pipelines" (project no. 241346-2; FP7-ENERGY-2009-1) is gratefully acknowledged.
FLUID FLOW IN CONSTRICTED TUBES AND POROUS DOMAINS USING LATTICE-BOLTZMANN AND MESHLESS SOLVERS

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Keywords: Meshless Point Collocation, Moving Least Squares, Lattice-Boltzmann, constricted tube, porous medium

ABSTRACT

In recent years, novel numerical methods, such as the Meshless [1] and the Lattice Boltzmann Methods (LBM) [2], have been developed and extensively studied, providing alternative approaches to more traditional numerical techniques for the study of equilibrium and dynamic properties of fluid systems. In the present work, the efficiency of Meshless methods and Lattice Boltzmann models as Computational Fluid Dynamics (CFD) solvers is examined in characteristic flow processes inside confined geometries. More specifically, we compare the accuracy and the computational efficiency of simulation codes based on the meshless point collocation method (MPC) using Moving Least Squares with velocity correction [3], along with the D2Q9, single relaxation Lattice Boltzmann model [4] for two-dimensional incompressible laminar flow problems in two confined geometries. Second-order fluid-solid no-slip conditions have been implemented in the LB approach, whereas typical no-slip conditions have been applied in the Meshless approximation. A tube with a step-wise constriction-expansion region, and the same tube with a porous medium region in place of the converging-diverging part are examined herein, and calculations are performed regarding the permeability and the local velocity profiles of the systems. In the first case, the vortices are examined with respect to the Reynolds number, whereas in the latter, the validity and the extension of the Darcy equation is studied with respect to the geometry characteristics and the velocity profiles in elevated Reynolds numbers.

Disc-shape (circular) granular media are used for the porous medium description, and the efficiency of the Meshless methods in the representation of the curvature of the geometric shapes is investigated in comparison with the pixelized form of the Lattice-Boltzmann grid (D2Q9). Results have shown that the Meshless approach, although more time-consuming than the Lattice-Boltzmann counterpart, is capable of producing flow field profiles with increased precision due to the detailed description of the internal boundaries of the porous domain.

REFERENCES

MULTISCALE CONSIDERATION OF PLASTICITY AND STRESS-STRAIN IN ENGINEERING MATERIALS (STUDY CASE: ALUMINUM ALLOY)

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Keywords: Multiscale, plasticity, stress-strain, nanoindentation, molecular dynamics, gradient elasticity

ABSTRACT

Tensile uniaxial experiment is widely used to evaluate the mechanical behaviour of bulk materials. During a classical tensile test, load-displacement data is obtained and the curve is converted to a nominal stress-strain curve. Typical tensile properties of probed materials, such as the yield strength, tensile strength, uniform elongation, total elongation, work hardening exponent (n-value), etc., can be obtained that are of a macro-, meso-scale.

Nanoscale measurements of mechanical properties play an important role in many emerging fields, such as surface engineering, magnetic storage disks, biomedical coatings and micro-, nano-electromechanical systems. In these systems, the bulk (i.e. non-surface region or interior) is typically strained in response to the stress of the surface. One of the challenges in studying the mechanical properties of these materials and specifically the local mechanical properties in a small volume of material having microstructural gradients is that the traditional methods, e.g. tensile test and microhardness test, are not applicable.

In contrast to the conventional indentation testing, in which the contact area is determined from a direct measurement of the dimensions of the residual impressions left in the sample surface upon the removal of load, the contact area in the nanoindentation test is determined by measuring the load (μN) and the penetration depth (nm) into the sample surface, continuously. Nanoindentation is used to evaluate the elastic constants, local yielding (failure of elasticity), local plasticity of materials in the micro- nano- scale. A challenge is the use of nanoindentation as a method of extracting equivalent stress–strain curves of materials at nanoscale and connection with meso- macro- scales. There are many drawbacks, i.e. the stress distribution between the nanoindenter and the sample is complex, and the definition of an equivalent nanoindentation strain remains a fundamental question as it depends on the indenter geometry, the penetration depth, the material, and the ratio of the elastic deformation to the total deformation. In addition, the current experimental nanoindentation testing systems exhibit significant difficulties in providing reliable results in very small depth penetrations (a few nm).

The difficulties with experimental methods at very small depths can, in general, be easily resolved by using molecular dynamics (MD) or an extension of continuum elasticity to describe a variety of problems at the nano scale and to simulate nanoindentation experiment. The classical theory of elasticity can be extended to the nanoscale by supplementing the equations of elasticity for the bulk material with the generalized Young–Laplace equations of surface elasticity.

In this work, the nanoindentation technique is applied on aluminum alloys. Stress-strain curves are extracted from loading-unloading curves. Finite Element Method (FEM) was performed to compare the resultant loading-unloading curves with the experimental ones (found to be in good agreement between, especially at depth of several hundreds of nanometer). In FEM the classical continuum plasticity framework incorporating Taylor dislocation model via strain gradient plasticity embedded in the constitutive equation may be adopted to take into account the nanoindentation size effect. In several studies of materials nanoindentation size effect is revealed, which shows an increase in stress (hardness) with decreasing applied load. The development of a MD simulation of a nanoscale uniaxial tensile test is also under investigated.

Development of a multiscale mathematical approach could significantly impact the issue of bridging the nano-, micro- and meso- (mm, cm) scales. For example, accurate determination of tensile properties from nanoindentation and the correlation with meso- scale results would have significant advantages and it is a matter of major challenge.
PARALLEL MULTISCALE COMPUTATIONS IN CHEMICAL VAPOR DEPOSITION PROCESSES

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Keywords: parallel processing, multiscale modeling, master-worker, MPI, chemical vapor deposition

ABSTRACT

An integrated parallel framework for performing multiscale computations in chemical vapor deposition (CVD) processes is presented. The macro- scale of a CVD reactor is linked with the micro- scale of a predefined topography of features on the wafer surface where the deposition occurs (Fig.1). A reactor scale model [1] which describes the transport phenomena along with the chemical reactions in the bulk phase of a CVD reactor is coupled with a feature scale model [2] which describes the profile evolution of the growing film inside micro-scale features on the wafer. The coupling of the co-existing scales is performed through a correction of the boundary condition for the species consumption along the wafer by a fixed point iteration procedure [1].

The computations in each scale are performed independently; when the macro- scale code “runs”, the micro-scale code is idle and vice versa. Thus, different parallel techniques can be utilized to accelerate the computations in each scale. The computations in the macro- scale are efficiently treated with the commercial code Ansys/Fluent and domain decomposition parallel techniques [3]. In the micro- scale, to deal with the time consuming computations, a master-worker [4] parallel technique is implemented since the computations in each boundary cell on the wafer surface are independent from each other. In both scales message passing interface is used for the communication between the processors. The efficiency of the computations, by using parallel processing techniques in both scales, is investigated. The computations are performed in high-performance computational cluster [5].

EVALUATION OF MAXIMUM SEISMIC DISPLACEMENTS OF STEEL FRAMES FROM RESIDUAL DISPLACEMENTS

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KEYWORDS: Moment-resisting steel frames, residual displacements; Maximum displacements;

ABSTRACT

The post-earthquake performance level of structures provides a very important source of information both for probable rehabilitation procedures and determination of structural response to probable oncoming aftershocks. This performance is described by the maximum deformation which is directly related to structural damage. On the basis of extensive parametric studies on moment-resisting steel frames, simple empirical equations are constructed for a simple and effective determination of the maximum seismic deformation from residual displacements, which can be measured in-situ after strong seismic events. It is found that the measure of residual deformation can be effectively used to evaluate the post-earthquake performance level of steel framed structures.

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THE SINGULAR FUNCTION BOUNDARY INTEGRAL METHOD FOR 3-D LAPLACIAN PROBLEMS WITH A BOUNDARY STRAIGHT-EDGE SINGULARITY

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Keywords: Singular Function Boundary Integral Method, Laplace problem, Edge Flux Stress Intensity Functions

ABSTRACT

Three-dimensional Laplace problems with a straight-edge singularity caused by two intersecting flat planes are considered. The solution in the neighbourhood of the straight edge can be expressed as an asymptotic expansion involving the eigenpairs of the analogous two-dimensional problem in polar coordinates, which have as coefficients the so-called edge flux stress intensity functions (EFIFs). The EFIFs are functions of the axial coordinate the higher derivatives of which appear in an infinite series in the expansion. The objective of this work is to extend the singular function boundary integral method (SFBIM) for solving the above problem and directly extracting the EFIFs. Approximating the latter by either piecewise constant or linear elements eliminates the inner infinite series in the local expansion and allows the straightforward extension of the SFBIM. As in the case of two-dimensional problems, the solution is approximated by the leading terms of the local asymptotic solution expansion. These terms are also used to weight the governing harmonic equation in the Galerkin sense. The resulting discretized equations are reduced to boundary integrals by means of the divergence theorem. The Dirichlet boundary conditions are then weakly enforced by means of Lagrange multipliers. The values of the latter are calculated together with the coefficients of the EFIFs. The SFBIM is applied to two test problems exhibiting fast convergence with the number of EFIFs, the number of the Lagrange multipliers, and the number of elements in the axial direction and yielding very accurate estimates for the EFIFs.
FINDING THE WETTING AND PINNING POINTS IN THE WIRE-PINNING PROCESS OF FILM CASTING

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ABSTRACT

Film casting involves melt flow through a slot die, across a small span, and onto a fast moving quench drum. In the “wire-pinning” casting process, a thin electrified wire close to the line of contact with the drum creates a strong pinning force that delays air entrainment to higher line speeds. Non-uniform wetting of the die lips by the extruded melt is frequently thought to be responsible for the formation of streaks, a defect in the machine direction. A finite element model of the film casting process with wire pinning was developed to assist in understanding what causes significant wetting of the lips and whether this can be avoided by electrostatic pinning. The simulations investigate the sensitivity of the static and dynamic wetting line locations on the die lands and to the imposed values of static contact angle and die-lip gap.
RHEOLOGICAL BEHAVIOR OF SELF COMPACTING CONCRETE: SIMULATION OF THE SLUMP FLOW TEST

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Keywords: Self Compacting Concrete, Slump Flow, Herschel-Bulkley Model, Spread, Computational Rheology, Finite Elements.

ABSTRACT

The slump flow test is used extensively as a means of determining the workability of self-compacting concrete (SCC). A frustum of a metallic cone is placed on a flat surface, filled with material and lifted to allow the material to flow. This quick and inexpensive method is widely standardized. According to the accepted standard the horizontal spread and the time required for the material to spread to a diameter of 500 mm provide measures of the flowability. In this work we use Lagrangian finite elements to simulate slump flow assuming that SCC behaves as a viscoplastic Herschel-Bulkley fluid. Our objective is to relate the rheological parameters to the spread and the spreading time. Numerical results are obtained for a wide range of these parameters.
THEORETICAL INVESTIGATION OF FLOW AND MASS TRANSPORT IN GRANULAR POROUS MEDIA FOR A REALISTIC SORPTION MECHANISM

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Keywords: Convection, diffusion, adsorption, mass transfer, flow, granular media.

ABSTRACT
This work aims to model the mass transport process from a moving Newtonian fluid to an assemblage of spherical solid absorbers. The convective / diffusive transport in a stochastically constructed 3-D assemblage of spherical particles under a realistic adsorption / reaction / desorption mechanism, is simulated by using the spatial/volume-averaging technique, where the appropriately simplified boundary-value problems are described and numerically solved for the flow velocity field and for the transport problem. The process was found to be controlled by the Peclet number as well as the geometrical properties (porosity) of the porous structure. Through model validation, it is also verified that the realistic sorption mechanism considered here, provides a reasonable estimation of the mass transfer coefficient.
ANALYSIS OF THE TOPOLOGICAL CHARACTERISTICS OF EARTHQUAKES IN REGIONS OF THE HELLENIC ARC BASED ON NETWORK THEORY

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ABSTRACT

The seismic activity is a highly complex natural process in the space-time-size domains given that the state of the seismogenic layer of the Earth is characterized by self-organized criticality. Over the last years, scientists have tried to quantify the topological characteristics of seismic activity in order to find possible correlations between earthquake events based on complex network theory[e.g. Baiesi and Paczuski, 2004; Suzuki, 2004; Baiesi and Paczuski, 2005]. Based on detailed data and depending on the region under study various scale free and small world structures have been reported. In this work, we quantify the relationship between the earthquake events along the Hellenic Arc which is the most seismogenic structure in the European-Mediterranean region. In particular, we study shallow seismicity (h < 40km) in the region extending from 34.5° to 40° N in latitude and from 19.5° to 30° E in longitude, thus covering the broad domain of the Hellenic Arc. The data were taken from the seismic catalogue of the Institute of Geodynamics, National Observatory of Athens, for the time period from 1 Jan. 2000 to 31 Dec. 2009. After testing the catalogue for data incompleteness on the basis of the magnitude-frequency linearity, we selected magnitude cut-off of 2.7. By linking in a systematic way in space successive events we constructed the underlying network that describes their evolution and extracted the statistical properties of the underlying topology. Based on detailed data including time, location, magnitude and depth of the earthquakes, we evaluated properties such as clustering, path length, degree distribution and betweenness. The aim is to look for possible statistical markers that would allow the classification of the activity in swarms, foreshocks, aftershocks and mainshocks. To our knowledge this is the first time that such an analysis is attempted in the Greek seismicity.

THE COMPLETE SET OF VECTOR ELLIPSOIDAL HARMONICS AND THE INDEPENDENCE OF THE EEG AND MEG MEASUREMENTS

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Keywords: Harmonic Functions, Ellipsoidal Geometry, Complete Vector Basis, Electroencephalography, Magnetoencephalography

ABSTRACT

In solving boundary value problems, involving vector fields, in terms of eigenfunction expansions, one usually has to assume the appropriate scalar expansions, for each one of the Cartesian components of the field, and leave the vectorial character of the problem to be handled by the coefficients of these expansions. This approach though creates a lot of difficulties when we attempt to satisfy boundary conditions. The reason is that, unless we are dealing with planar boundaries, where the Cartesian structure is appropriate, the boundary of the fundamental domain does not conform with the intrinsic geometry of the chosen eigenfunctions. What we actually need is to cast the vectorial structure of the problem, not to the coefficients but rather to the eigenfunctions of the corresponding expansion. Nevertheless, this is by far a not easy task and as it was shown in the late 40’s, even for the Laplace equation, there are only a few coordinate systems that allow orthogonal vector eigenfunctions. The spherical system is one of them, as it was demonstrated by Hansen in 1935. The criteria, that were stated over 60 years ago, for the existence of vector harmonics in any particular system, are far from being satisfied in the case of the ellipsoidal system, which basically models anisotropic behavior. In the present report, we scrutinize the character and the peculiarities of the vector Laplace operator in ellipsoidal coordinates and we tried to identify were the general theory breaks down. Once we identified the problem, we bypass it by introducing, besides the classical one, a second topological structure which secures the orthogonality of the subspace that fails to be orthogonal with respect to the classical inner product. This way we manage to have a complete system of surface vector eigenfunctions that can be used to solve vector problems in ellipsoidal geometry. An application is included, that shows the independence of the electroencephalographic and magnetoencephalographic measurements and at the same time, it identifies the subspace of the neuronal current that provides information to both of these brain imaging techniques.
A ROBUST, PRACTICAL, AND GENERAL METHOD FOR COUPLED ITERATIONS OF BLACK-BOX NONLINEAR SOLVERS BY AN APPROXIMATE BLOCK NEWTON METHOD

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Keywords: Multiscale coupling, Approximate Newton methods, Modular iterations, Crystal growth.

ABSTRACT

A major thrust of our research activity is the solution of melt crystal growth problems that are characterized by continuum phenomena that are highly nonlinear and strongly coupled. The problem complexity presents a significant technical challenge, requiring the integration of a large-scale furnace model with a strongly coupled, multi-physics, transport problem of the Stefan, moving-boundary type. Problem nonlinearity can be severe, due to high-temperature, radiative heat transfer and strong, richly structured melt flows of a transitional nature. Robust computing of steady-state solutions under these conditions can be achieved by Newton-Raphson iteration, but its desirable quadratic convergence property relies on our ability to compute a sufficiently accurate approximation to the inverse of a Jacobian matrix of the global system of equations.

It is costly to develop monolithic software that simultaneously represents all chosen phenomena at all scales in a single model of melt crystal growth. From a practical standpoint, problems of this scope favor a partitioned approach, in which a few major subdomains of the problem are tackled independently by existing software best suited to the task. Such methods can be used to link together existing best-in-class tools to tackle complex multi-physics and multi-scale problems, without requiring extraordinary programming effort.

Towards this end, we have developed an approximate block Newton (ABN) method to couple arbitrary, black-box nonlinear solvers [1]. This ABN method preserves the quadratic approximation properties of an exact Newton iteration. The notion of a solver is abstract, encompassing any interpolations or other transformations of data exchanged between solvers. It is shown that the method behaves like a Newton iteration preconditioned by an inexact Newton solver derived from subproblem Jacobians. The method is demonstrated on several conjugate heat transfer problems modeled after melt crystal growth processes [1,2]. Whereas a typical block Gauss--Seidel iteration fails about half the time for such problems, quadratic convergence is achieved by the ABN method under all conditions studied. Prospects for quantitative process modeling and the ability to represent three-dimensional and transient phenomena in bulk crystal growth are also discussed.

REFERENCES


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APPLICATION OF THE FICTIONICIOUS DOMAIN/LAGRANGE MULTIPLIER METHOD ON THE SIMULATION OF THE AORTIC VALVE

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Keywords: Fictitious Domain, Lagrange Multiplier, Fluid Structure Interaction, Aortic Valve

ABSTRACT

We study numerically the nonlinear interaction of a three-dimensional representation of an aortic heart valve, composed of three hyperelastic leaflets of finite density attached to a stented vessel under physiological flow conditions. Blood flow is caused by a time varying pressure gradient that mimics that of the aortic valve and corresponds to a peak Reynolds number equal to 4,050. Here, we fully account for the shear-thinning response of the blood [1], contact effects and large deformations of the leaflets, by solving the momentum and mass balances for both phases. The mixed finite element/Galerkin method along with linear discontinuous Lagrange multipliers for coupling the fluid and elastic domains are adopted [2]. Moreover, a series of challenging numerical issues such as the finite length of the computational domain and the conditions that should be imposed on its inflow/outflow boundaries, the accurate time integration of the parabolic and hyperbolic momentum equations, the contact between the leaflets and non-conforming mesh refinement in a part of the domain is successfully addressed. Calculations for the velocity and the shear stress fields of the blood reveal that boundary layers appear on both side of a leaflet. The one along the ventricular side transfers blood with high momentum from the core region of the vessel to the annulus or the sinusoidal expansion, causing the continuous development of flow instabilities. At peak systole vortices are convected in the flow direction along the annulus of the vessel, while during the closure stage of the valve an extremely large vortex develops in each half of the flow domain [3].

REFERENCES


DYNAMICS OF ERYTHROCYTES IN THE MICROCIRCULATION VIA A NON-STIFF CYTOSKELETON-BASED CONTINUUM COMPUTATIONAL ALGORITHM

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Keywords: Erythrocyte, Microcirculation, Cytoskeleton

ABSTRACT

The motion of erythrocytes through vascular microvessels has long been recognized as a fundamental problem in physiology and biomechanics, since the main function of these cells, to exchange oxygen and carbon dioxide with the tissues, occurs in capillaries. Unfortunately, studies on the flow dynamics of erythrocytes still constitute a challenging problem in any type of research owing to the micron-size of the cell and its complex multi-layered membrane.

In the area of our interest (i.e. computational investigations), several continuum and molecular-based models have been developed in the recent decades to study erythrocytes. In the continuum models, treating the erythrocyte membrane as a two-dimensional elastic solid with large area-dilatation modulus results in a very stiff computational problem especially for three-dimensional investigations. On the other hand, cytoskeleton-based molecular algorithms were able to model efficiently the global area-incompressibility of the skeleton, but their applicability to flow problems is usually restricted owing to large computational cost.

In this talk, we show that, by combining the current experience on erythrocyte computational algorithms via both continuum and molecular modelings, we develop a cytoskeleton-based continuum algorithm which accounts for the global area-incompressibility of the skeleton via a non-stiff, and thus efficient, procedure. In addition, we investigate the erythrocyte dynamics in shear flows for moderate and strong capillary numbers and small to moderate viscosity ratios. These conditions correspond to a wide range of surrounding medium viscosities and shear flow rates, and match those used in ektacytometry systems and the tank-treading frequencies in vivo. The tank-treading period is shown to be inversely proportional to the shear rate and to increase linearly with the ratio of the cytoplasm viscosity to that of the suspending medium. Our modeling also predicts that the cytoskeleton undergoes measurable local area dilatation and compression during the tank-treading of the cells.
ABSTRACT

The study of the interfacial dynamics of artificial or physiological capsules (i.e. membrane-enclosed fluid volumes) in Stokes flows has seen an increased interest during the last few decades due to their numerous engineering and biomedical applications. Artificial capsules have wide applications in the pharmaceutical, food and cosmetic industries. In pharmaceutical processes, for example, capsules are commonly used for the transport of medical agents. In addition, the motion of red blood cells through vascular microvessels has long been recognized as a fundamental problem in physiology and biomechanics.

In the present study we investigate computationally the steady-state motion of an elastic capsule in a microfluidic channel. In particular, we consider a slightly over-inflated elastic capsule made of a strain-hardening membrane with comparable shearing and area-dilatation resistance. When the hydrodynamics forces on the membrane increase, the capsule develops a pointed downstream edge and a flattened rear (possibly with a negative curvature) so that the restoring tension forces are increased as also happens with droplets. Membrane tensions increase significantly with the capsule size while the area near the downstream tip is the most probable to rupture when a capsule flows in a microchannel.

By combining basic physical principles and geometric properties, we develop an asymptotic analysis that explains the power laws we found for large capsules; our analysis is independent of the type of the membrane which suggests that the scaling laws we found in this work should also be valid for other types of artificial and biological capsules such as for the motion of erythrocytes in the microcirculation.
FINITE ELEMENT MODELING OF POROUS PIEZOCOMPOSITE MATERIALS WITH DIFFERENT CONNECTIVITY AND APPLICATIONS FOR ANALYSIS OF ULTRASONIC TRANSDUCERS

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Keywords: Coupled Problems, Finite Element Method, Piezoelectric Composite, Effective Moduli Method, Ultrasonic Transducer.

To calculate the effective moduli for porous piezocomposites with different types of connectivity it was developed an approach based on the using of the finite element technology, the effective moduli methods and on the modeling of representative volumes. Obtained effective moduli were applied for the calculation of piezotransducer which made of porous piezoceramics with effective moduli. New computer models of piezomaterials’ representative volumes for porous piezoceramics with different types of connectivity (composites of 3-0 connectivity with closed porosity, 3-3 connectivity composites with open porosity and 0-3 connectivity composites) were developed. Finite element models of high-porous ceramics (with open type and closed type pores) were obtained using a new cluster models that take into account the direction of the polarization vector, associated with their spatial orientation. The following methods for generating a representative volume of the two-phase cubic piezocomposite with cubic elements were implemented: a random method, method of the initial concentration, the method of longitudinal fiber layout, the method of transversal fiber layout, the DLA (diffusion limited aggregation) Witten-Sander method, and the DLA “growth from the plane” method, etc.

To take into account the inhomogeneous polarization, the electrostatic problem for the dielectric composite was previously solved and the electric field was founded. Such problems were modeling the piezoceramic’s polarization process. Further, the polarization vector directions and values for piezoceramic matrix of the multiple-phase piezocomposite have been finding. As a result we had a representative volume for the piezocomposite with inhomogeneous properties of piezoceramic matrix (generally, near the pores).

To determine the effective moduli the sets of problems for a representative volume under the special boundary conditions were solved. Four types of boundary conditions that provide the homogeneous distributions of the field characteristics gradients in case of homogeneous media were considered. In the first type the displacements and the electric potential on the volume’s planes were specified, in the second version – displacements and the normal component of the electric induction vector, in the third version – the stress vector and the electric potential, and finally in the fourth type – the stress vector and the normal component of the electric induction vector. These problems were solved numerically using software specially developed for the FE package ANSYS. Using the averaging procedure the effective moduli of porous piezocomposite materials were obtained. The influence of both the various representative volume structures and taking into account the inhomogeneous polarization on the effective modules was analyzed. A comparison of the calculated porous piezocomposite characteristics and the well-known experimental data was carried out.

The efficiency of the proposed models and finite element approximations was demonstrated by the analysis of a spherical focusing porous piezoceramic transducer, loaded on the acoustic medium. Using the finite element technology and software tools, the working frequencies of the electric resonance and antiresonance for the thickness oscillations were obtained, gain-frequency characteristics for both free and loaded piezotransducer were calculated, and the focal area under the load on the acoustic medium at a resonance frequency was defined. Also the case of a multi-electrode piezotransducer made of porous piezoceramics was considered. It was noted that the multi-electrode coating allows to control the view of the focal area at the working acoustic medium and, thus, to improve the efficiency of the transducer with a powerful ultrasound.
A BEAM ELEMENT FOR POSTBUCKLING ANALYSIS USING BEM

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Key words: Nonlinear Analysis, Large Deflections, Postbuckling, Shear center, Boundary element method.

ABSTRACT

Postbuckling behaviour of beams is of fundamental importance in the design of structures subjected to heavy transverse and/or compressive loading. This beam postbuckling analysis becomes much more complicated in the case the cross section’s centroid does not coincide with its shear center (monosymmetric or asymmetric beams), leading to the formulation of a highly nonlinear flexural-torsional postbuckling problem. The nonlinearities involved (of geometrical nature) are due to the nonlinear kinematic relations and to the second order approximations for the deflection – curvature relations.

In this paper, the postbuckling analysis of beams of arbitrary cross section is presented taking into account moderate large displacements, large angles of twist and adopting second order approximations for the deflection – curvature relations. Starting from a displacement field without any simplifying assumptions about the angle of twist amplitude and based on the total potential energy principle, four highly coupled nonlinear governing differential equations are derived taking into account the shortening and warping effects and the Wagner’s coefficients due to the asymmetric character of the cross section. The arising four boundary value problems with respect to the transverse displacements, to the axial displacement and to the angle of twist are solved using the Analog Equation Method [1], a BEM based method. The essential features and novel aspects of the present formulation compared with previous ones are summarized as follows.

i. The present formulation is applicable to arbitrarily shaped symmetric, monosymmetric or asymmetric thin or thick walled cross sections occupying simple or multiple connected domains.

ii. The proposed method can be employed to beams supported by the most general boundary conditions including elastic support or restraint.

iii. The beam is subjected to the combined action of an arbitrarily distributed or concentrated axial, transverse and torsional loading.

iv. The proposed formulation does not stand on the assumption of a thin-walled structure and therefore the cross section’s torsional rigidity is evaluated exactly without using the so-called Saint –Venant’s torsional constant.

v. The developed method takes into account second order approximations for the deflection – curvature relations.

vi. Both the Wagner’s coefficients and the shortening effect are taken into account.

vii. The proposed method employs a BEM approach (requiring boundary discretization) resulting in line or parabolic elements instead of area elements of the FEM solutions (requiring the whole cross section to be discretized into triangular or quadrilateral area elements), while a small number of line elements are required to achieve high accuracy.

Numerical examples are worked out to illustrate the efficiency, the accuracy and the range of applications of the developed method. Conclusions of great practical interest are drawn.

REFERENCES

INELASTIC POUNDING OF ADJACENT REINFORCED CONCRETE STRUCTURES UNDER MULTIPLE EARTHQUAKES

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Keywords: Inelastic analysis, Pounding, Multiple earthquakes

ABSTRACT

This paper examines the effect of collision between adjacent reinforced concrete (RC) buildings under repeated earthquakes. Two five-storey and two eight-storey frames are examined, which have been designed in accordance to European codes EC2 and EC8. These frames were combined together to examine 3 different combinations (pairs) of adjacent RC structures, where in any case, one five-storey and one eight-storey frame placed in contact or in distance with gap equal to 0.01m, 0.02m or 1.00m. The behaviour of frames is examined using dynamic inelastic analysis under real seismic sequences. Various parameters are investigated as the maximum horizontal displacement of top floor, ductility of columns, permanent displacements etc. Furthermore, the effect of the collision of the frames is also investigated for the aforementioned values of gaps between the adjacent frames. It is concluded that the effect of collision of adjacent frames seems to be unfavourable for the structures as well as the seismic sequences have more severe impacts compared to the isolated seismic events.

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CONTINUOUS INTERIOR PENALTY FINITE ELEMENT METHOD FOR STRAIN
GRADIENT ELASTICITY

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Keywords: Gradient Elasticity, Continuous Interior Penalty, Finite Element.

ABSTRACT

This work revolves around the design of a continuous interior penalty finite element method for strain gradient elasticity, through the use of non-conforming finite elements. Initially, we use an one-dimensional model problem, following the concepts of both Toupin and Mindlin theory of linear elasticity, for which we define the interior penalty finite element method on finite element spaces consisting of piecewise continuous polynomials. In addition, the resulting method involves only the primary variable, which is advantageous over standard mixed approaches as it refrains from introducing additional unknowns and related difficulties.

Furthermore, the main feature of the new method is the weak enforcement of continuity of first and higher-order derivatives by means of stabilizing terms on both the interior and exterior boundaries. Given the fact that the stabilizing terms are of crucial importance for the convergence of the method, we proceed with the definition of the stabilization parameters. Finally, consistency, stability and subsequently convergence are shown analytically.
A MIXED FINITE-VOLUME-ELEMENT (FVE) FORMULATION FOR THE SOLUTION OF TYPE-III STRAIN GRADIENT ELASTICITY PROBLEMS

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Keywords: Finite volume, finite elements, mixed formulation, first strain gradient elasticity.

ABSTRACT

The dependence of the macroscopic mechanical behavior on the micro-structure of materials is demonstrated in the gradient theories of elasticity. The first foundations were set by Mindlin in 1964, and three forms of the Linear Strain Gradient Theory –LSGT- were analyzed. In the present work a computational approach for the solution of Type- III-LSGT is performed using one microscopic variable. The method adopted is a mixed Finite Volume-Element (FVE) one, in which equilibrium around vertex-centered finite volumes is assumed. The fields of displacement, rotation, couple-stresses and double-stresses are selected as primary variables. The method is applied in 1D LSGT problems, and comparison with analytic solutions shows excellent agreement between the results.
GENERALIZED VARIATIONAL PRINCIPLE AND ENERGY THEOREMS FOR LINEAR STRAIN GRADIENT ELASTICITY

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Keywords: Generalized variational principles, energy theorems, first strain gradient elasticity, Hellinger-Reissner principle, Fraeijs-de-Veubeke-Hu-Washizu principle, He’s semi-inverse method.

ABSTRACT

Generalized continuum theories aim at developing material behavior models that take into account the micro-structure of materials. A well-established theory is the linear strain gradient elasticity, developed by Mindlin in 1964, in which the strain energy density is a positive-definite functional of the strain (as in classical elasticity theory) and the second gradient of the displacement field or the first gradient of the strain. The resulting mathematical models include partial differential equations of at least order-4 and complicated generalized boundary conditions that make the research of analytical solutions quite difficult. Thus, the most secure approach seems to be the numerical one, and in particular the method of finite elements method, which is based on the variational formulation of the problem ahead. In this paper, He’s semi-inverse method is applied to establish a generalized variational principle of five main tensor variables. The resulting generalized energy functional is then constrained by geometrical, constitutive and boundary conditions equations to obtain a family of energy theorems of the kind of "Hellinger-Reissner" and "Fraeijs-de-Veubeke-Hu-Washizu" principles, containing two, three and five main variables. All formulated energy theorems may be used to develop mixed finite element models. The computational effort by means of matrix condition number, convergence, error analysis, etc. may also be investigated and discussed.
EFFECT OF TRIGGERING ON THE ENERGY ABSORPTION CAPACITY OF ALUMINUM SQUARE TUBES SUBJECTED TO OBLIQUE LOADING

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Keywords: Absorbing Energy, Trigger, FEM simulation, Progressive buckling.

ABSTRACT

Aluminum alloys are increasingly used in structures where low weight is important. The ecological aspect of weight savings of up to 25% compared to conventional steel structures makes aluminum an attractive material in the automotive industry. The lower weight reduces the fuel consumption and the emission of carbon dioxide. Aluminum also has the ability to be recycled, which also gives environmental advantages. The axial folding of metal tubes has been known for several decades as an excellent energy absorbing mechanism. Today, Energy-absorbing systems are frequently used in vehicles to protect passengers and the cars structure during accident. The crash box is designed to absorb energy at low speed impacts. Its purpose is to control the initial kinetic energy during impact, and at the same time avoid permanent deformations in the rest of the car body. The energy absorber will seldom be subjected to either pure axial loading or pure bending during an actual crash event, but rather a combination of the two load cases. According to requirements in the automotive industry, the bumper system should endure a load applied with a 30° load angle to the longitudinal axis. In an oblique impact, the crash boxes will be subjected to both moments and axial forces. If the crash box collapses globally, the energy absorption is lowered compared to axial crushing, and both moments and axial forces will be transferred to the rest of the vehicle’s structure. Although studies in this area are limited, some investigations have been carried out numerically. Geometrical discontinuities as ordinary triggers are used in energy absorber structures. Triggers make crushing process easier and decreases maximum crushing load and change collapse process and crushing modes. Despite effects of triggers are investigated in the specimens subjected to axial loading, effect of triggers on the energy absorption under oblique loading is not investigated. The main objective of this study on obliquely loaded specimens was to examine their energy absorbing capability, and the effects of triggers. The behavior and energy-absorbing capability of obliquely loaded square thin-walled aluminum columns were studied through quasi-static FEM-analyses with LS-DYNA. Additionally, the experimental tests were performed, mainly to verify a numerical model of the obliquely loaded columns. The numerical analyses were able to predict the experimental results with reasonable accuracy. The results of this research show that the triggers change the collapse processes and folding modes from global buckling mode to progressive buckling. Therefore, the maximum load is reduced; absorbed energy and crush force efficiency are increased.
MATHEMATICAL MODELING OF THE STRESS–STRAIN CURVES OF AZ80 MAGNESIUM ALLOY AT VARIOUS TEMPERATURE AND STRAIN RATE

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Keywords: Mathematical model, AZ80 magnesium alloy, Tension and compression, genetic algorithm.

ABSTRACT

Magnesium alloys represent poor formability and very limited ductility at the room temperature because of hexagonal closed pack (HCP) structure. That is why magnesium alloys are usually deformed under warm or hot conditions. The deformation behavior of AZ80 magnesium alloy has been investigated in various temperature and strain rate range. During hot working, concurrent strain hardening and flow softening are commonly observed in some materials such as magnesium alloys, steel and aluminum alloys. Due to obtaining the stress-strain behavior of these materials is complicated, time and cost consuming procedure. Hence, a mathematical model can be useful to predict the stress-strain behavior of these alloys. In this study a mathematical model has been developed to predict the stress-strain curves of AZ80 for tension and compression. This model is based on a phenomenological representation of the shape of the stress-strain curves and the traditional theories for constitutive equations which incorporate the power low. In this model curve was divided in two stages. The first component, models the work hardening part up to peak stress. And the second component predicts the stable and softening behavior of alloy. The parameter of this model also obtained and optimized whit genetic algorithm. In addition F.E.M simulations for tension and compression have done. The experimental tests confirm the result of the mathematical model and F.E.M simulations.
THREE-DIMENSIONAL NUMERICAL SIMULATION OF PLAQUE FORMATION AND DEVELOPMENT IN THE ARTERIES

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Keywords: Plaque formation and development, Computational Model, IVUS and histology matching

ABSTRACT

Atherosclerosis develops from oxidized low-density lipoprotein molecules (LDL). When oxidized LDL evolves in plaque formations within an artery wall, a series of reactions occur to repair the damage to the artery wall caused by oxidized LDL. The body's immune system responds to the damage to the artery wall caused by oxidized LDL by sending specialized white blood cells—macrophages (Mphs) to absorb the oxidized-LDL forming specialized foam cells. Macrophages accumulate inside arterial intima. Also Smooth Muscle Cells (SMC) accumulate in the atherosclerotic arterial intima, where they proliferate and secrete extracellular matrix to form a fibrous cap.

In this study, experimental model of plaque formation on the pig left anterior descending coronary artery (LAD) is simulated numerically using a specific animal data obtained from IVUS and histological data. The 3D blood flow is governed by the Navier-Stokes equations, together with the continuity equation. Mass transfer within the blood lumen and through the arterial wall is coupled with the blood flow and is modeled by the convection-diffusion equation. LDL transport in lumen of the vessel is described by Kedem-Katchalsky equations. The inflammatory process is solved using three additional reaction-diffusion partial differential equations.

Matching of IVUS and histological animal data is performed using 3D histological image reconstruction and 3D deformation of elastic body. We developed optimization method to simulate plaque volume development at specific LAD position in order to fit 3D histological observation. Fully 3D concentration of oxidized LDL, macrophages, cytokines indicates that there is a newly formed matter in the intima, especially in region where histological data have found plaque position.

This computer model is based on partial differential equations with space and times variables and it describes the biomolecular process that takes place in the intima during the initiation and the progression of the plaque. The understanding and the prediction of the evolution of atherosclerotic plaques either into vulnerable plaques or into stable plaques are major tasks for the medical community.
APPLICATION OF THE MAXIMUM SCORE MAXIMUM PROFIT ESTIMATOR TO STOCKS OF THE BANKING SECTOR IN THE ATHENS STOCK EXCHANGE

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Keywords: maximum score, multi-objective, evolutionary algorithms, financial time-series, mathematical programming.

ABSTRACT

We are familiar with the maximum score estimator of Manski [1]. A generalization of the maximum score estimator is the maximum profit estimator of Skouras [2]. The general case is the maximum weighted score estimator of Florios and Skouras [3]. Recently, we have discussed the multi-objective estimator maximum score maximum profit (MS-MP). In this paper, we study the computational characteristics of MS-MP in a study of four stocks of the Banking Sector from the Athens Stock Exchange (ASE). The time interval of the analysis is 2001-2009 regarding daily close prices. This results in sample sizes of approximately 2250 observations. The estimation techniques that are used are Non Dominated Sorting Genetic Algorithm II (NSGA-II) [4] and the $\varepsilon$-Constraint method of mathematical programming. The comparison of the two estimation techniques results in a tie and the choice of technique depends on the familiarity of the user with available methods and the availability of software. Results show that the studied greek bank stocks are rather predictable compared to American Dow Jones Chemicals stocks. The obtained score values for the studied greek banks vary from 54% to 58% and the profit values vary from 0.40% to 0.80%. As score measures the direction and profit measures the magnitude of the price movement, we conclude that the MS-MP model predicts 8%-16% better compared to the naïve predictor of score 50% that would predict the direction of the market half of the time. Also, if we have in mind that transaction costs are approximately 0.30% for internet trading, there is a substantial margin for profits since the average profit is 0.40% to 0.80% per day. Future analysis should include out-of-sample considerations for the score and profit metrics. Finally, future research may be directed to the evaluation of alternative mathematical programming techniques and/or evolutionary algorithms.

References
CORRELATION BETWEEN GROUND MOTION INTENSITY MEASURES AND DAMAGE INDICES IN CASE OF AN ASYMMETRIC 3D R/C BUILDING

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Keywords: Ground motion, Intensity measure, Damage indices, R/C Asymmetric building.

ABSTRACT

According to Performance Based Design, structures should be designed so as to meet specific response objectives due to ground motions of a certain intensity level. A number of ground motion intensity measures have been proposed by many researchers over the years. These intensity measures are used for scaling earthquake records in order to evaluate the structural performance. Many researchers have investigated the efficiency of commonly used ground motion intensity parameters by correlating them to the corresponding structural damage. However, all previous investigations have been restricted to plane frames.

The present paper investigates the correlation between a number of widely used ground motion intensity measures and the behavior of an asymmetric single storey r/c building. The overall structural behavior and damage is expressed and quantified in form of the modified Park and Ang damage index. The investigated seismic intensity measures are various peak ground intensity parameters as well as spectral and input energy parameters. Nonlinear time history analyses of the r/c building due to seven bi-directional ground motions are performed. The ground motions are represented by: a) the correlated recorded accelerograms, b) the corresponding uncorrelated accelerograms and c) the completed correlated accelerograms. In an attempt to examine the influence of seismic incident angle, the two horizontal accelerograms of each ground motion are applied along horizontal orthogonal axes forming with the structural axes an angle of \(0^\circ, 10^\circ, 20^\circ, \ldots, 360^\circ\). Then, the maximum damage index for each individual pair of accelerograms of the aforementioned ground motions over all seismic incident angles is computed. Also, the seismic intensity parameters corresponding to each individual pair of accelerograms (recorded, uncorrelated and completed correlated) have been calculated. Finally, the correlation between the calculated maximum damage indices and the ground motion intensity measures is determined and expressed using the Pearson correlation coefficient. The correlation coefficients between the different ground motion intensity measures have also been evaluated.

The results show that

(a) the ground motion intensity measures computed from recorded, uncorrelated and completed correlated accelerograms corresponding to the same ground motion are different, and

(b) the intensity measures that are strongly correlated to the damage index, whether the latter is caused by recorded, uncorrelated or completed correlated pairs of accelerograms, are the Arias intensity and the cumulative absolute velocity.
PERFORMANCE-BASED SEISMIC DESIGN FRAMEWORKS USING STRUCTURAL OPTIMIZATION

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Keywords: Performance-based design, Reliability-based optimization, Particle swarm optimization, Pushover analysis, Life-cycle cost, Single and multiple design objectives

ABSTRACT

We present the application of alternative problem formulations for the performance-based seismic design of steel frames. The design methods discussed are all expressed in a metaheuristic structural optimization environment. We show that advanced – linear or nonlinear, static or dynamic – analysis procedures can be accommodated within a structural optimization algorithm, thus replacing the conventional trial-and-error design process. The proposed procedures are expressed both in deterministic and/or probabilistic formats, the former applying directly the performance-based design concept and the latter being a more elaborate approach where the engineer can set his/her preference on the limit-state failure probabilities, or on the mean annual frequencies of a limit-state being exceeded. Furthermore, one or more objective functions that represent the initial cost or the cost of future earthquake losses during the lifetime of a structure may be taken into consideration during design. The problems discussed are consistent with design-code provisions and consider the response at a number of limit-states, ranging from serviceability to collapse. The procedures are compared on a four-storey steel braced frame. The Particle Swarm Optimization was chosen to solve the structural optimization problem. We show that increased control on the structural performance is obtained since more elaborate analysis procedures are adopted to estimate the structural response. Compared to the current design practice, all problem formulations lead to structures of improved seismic performance and reduced cost.
INVESTIGATION OF SHEAR INSTABILITY IN ORTHOGONAL MACHINING OF TI6AL4V ALLOY USING THE FINITE ELEMENT METHOD

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Keywords: Segmented Chip, Shear Instability, Adiabatic Shear Bands, Crack Generation.

ABSTRACT

During orthogonal cutting of Ti6Al4V alloy the chip is segmented, suggesting the emergence of some kind of instability during plastic deformation of the material. The segmented chip formation occurs from low cutting speeds and persists even at very high speeds, but with a notable change of the chip morphology. Considerable research efforts have been conducted worldwide to explain the underlying physical mechanisms of the segmented chip formation, and several theoretical models have been proposed. Theoretical models based on thermally aided shear instability which results to adiabatic shear bands formation proposed to explain the plastic instability of the material at high deformation rates. Unfortunately, these models cannot provide answers at low deformation rates. On the other hand, fracture models which consider machining as a mechanism of ductile or brittle fracture explain the segmented chip formation as a periodic crack generation mechanism. Despite the above theoretical approaches, the phenomenon is still not well understood. The objective of this work is to investigate the mechanisms of catastrophic shear instability during orthogonal cutting of Ti6Al4V alloy based on coupled thermomechanical rigid viscoplastic finite element simulations in a wide range of cutting speeds.
MULTISCALE COMPUTATIONS IN CHEMICAL VAPOR DEPOSITION PROCESSES: COUPLING A REACTOR WITH A FEATURE SCALE MODEL

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Keywords: Multiscale modeling, Computational Fluid Dynamics, Chemical Vapor Deposition, Ballistic Model, Level Set Method.

ABSTRACT

Chemical vapor deposition (CVD) is a chemical process for producing thin solid films from gaseous compounds, the precursors. CVD is performed in special designed reactors, the CVD reactors, equipped with characteristic surfaces, the wafers, which are exposed to one or more precursors. The precursors react on the wafer surface to produce the desired deposit. The produced films are utilized to a wide range of applications; from semiconductor and micro- sensor devices to micro- and nano-electromechanical systems. Nowadays, the size of these devices shrinks to lower scales and the specifications of the films (thickness, uniformity, surface morphology) refer to properties in micro- or nano-scale. Thus, the single scale conventional CVD modeling methods are not adequate. More advanced, multiscale modeling methods ought to be implemented for studying the phenomena in the co-existing (multiple) scales, in e.g. the filling of a micro- trench or the roughness development during deposition.

In this work, computations in the micro-scale of a predefined topography on the wafer are coupled with computations in the macro-scale of a low pressure CVD reactor (Fig.1). In particular, a link of the reactor operating parameters with the film growth evolution is performed by coupling a reactor scale model (RSM) with a feature scale model (FSM). The RSM consists of the partial differential equations describing the transport phenomena in the reactor bulk phase which are numerically solved by a commercial code [1]. The FSM [2] consists of three sub-models: A ballistic model for the species’ transport inside features (e.g. trenches), a surface chemistry model, and a profile evolution algorithm based on the level set method. The coupled computations are accomplished by correcting the boundary condition for the consumption of species on the wafer [3]. Computational information “flows” from the macro- to micro-scale and vice versa in the course of the simulation. The case study is CVD of Silicon; a key material in the semiconductor industry and in photovoltaic applications. The effect of a) the reactor operating parameters (wafer’s temperature, operating pressure, mole fraction of the precursor at the inlet) and b) the predefined topography on the consumption rate of the species is investigated. The time consuming computations in the micro-scale are efficiently treated with a master-worker parallel technique [4].

Figure 1. (a) Macro-scale: Schematic of a CVD reactor. (b) Micro-scale: Predefined topography on the wafer surface.

MULTISCALE BLOCK MATCHING FOR CAROTID ARTERY WALL MOTION ESTIMATION FROM B-MODE ULTRASOUND

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Keywords: multiscale block matching, Kalman filter, motion analysis, ultrasound, carotid artery.

ABSTRACT

Block matching (BM) has been previously used to study carotid artery wall motion from B-mode ultrasound image sequences [1]. This paper proposes the combination of BM with multiscale analysis based on the decomposition of images using a 2D discrete wavelet transform (DWT). The wavelet-based multisiresolution approach has been used to characterize atherosclerotic tissue from B-mode ultrasound [2]. Multiscale BM (MBM) exploits the information obtained with BM from the approximation sub-images at different spatial resolution scales of the images, obtained by the DWT. Kalman filtering, which has been successfully incorporated in BM-based motion analysis [3], was selected to compose the radial and longitudinal motion estimation of a region of interest (ROI) as a nonlinear combination of motion estimates between successive approximation sub-images. The repetition of MBM nine times by estimating a ROI’s position at the highest decomposition level of the first image of a sequence within a 3×3 window, followed by mean or median filtering of the results, created two additional methods, namely MEANMBM and MEDMBM. All methods were optimized and evaluated on noise-free and noisy synthetic image sequences through the calculation of the warping index. MBM, MEANMBM and MEDMBM enhanced the accuracy of motion analysis of the arterial wall, yielding average error reductions of 63%, 69% and 70%, respectively, for total displacements compared to BM. MEDMBM minimized the warping index with respect to BM (Fig. 1) and could be considered as a reliable computational tool for arterial wall motion estimation from B-mode ultrasound.

Figure 1. Examples of radial (RP) and longitudinal (LP) positions of a ROI located in the posterior wall-lumen interface in the first image of a noisy (top row) and a noise-free (bottom row) synthetic sequence, using BM and MEDMBM.

REFERENCES

NUMERICAL MODELLING OF THE PULL-OUT OF INCLINED HOOKED STEEL FIBRES FROM HIGH-STRENGTH CEMENTITIOUS MATRIX

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Keywords: hooked steel fibres, inclination angle, pull-out strength, high-strength cementitious matrix, three-dimensional finite element modelling.

ABSTRACT

Concrete is a brittle material with a low tensile strength. It has been proved that the addition of steel fibres in concrete or in most kinds of cementitious mixtures, can improve significantly their tensile strength. The beneficial effect of the fibres becomes obvious after matrix cracking has occurred, as they tend to restrict the growth of cracks and undertake the tensile forces immediately after the exhaustion of the tensile strength of the matrix. As each crack continues to open, the fibres that are “bridging” the crack are being pulled-out from the cementitious matrix. Thus, it can be said that the post-cracking behaviour of a steel-fibre reinforced cementitious matrix (SFRCM) is influenced by the effectiveness of the steel fibres in the mixture. The effectiveness of a single fibre can be determined through the load – slip curve which is obtained by the pull-out test of the fibre.

Considering a specific type of hooked steel fibres and for a given volumetric ratio of these fibres in the mixture, the post-cracking properties of the SFRCM are influenced by the random distribution of the fibres in the mixture and consecutively, their random orientation. The fibres added in a cementitious matrix are oriented randomly with respect to the cracking plane. The pull-out behaviour of the fibres that are oriented perpendicularly or almost perpendicularly to the formed crack is dominated by the debonding of the fibre-matrix interface, the friction mechanism and the plastification of the hook due to bending, during the fibre’s slip. However, the fibres which are not oriented perpendicularly or almost perpendicularly to the formed crack, exhibit a more complex behaviour due to additional friction mechanisms, the bending of the fibres at the crack surface and the possible spalling of the matrix. Therefore, fibres with different inclination angles with respect to the cracking plane and for a given crack width can result to different maximum strength values.

This work focuses on the numerical modelling of the pull-out of inclined hooked steel fibres from high-strength cementitious matrix. The pull-out of the fibres is studied by means of accurate three-dimensional finite element models which take into account the non linearities that are present in the physical model, such as the non-linear bonding between the fibre and the matrix in the early stages of the loading, the unilateral contact between the fibre and the matrix, the friction at the contact areas, the plastification of the steel fibre and plastification and cracking of the cementitious matrix. The bonding properties of the fibre-matrix interface considered in the numerical model are based on experimental results of pull-out tests on straight fibres. The paper studies the effects of different inclination angles of the fibres to the load-displacement pull-out curves. The three-dimensional numerical models presented in this work are based on the respective models of aligned hooked steel fibres proposed in [1].

TOP-DOWN ANALYSES OF THE GENETIC CONTROL OF YEAST GROWTH UNDER A RANGE OF PHYSIOLOGICAL CONDITIONS

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Keywords: fitness, genomics, metabolic control analysis, proteasome, ribosome, systems biology, yeast.

ABSTRACT

Large-scale analyses are a fundamental approach in the effort to proceed from genome sequences to systems biology. Molecular tags that allow the identification of every single deletion strain enable parallel competition experiments and genome-wide fitness analysis. An almost complete collection of yeast mutants (96\% of all annotated ORFs) has been used in competitive growth assays under certain environmental conditions. This was accomplished by coupling the molecular barcoding strategy with hybridization-array analysis. By ranking all strains in order of the relative change in their abundance in the population, fitness can be quantitatively analysed.

This study reports the identification of yeast genes displaying a haploinsufficient/haploproficient phenotype in various experimental conditions, including carbon-, nitrogen- and phosphorus-limitation and upon exposure to chromium and grape-juice (GJ). An over-representation of ORFs exhibiting haploinsufficiency has been observed on chromosome III under all three nutrient limitations and in the presence of Cr and GJ. Since chromosome III harbours the genetic loci that determine mating type in yeast, this accumulation of haploinsufficient genes might be due to selection against the loss of chromosome III from diploid cells. A “selective” haploinsufficiency occurs among components of the 19S proteasome sub-complex during Cr stress following observations about the highly significant haploproficiency of the 26S “nanomachine” subunits under N-limitation, while treatment with Cr seems to “reverse” the haploproficiency exhibited by ribosomal protein genes in the C-limited environment; this may reveal a potential interplay between the translational apparatus and the 26S proteolytic machinery to limit Cr toxicity. Additional genome-wide analyses demonstrated the potential importance of protein clearance systems for survival of desiccation in yeast.

The integration of these distinct population-profiling data sets provided information, suggestions, and evidence which pave the way for the assessment of the contribution of all yeast genes to growth rate and fitness. Nevertheless, the real challenge is to elucidate why the growth rate of yeast is affected by these specific gene deletions under these conditions. Having identified classes of genes encoding proteins with, in the terms of Metabolic Control Analysis (MCA), high flux-control coefficients, an endeavour should be made to model the pathways for protein synthesis and protein turnover. A major motivation to define the system (i.e. the yeast cell) from the bottom up is previous evidence for significant effect from the top down. The MCA framework can be combined with linear programming methods for metabolic network analysis and experimental validation of the reconstructed model, using mainly metabolomics and metabolic flux analysis, and, selectively, transcriptomics and proteomics. Bridging the gap between quantitative phenomics and MCA is a challenging task and complementary bottom-up and top-down modelling approaches in yeast as model system could play a key role to accomplish it. Extending the proposed strategy to mammalian cell lines might be attempted towards decoding fundamental properties of all eukaryotic cells and furthering our understanding of the mechanisms of life.
OPTIMIZATION OF THE ELECTROMAGNETIC CHARACTERISTICS OF A 3-PHASE SQUIRREL-CAGE INDUCTION MOTOR USING FEM

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Keywords: Induction motor, FEM analysis, Optimization.

ABSTRACT

The Induction motor forms the 85% of industrial applications, due to its simple manufacturing, reliability and steadiness. Far more than 95% of an electric motor life cycle cost is energy cost. Substantially, lowering motor losses will have a significant impact on one country’s energy consumption. Induction motor design principles have not changed dramatically over the years, while the tools and knowledge of the engineers have improved considerably. Extensive research has been carried out in the last years aiming to high efficiency motors through the optimization of the motors design characteristics. Together with the development of the computer’s science, FEM has also been developed and extensively used by researchers to aid in such problems.

The optimization of the motor geometry has the second greater impact of the possible areas of improvement for the induction motors performance, after the improvement of the active material. Besides that, it is worldwide the least cost-consuming method of induction motors improvement. Firstly, the design optimization process is carried out with the use of simulation models under computer analysis, in order to reshape the motors blueprints. Then, the optimized motor is manufactured. It is obvious that the cost of the process described above, is extremely low while the cost of the manufacturing process remains at the same level.

It is well known that every motor designer confronts a significant dilemma while designing an induction motor. If the rotor’s resistance is high then the motor’s starting torque will be high and the starting current low. On the other hand, the pullout torque occurs at a higher slip causing less part of the air-gap power to transform into mechanical power and consequently reduction of the motor’s efficiency. An induction motor with low rotor resistance presents low starting torque and great starting current but its efficiency under normal load is high. So, an induction motor designer is obliged to choose between the following two conflicting demands, depending on the application: Improved starting performance or high efficiency. NEMA (National Electrical Manufacturing Association) has divided induction motors in four classes (A, B, C, D), depending on the rotor’s geometrical characteristics.

In this work, a 3-phase, 4kW, 400V cast aluminium induction motor with 36 stator and 28 rotor slots has been simulated with the software OPERA Electromagnetic Fields. This first model has been created so that the geometric variables of the rotor are parameterized. The parameterized model has been optimized under three different criteria, covering every possible application with the use of the Optimizer, which is an application of the OPERA. In both three optimization processes, all the parameterized geometric variables of the rotor are taken into account. The first of these three processes occurred to a model with optimized starting behaviour, whereas the second to a model with optimized mechanical output power at nominal speed and the third to a model with optimized efficiency at nominal speed. In all simulations, the electromagnetic analysis was 2D AC steady-state. The analysis considers the models non-skewed and takes into account the non-linear B-H magnetic characteristic of the stator and the rotor iron core. The stator resistance used in the analysis, was measured by DC current injection in the real induction motor.

The purpose of this work is: by keeping the stator intact, to acquire new rotor geometries which will lead to the production of motors with optimized some electromagnetic characteristics, depending on the application requirements. For an induction motor manufacturer this means that, practically with the same production cost, improved motors can be produced, exploiting the results from FEM optimization analysis. Also, faster and cheaper production of models under special client requirements can be achieved, under minimum new designing process.
A REVIEW ON MULTISCALE MODELING IN COMPLEX BIOLOGICAL SYSTEMS: THE TUMOR GROWTH PARADIGM

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Keywords: Multiscale modeling, complex biological system, nano drug delivery

ABSTRACT

Multiscale modeling is a large field that has in root in physics. Over the years a multiscale physics was the main inspiration for developing multiscale mathematical theories. Models have been developed in the microscopic (e.g. molecular dynamics, cellular automata etc), mesoscopic (e.g. kinetic theory, monte-carlo methods etc) and macroscopic scale (continuum models). Multiscale algorithms attempt to bridge the scales and allow for a consisten flow of information.

Tumor growth has been recognized as a prototype complex biological system. Typically, it is a result of events at the intracellular (e.g. signaling pathways), intercellular (e.g. cell-cell adhesion/communication), and tissue (e.g. mechanical pressure due to host constraints) scales. To gain insight, tumor and developmental biologists have gathered a wealth of molecular and cellular measurements including genetic and immunohistochemical measurements. Using an empirical approach, correlations are drawn from the data at the small scale to the tissue scale behavior. Bridging these scales is a significant challenge. Development of multiscale mathematical approaches could significantly impact the issue of bridging the nano (nm)-micro (μm) to the macro (mm, cm) scales and the development of theory that can guide the application of therapies based on nano drug delivery. Here we attempt to review and analyze the application of multiscale models on the problem of tumor development.
MRNA-MICRORNA NETWORK INTEGRATION REVEALS BREAST CANCER SUBTYPE INTERACTIONS

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Keywords: transcriptional, post-transcriptional, network, microRNA.

ABSTRACT

We have recently developed a new method (mirConnX) that combines gene expression data with prior information to calculate gene network modules of transcription factors, miRNA genes, and their corresponding targets. The advantage of mirConnX is that it uses sequence (static) information to define interaction priors between genes, which then help reduce the large number of false positives other algorithms generate. A prior, static network is pre-calculated consisting of computationally predicted transcriptional regulations (transcription factor motif scanning of the genomic regulatory sequences) and post-transcriptional regulations (microRNA target predictions), as well as known interactions supported by literature evidence. The dynamic network is based on mRNA and –if available– microRNA expression data and is inferred using an association measure of choice. Various correlation coefficient measures are currently available, while mutual information will be added in the near future. The static and dynamic networks are then integrated using an integration function. When applied on a breast cancer dataset that became recently available, mirConnX was able to uncover known pathways and identify potentially interesting miRNA-mRNA interactions.
ON DRUG DELIVERY SIMULATION – MODELLING MOTION OF CIRCULAR AND ELLIPTICAL PARTICLES IN LAMINAR FLOW

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Keywords: micro/nano-particles, FE/DPD modeling, shear flow, biomedical applications

ABSTRACT

The intravascular delivery of nanoparticles for biomedical imaging and therapy becomes very powerful and promising tool in cardiovascular and oncological applications. Nanoparticles can be loaded with drug molecules and contrast agents and transported by the blood flow through the circulatory system. They are generally decorated with ligand molecules which are able to interact specifically with antigens expressed over diseased cells (target cells).

In this work, we use the finite element (FE) and dissipative particle dynamics (DPD) approach to model the motion of circular and elliptical particles in a 2D shear laminar flow. Three examples are considered: i) evaluation of the drag force exerted on a circular particle moving in a stagnant fluid, ii) rotation of an elliptical particle around its center in a shear flow, and iii) motion of an ellipsoidal particle in a linear shear flow. For all cases, we found a good agreement with theoretical and finite element (FE) solutions available. These results show that the FE and DPD methods can effectively be applied to model motion of micro/nano-particles at the mesoscale. The method proposed can be used to predict the performances of intravascularly administered particles for drug delivery and biomedical imaging.
A KINETIC-METABOLIC MODEL TO STUDY THE ROLE OF CELL ENERGETIC STATE ON METABOLIC FLUX REGULATION

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Keywords: Metabolic modelling, kinetic modelling, cell energetic, CHO cells, plant cells.

ABSTRACT

Welcoming fundamental life sciences to meet engineering applications, systems biology has now became a federating buzzword. However, ultimately, this approach can lead to highly useful tools, such as predictive mathematical models, which will be beneficial to the biotechnology, biomedical and medical fields. For instance, such models can help to better the productivity and the reproducibility of bioprocesses, as well as to enhance our understanding of a disease or the development of more efficient therapies.

For being predictive, such models need to describe, to our point of view, enzymes kinetic as well as metabolic network regulation. Following this concept, we are developing and challenging a kinetic-metabolic model approach to describe eukaryotic cells behaviour. The model describes nutrient uptake (glucose and glutamine) and metabolite production (lactate and glutamate), glycolysis, pentose phosphate pathway, TCA cycle, phosphorylative and non-phosphorylative respiration from mitochondrial proton leak phenomenon. Metabolic flux kinetic regulation is described from cell energetic and redox states, and from other known effectors or inhibitors concentration.

This model approach has been used successfully to simulate and predict, as well as to control and optimize, plant cell cultures for the production of secondary metabolites. The approach has also been transposed to Chinese hamster ovary (CHO) cells, and different mathematical representations for the regulatory schemes have been tested. Model structure will be presented and model parameters calibration on experimental data for the different cell types and cell lines will also be presented and discussed. In this work, we show that a unique model structure can be used to simulate different plant cell and CHO cell lines. Perspectives on the use of such modelling approach as an in silico tool will be discussed.
THERMAL - STRESS ANALYSIS OF A 3 DIMENSIONAL END – PLATE STEEL JOINT

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Keywords: Thermal – stress analysis, Steel connections, Contact mechanics

ABSTRACT

The mechanical behaviour of a steel connection under elevated temperatures simulating fire conditions, is under investigation. A three dimensional finite element analysis model has been developed, for the simulation of an extended end - plate steel joint. Unilateral contact and friction laws taken from non - smooth mechanics have been applied to the interface connecting the end - plate with the column flange. Material and geometric nonlinearities have been implemented to the mechanical model. The proposed thermo - mechanical analysis is divided into two phases. A thermal model is initially developed; within this model only thermal loads and elevated temperatures are applied to the surfaces of the beam and the column of the connection. The data obtained from this model, e.g. the distribution of temperatures as well as the heat fluxes developed on the structure, are imported to the mechanical model where mechanical loads are also considered. The influence of the elevated temperatures on the mechanical behaviour of the joint is then studied. Comparison between the results obtained from the model with and without high temperatures, has been taken place. Different thermal load combinations have been applied to the connection, for the investigation of their impact on the mechanical behaviour of the structure.
A COMPUTATIONAL MODEL FOR STIRRUPS’ RESPONSE OF REINFORCED CONCRETE UNDER DYNAMIC LOADING

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Keywords: Reinforced concrete, Stirrups, Dynamic load, Strain gauges, Finite elements.

ABSTRACT

In this work a reinforced concrete beam-column connection is simulated using an elastic model. The specimen was fully clamped at the base of the column and a dynamic load was applied at the end of the beam.

At the real scale model, strain gauges were attached on the stirrups of the reinforcement so as to measure their strain. Then the reinforcement was put into concrete. The dimensions of the column and the beam were 152x29x29 cm³ and 157x29x29 cm³, respectively. The real scale model was fixed into a concrete slab at its base and a compressive dynamic load was applied at the end of the beam using an MTS machine.

3D solid finite elements were used for the simulation of the concrete, truss elements for steel reinforcement and a perfect bond condition was assumed between them. Truss elements with cyclic cross section of radius 8mm and 12mm respectively simulate transverse and longitudinal reinforcement. The solid element meshing was performed in a way that the nodes of the solid elements coincide with the nodes of the truss elements. The bottom of the column is clamped. A sinusoidal dynamic load with frequency of 2Hz, 4Hz, 8Hz and amplitude 2.07 mm was applied for 16 sec as a line load at the upper edge of the end of the beam. Transient analysis of the simulation gives results of strains at the locations where the strain gauges were attached on the scale model. A spectral analysis was performed using Fourier transformation.

The aim of this work is to check whether the numerical simulation results are consistent with the experimental data. The frequency where the maximum amplitude is observed and the maximum stains were compared. Numerical results and experimental data were found to be in good agreement.
DESIGN AND IMPLEMENTATION OF A GENERAL PURPOSE FINITE ELEMENT LIBRARY

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Keywords: object-oriented programming, parallel processing, extensibility, finite element library.

ABSTRACT

The design and implementation of Finite Element Analysis programs have always tried to fulfill the requirements of flexibility, efficiency and extensibility. Flexibility may be defined in different ways: (a) the minimum of knowledge of the entire program is required to work on a portion of the code, (b) easiness on reusing code, (c) changes within the data structures does not affect the whole program, (d) interdependencies between the components of the design are easy to determine and/or (e) the integrity of the data structures is assured. Efficiency, defined by means of minimizing the computational time needed for a numerical simulation, has been always a desirable; in fact, flexibility (and even readability and maintainability of the code) is frequently sacrificed in favor of performance. Finally, extensibility refers to the ability that a Finite Element library provides to both developers and users to easily extend its functionality according to their needs.

An overview of recent trends in the design and implementation of a general purpose finite element library is presented in this paper. The use of advanced object-oriented techniques including data abstraction, encapsulation, polymorphism and inheritance in order to boost flexibility of the code base is discussed. Parallel computing architectures like distributed memory systems and shared memory multiprocessing, as well as recently introduced approaches to task-based and data-based parallelism across heterogeneous platforms are compared with respect to performance gains in typical finite element applications. Finally the extensibility and the parametrization of a finite element code base using a scripting language is explored.

The most interesting of the above mentioned techniques are demonstrated in nemesis, an experimental finite element code, implemented by the author. A number of examples are presented, showing the use of the library in typical applications.
ON THE FORMULATION OF A SPECTRAL RETURN MAPPING ALGORITHM 
FOR NONSMOOTH MULTISURFACE VISCOPLASTICITY

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Keywords: return mapping, spectral theorem, multisurface, viscoplasticity.

ABSTRACT

Plasticity models defined by more than one yield surfaces intersecting nonsmoothly are frequently met in many engineering applications, especially in soil and rock mechanics. Furthermore the theory of viscoplasticity is often used to describe the post yield, rate-dependent behavior of solids, including phenomena as creep and relaxation.

This paper presents the formulation and numerical implementation of nonsmooth multisurface viscoplasticity models. In particular, the case where the boundary of the elastic domain is composed of several smooth yield surfaces intersecting nonsmoothly is examined. This implies the presence of singularities in the boundary of the elastic domain, which introduce severe numerical complexities. As a result, different theoretical approaches, algorithms and computer implementations have been proposed to overcome the above mentioned problem, usually requiring specific treatment for each plasticity model. Additionally it can be easily proven that the typical Perzyna viscoplastic model cannot be meaningfully generalized to elastic domains bounded by multiple surfaces.

The algorithm presented in this work, is based on the spectral representation of stresses and strains according to the Spectral Theorem [1] and a return mapping scheme [2] in the principal stress space. Furthermore, the rate-dependent response is assumed to be governed by a suitable generalization of the Duvaut-Lions viscoplastic model [3]. These assumptions lead to a general, efficient, elegant and robust numerical scheme that overcomes the above mentioned difficulties.

The accuracy, performance and stability of the proposed algorithm are thoroughly examined through typical multisurface models.

REFERENCES

WETTING PHENOMENA ON MICRO-STRUCTURED SURFACES

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Keywords: wetting phenomena, micro-structured surfaces, Lattice-Boltzmann.

ABSTRACT

The design of surfaces with fully controllable wetting properties is a research area, with applications ranging from self-cleaning to versatile handling of liquids at the micro-scale without the use of mechanical parts. It is well known that roughness enhances the wetting properties of solids [1]: hydrophobic surfaces become super-hydrophobic and hydrophilic surfaces can become super-hydrophilic through the appropriate design/modification of their roughness. Microlithography techniques enable the fabrication of surfaces with desired roughness, periodic or not, through the construction of micro-pillar configurations with circular or rectangular cross section.

We model wetting of liquids on micro-structured surfaces at the micro-scale. In particular, a two phase flow analysis is implemented using the Lattice Boltzmann method, since the analysis at the continuum using the classical Navier-Stokes equations is prohibitive for flows around complex geometries at the micro-scale. A computational framework linking micro-scale (velocity distribution of fluid particles) and macro-scale (velocity and pressure field) is developed and enables the systematic solution space exploration via the so-called “equation-free” methodology [2]. Multiple wetting steady states are computed and their relevant stability is quantified through the application of matrix-free methods. In this context, the systematic study of the dependence of the wetting states on the geometric features of roughness (i.e. pillar size and shape) is feasible.

We present computations performed for a benchmark problem of a droplet wetting a single pillar. The dependence of the wetting states on the geometric characteristics of the pillar is studied and the results are compared with the computational solutions of the Young-Laplace equation, solved by the standard finite element method.

REFERENCES


AXIAL VIBRATION OF VISCOELASTIC BARS USING THE FINITE-ELEMENT METHOD

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Keywords: Finite element method, viscoelasticity, longitudinal wave propagation.

ABSTRACT

An efficient alternative solution for the finite-element implementation of the axial vibration of viscoelastic bars is discussed in this paper. The effect of viscoelasticity on the dynamic response is accounted for by a convolution integral avoiding the difficulties associated with the fractional time-derivatives used in conventional models for viscoelasticity. An accurate numerical approximation for the obtained convolution integral is proposed. This numerical approximation allows for easy implementation of the finite-element procedure in the time domain as it only introduces additional terms to the mass matrix and the force vector. The additional terms are calculated from quantities obtained in the previous time step. To validate the proposed numerical procedure, a few simple examples are presented and solved by the existing direct methods as well as the alternative method. The examples include the computation of the dynamic axial response of a viscoelastic bar fixed at one end and subject to a step or sinusoidally varying load at the other end. It is concluded that the new method is valid and works satisfactorily.

REPRESENTATIVE FIGURES

Fig. 1. Displacement at the end and middle of a viscoelastic bar subjected to a step axial force for two different materials.
DESIGN OF TURBOMACHINERY BLADINGS USING "T4T".

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Keywords: Turbomachinery, Blade Definition, Parametric Design, NURBS.

ABSTRACT

Although many researchers are involved in the geometrical design (as well as optimization) of turbomachinery components very few methodologies have been presented so far in the open literature concerning the parametric modeling of bladings. The utilization of a commercial CAD package to directly construct the parametric model of a turbomachinery blading is a usual approach, with the obvious advantage that all the infrastructure of the CAD package can be used. However, a separate parametric model for every different type of blading should be built, and the designer has to rely on the available geometric modeling tools of the specific software, without the ability of introducing alternative geometric manipulation methodologies.

A software tool for the conceptual design of turbomachinery bladings named “T4T” (Tools for Turbomachinery) is presented in this paper, which provides the ability to interactively construct parametric 3D blade rows of various types, for single- and multistage machines. A complete parametric design procedure has been adopted, while the generic approach, used in the design procedure, allows for the production of a variety of different rotating machinery components. Although the basic design parameters used for the blades as well as the hub and shroud surfaces construction correspond to 2D sections, the resulting geometries are modeled as fully 3D surfaces and can be exported to other CAD or analysis software via standard exchange protocols, incorporated to T4T.

The object oriented structure of the code enables the easier handling of the various types of geometrical entities (blade sections, 3D blades, hub and shroud curves and surfaces) for single and multistage machines. The geometry definition is based on NURBS curves and surfaces; the blades as well as the hub and shroud surfaces are initially developed in 2D space by defining their cross-sections, and afterwards are translated in 3D space, through standard surface generation techniques such as lofting, or revolving. The definition of blades’ cross-section is based on the use of a camber line and an imposed “thickness distribution” which defines the positions of either the control points or interpolation points of a single NURBS curve. The all-NURBS surface definition strategy was adopted from the beginning of the development of T4T software, which renders the software compatible with the majority of CAD, mesh generation and analysis software, and allows for the use of a small number of design parameters, even for complicated designs.

The software’s structure and geometric algorithms, as well as new features of T4T software are presented in this paper, along with sample turbomachinery designs, selected to demonstrate the capabilities of the software to easily produce different types of turbomachinery, either through the use of its graphical user interface or through a fully automated procedure, developed for optimization purposes.
DYNAMIC RESPONSE OF SINGLE DEGREE OF FREEDOM OSCILLATORS WITH STOCHASTIC MATERIAL PROPERTIES

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Keywords: Stochastic Finite Element Analysis; Dynamic Variability Response Functions; Upper bounds

ABSTRACT

This work presents a methodology for calculating the mean and variability response of linear dynamic single degree of freedom stochastic systems using the concept of the so called Mean and Variability Response Functions (MRF and VRF), recently proposed for statically determinate and indeterminate stochastic systems [1-3] under static loading. Consequently, respective integral expressions are formulated (involving Dynamic VRF and Dynamic MRF) for the estimation of the transient system variance and mean response. The oscillator examined is subjected to two different load cases: a sinusoidal load at the end of its length and an earthquake load following the accelerogram of the el-centro earthquake. The stochasticity of the system results from the selection of a random stochastic field for the inverse of the elastic modulus (flexibility). Any changes to both the Spectral Density Function (SDF) and the marginal probability density function of the stochastic field appear to leave DMRF and DVRF unaffected although this has yet to be proven analytically. This feature gives this methodology a significant advantage providing with an insight into the mechanisms controlling the system responses as well as establishing an easy way to perform sensitivity analyses. Furthermore distribution-free upper bounds can be established all together in a computationally efficient manner. Any results obtained compared with estimates from brute-force Monte Carlo simulations.

REFERENCES

BUILDING FIRE BEHAVIOUR IMPLEMENTING GYPSUM PLASTERBOARDS CONTAINING PHASE CHANGE MATERIALS: A CFD STUDY

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Keywords: CFD, Fire, Gypsum plasterboard, Phase Change Material, LES.

ABSTRACT

A contemporary technique to increase the thermal mass of a building element is to incorporate a Phase Change Material (PCM) into its volume; in this case, the thermal energy absorbed (or released) during the PCM’s transition from solid to liquid phase (or vice-versa) results in a reduction of the indoor temperature fluctuations, thus affecting favourably the required total energy consumption for heating and air-conditioning purposes. Recently, gypsum plasterboards incorporating paraffin-based PCMs, encapsulated in millimetre scale polymer spheres, have become commercially available. The solid-liquid phase change occurs in the temperature range typically found in indoor environments (20-26°C). However, in the event of a fire, building materials may be exposed to substantially higher temperatures (over 800°C). In this case, the paraffins, exhibiting boiling points below 350°C, are expected to evaporate; if the encapsulation spheres fail, the produced paraffin vapours will be released to the porous structure of the gypsum plasterboard and, through mass diffusion, will emerge to the fire region, where they will ignite, thus adversely affecting the fire resistance characteristics of the building.

The effect of PCM addition is investigated by performing detailed numerical simulations of the developing flow and thermal fields in a building constructed using gypsum plasterboards and exposed to fire conditions. The Fire Dynamics Simulator CFD code is utilized for the simulations; the turbulent flow is described using the LES approach, whereas combustion is simulated using a two-step mixture-fraction model. The temperature variation of the various materials’ thermo-physical properties is taken into account by using information obtained by means of Differential Scanning Calorimetry. A conjugate heat transfer model is used to calculate the dynamically varying wall temperature; the paraffin evaporation process is modelled and the produced vapours are introduced to the flow-field as an additional gaseous “fuel” source. The CFD code is validated by utilizing available experimental data, obtained in a standard ISO 9705 fire room exposed to an n-heptane pool fire. The detailed predictions of the temporal evolution of wall surface temperature, gas mixture velocity and temperature, species concentrations and smoke movement are used to assess the effect of PCM addition to the gypsum plasterboard.

Figure 1. Predictions of flame envelope, smoke concentrations, gas mixture velocity and temperature 30 min after the fire initiation.
SIZING OPTIMIZATION OF COLLAPSE-RESISTANT FRAMES

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Keywords: Structural optimization, Limit load, Progressive collapse, Column removal, Alternate load path.

ABSTRACT

Structural design optimization has progressed over the last decades to a valuable computational tool, which assists the engineer in making best use of structural material, in order to detect a feasible and cost-effective design satisfying certain pre-specified constraints. Typically, the aim is to minimize the cost (or weight/material volume) of the structure under consideration subject to behavioral constraints imposed by design codes. Such constraints are mainly associated with member stresses and nodal displacements or inter-storey drifts. In addition to these design code provisions referring to local/member resistance, additional design requirements on system resistance and safety against local failure are increasingly considered in recent years. Local failure may trigger progressive collapse of a structure, therefore insensitivity to local failure is an important property of the structure, which needs to be considered during the design process.

The present work presents a sizing optimization procedure for collapse-resistant elastoplastic steel frames. Mathematical and evolutionary optimization algorithms are employed to minimize structural cost subject to constraints associated with: (a) Eurocode 3 provisions for safety of structural members, (b) structural system resistance and (c) progressive collapse resistance. A method based on the notional removal of key-elements of a frame is used to direct the optimizer towards identifying a structural design, which provides adequate alternate load paths when local failure occurs in the structure. The numerical examples tested demonstrate the effectiveness of the proposed optimization approach.

Of particular importance is also the investigation of the variation in the structural cost achieved when collapse resistance constraints are incorporated in the design process. By enforcing the satisfaction of additional design requirements on system resistance and safety against local failure, structural cost is inevitably increased due to the need for extra weight/material volume. This increase is quantitatively explored by comparing designs obtained with and without collapse resistance constraints.
NUMERICAL COMPUTATION OF THE PERFORMANCE CURVE OF A PELTON TURBINE USING THE SMOOTHED PARTICLE HYDRODYNAMICS METHOD

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Keywords: Pelton turbine, performance curve, Smoothed particle hydrodynamics, mesh less methods, numerical simulation.

ABSTRACT

Pelton turbines are impulse hydraulic turbines suited for high hydraulic water head at relatively low flow rates. The operation of the turbine is based on the interaction of a high velocity water jet with a rotating runner, thus free-surface, unsteady flow with moving boundaries develops. The simulation of the flow using traditional Eulerian representation of the computational domain is a difficult computational task, due to the complexity of the mesh generation on such geometry and the different time and length scales involved. Moreover special treatments are required for the simulation, such as the Volume of Fluid (VOF) method, sliding meshes and mesh adaptation. Representation of such flows would be easier using a Lagrangian point of view. However techniques utilizing moving grids suffer from mesh distortion and grid reconstruction is essential at regular intervals. It would be beneficial to use a method which does not need a computational mesh to discretize the equations of fluid motion. A promising method that fulfils the previously mentioned requirements (Lagrangian and mesh-less) is Smoothed Particle Hydrodynamics, or in short SPH.

SPH was developed by B. Gingold and J. Monaghan, and independently by L. Lucy in 1977, initially for the simulation of complex astrophysical phenomena, but soon the method was extended to model the behavior of solids and fluids. The basic concept is to discretize the simulated medium in a finite set of elements that are called particles. Each element carries its own mass and the respective properties of the medium. Field functions and differential operators appearing in PDEs, governing the behavior of the described medium, can be expressed with summation approximations using a smoothing function on a finite support domain around each computational element, without using a computational mesh.

SPH is being increasingly used to model fluids, since it presents some advantages over the traditional grid-based methods: It guarantees mass, momentum and energy conservation. Adopting a Lagrangian point of view means that there is no need to calculate the convective part, which is a source of numerical diffusion, since it is included in the Lagrangian derivative. Also using a mesh-less discretization from an arbitrarily distributed set of particles, without connectivity, enables the easy representation of complex geometries and of moving/deforming boundaries. Moreover SPH handles naturally free surfaces, without using any special treatments for interface tracking and without diffusion at the interface. The above main characteristics of SPH makes it very appropriate for the simulation of the violent free surface flow developed on the blades/buckets of impulse water turbines, like the Pelton and the Turgo type.

To this purpose, an SPH-based computer code has been developed in our laboratory and verified against various test cases from the literature, such as jet impingement on a flat plate, as well as using laboratory measurements in a Pelton turbine injector. Also, the SPH algorithm was used for the prediction of the flow pattern and force field in a static Pelton turbine bucket under different impingement angles and performed satisfactorily in comparison with a mesh based commercial software, while being considerably faster. This is attributed to the easy parallelization of the SPH algorithm, since the calculation of the characteristics for each particle is independent from all other particles.

In the present work we have used the SPH algorithm to predict the characteristic performance curve of a Pelton turbine. The characteristic turbine curve is very important, since it provides information about the performance and the energy efficiency of the turbine at different operating conditions (flow rate, total pressure difference, revolutions per minute of the runner, etc.). The computed performance curve shows the same trends with the experimental curve. Small discrepancies occur between the two curves, but with the use of a higher resolution in the SPH simulation or the use of a correction factors, these differences are minimized.

The main purpose of our research is the design of a turbine with optimal efficiency at full and part load conditions.
SYSTEM REDUCTION FOR NONLINEAR MULTISCALE DYNAMICAL SYSTEMS: MANIFOLD COORDINATES

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Keywords: System reduction, multiscale problems, manifold coordinates, macroscopic models, microscopic models.

ABSTRACT

The primary scope, when monitoring and analyzing time-evolving systems modeled in the microscopic level, is the prediction of measurable macroscopic, or coarse grain, quantities. However, the presence of a wide range of time scales usually prohibits numerical simulations in the microscopic level. This challenge in numerical modeling cannot be accommodated only by the overwhelming development of computer software and hardware; i.e. in code language and parallel computing. Advancement is also required in mathematical modeling and numerical algorithmic tools. The present work aims towards this direction. In some cases, specific closures allow the derivation of macroscopic simplified models, which are amenable to numerical simulations (e.g. turbulence). Unfortunately, in most cases such closures are not available. Thus, the development of algorithmic tools for the identification of macroscopic models has lately received great attention. In the deterministic setting, most often such systems are usually modeled as $N$ coupled autonomous stiff ODEs, the dynamics of which exhibit $M$ time scales of dissipative nature that are much faster than the rest. While these fast time scales become exhausted, the solution is quickly attracted and eventually evolves on a $(N-M)$-dimensional surface in the phase space; usually referred to as the Slow Invariant Manifold (SIM). The motion along the SIM is related to the macroscopic (continuum) description level, while the fast dynamics of the microscopic (detailed) level are responsible for directing and confining the solution on it. Employing the well-established Computational Singular Perturbation (CSP) method, a new low-dimensional system of non-stiff ODEs is formulated, which governs the slow evolution on the SIM. This reduced sized system is based on a new set of “manifold” variables, i.e. the macroscopic variables, the coordinates of which lie on the SIM. Of all such possible coordinates systems delivered by the method, the selection of the most appropriate one depends on the goals set by the investigator, regarding both the physical meaning of the low dimensional set of new variables, as well as, the simplicity of the mathematical model that governs their slow evolution. The validity of the proposed methodology is demonstrated on the basis of simple examples.

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INTEGRATING GENE REGULATORY AND METABOLIC MODELS TO PREDICT MICROBIAL GROWTH KINETICS

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Keywords: Metabolic Engineering, Genetic Circuit, pWW0 Plasmid, Pseudomonas putida, Dynamic Model

ABSTRACT

Monitoring of bioprocess performance is generally conducted by measuring macroscopic operating parameters, ignoring the molecular interactions controlling the process. However, in many cases biomass utilization and substrate consumption patterns cannot be accurately predicted by models developed merely based on bulk measurements, due to regulation at both the enzyme and the genetic level [1]. The application of experimentally validated models of key genetic circuits to improve the description of the kinetic properties of a microorganism has not been demonstrated yet. The combination of advanced genetic techniques with mathematical models capturing essential quantitative features of experiments can bring a breakthrough from descriptive and empirical approaches to a modern form of mathematical reasoning enriching our understanding of bioprocesses [2]. Thus, mathematical modelling approaches employed to study the function of key genetic circuits for a bioprocess can reveal important links of the particular circuit to the function of the biological system.

Herein, we integrate two dynamic models in the regulatory and metabolic cellular level to describe the m-xylene degrading behaviour of Pseudomonas putida. To this end we have previously paved the way with the development of a mathematical model of the Ps/Pr node of the pWW0 (TOL) plasmid encoded by P. putida mt-2, involved in the metabolism of m-xylene [3]. We present a growth kinetic model of the strain and its novel coupling with the genetic circuit model, which is extended to include the function of Pu and Pm promoters of the network that control the transcription from its catabolic operons. Estimation of model parameters and validation of the model’s predictive capability were successfully performed in batch cultures of mt-2 fed with different concentrations of m-xylene, as confirmed by relative mRNA concentration measurements of the promoters encoded in TOL.

We have built and validated a mathematical model that captures the essential regulatory features of TOL taking into account the observed dynamics of the regulatory circuit in a quantitative manner. The dynamic behaviour of the genetic circuit has been coupled to the growth kinetics of the strain developing a systematic framework that links molecular-level understanding of a system to macroscopic bioprocess behaviour. We demonstrate that substrate consumption and biomass production can be decoupled and described in a mechanistic way based on the molecular phenomena controlling each of the two processes, while the presence of non-constant yields can be also considered reducing the error often generated when constant yield is assumed. Future studies can use the modelling framework developed here in conjunction with the current progress in molecular biology to decipher more detailed models of the relationship between the dynamics of key circuit components and how their underlying biochemical interactions affect the function of biological systems.

REFERENCES

POLLUTANT DISPERSION STUDY IN ASYMMETRIC STREET CANYONS USING LARGE EDDY SIMULATION

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Keywords: CFD, ADREA-HF, LES, Code parallelization, Street canyons, Dispersion

ABSTRACT

Computational Fluid Dynamics (CFD) is a powerful technique to investigate the pollutant dispersion in urban areas. The street canyons, which are the basic modules of the cities, are of particular research interest and they present significant difficulties in their modeling, despite their rather simple geometry. In the current study, an advanced turbulence modeling methodology is used to address the problem and more specifically the Large Eddy Simulation (LES), recently incorporated into the ADREA-HF CFD code \cite{1}. The case considered is the two-dimensional street canyon with a wind direction perpendicular to the street axis and a pollution source at the street level. Firstly, the code is evaluated against experimental data from Hoydysh and Dabberdt \cite{2} and then a number of asymmetric canyons, i.e. canyons with buildings of different heights, is examined. Reynolds Averaged Navier Stokes (RANS) results obtained with the PHOENICS CFD code using the RNG $k$-$\varepsilon$ turbulence model are also presented, along with comments about the performance of RANS comparing to LES. The differences in the flow patterns and the pollutant dispersion between symmetric and asymmetric street canyons are highlighted. The work is focused on the step-down canyons, which present a very interesting feature: At a particular height ratio of the two buildings that form the street-canyon, the flow regime changes and the main recirculation vortex inside the canyon reverses, affecting the pollutant concentrations considerably. Using both RANS and LES simulations, the critical height ratio mentioned above is determined satisfactorily. The instantaneous flow and concentration patterns from LES, provide a deep insight of the phenomena occurring and reveal an unsteady behavior. Some of the results are presented in the following figures. In figure 1 it can be noticed that the predicted pollutant concentration values show fairly good agreement with experimental data, especially for LES. Figures 2a and 2b demonstrate the influence of a small height ratio change in the pollutant concentration patterns.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure1}
\caption{Comparison with experiment (1) and differences in pollutant dispersion depending on $h_1/h_2$ (2).}
\end{figure}

REFERENCES


MODELING OF THREE-DIMENSIONAL FLOW, HEAT TRANSFER AND STRESS ANALYSIS IN HDPE EXTRUSION DIE

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Keywords: Finite Element Analysis, Polymer Flow, HDPE, Extrusion Die

ABSTRACT

A three-dimensional numerical model was developed to investigate the non-isothermal, non-Newtonian polymer flow through a spider die used in the HDPE (High-Density Polyethylene) extrusion process. This model, based on the Multiphysics FE code COMSOL, was used to calculate the pressure flow and temperature distribution in the spider die in the case of the industrial-scale extrusion of HDPE pipes. The model also accounted for viscous heating.

Furthermore, a numerical analysis of the stresses exerted on the spider legs of extrusion dies, using the Arbitrary Lagrangian-Eulerian (ALE) technique, showed that the maximum stresses developed on the die during the extrusion process revealed that, even the spider legs – which are the weakest members of the die – can withstand the applied stresses, during the die operation.

Finally, the results obtained from the FE-analysis, were applied in the design and fabrication of the optimal spider-die, selecting IMPAX (tool steel) as fabrication material.

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Nonlinear System Identification of Vibroimpact Dynamics

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Keywords: Nonlinear System Identification, Vibroimpact Dynamics, Reduced Order Modeling

ABSTRACT

The EMD method combined with the Hilbert spectral analysis, which was introduced in Huang et al. [1] identifies in the characteristic time scales in the data and is claimed to be adaptive and highly efficient, which makes it more suitable for nonlinear and nonstationary data sets. Recently [2,3] a physics-based foundation for EMD has been proposed, making it suitable for reduced order modeling of nonlinear systems. In this paper, we analyze the response of a 1.3 m long cantilever beam, fixed at one end, constrained by two rigid barriers from clearances at 1.185 m, and excited by a pulse force at 0.4 m from its fixed end. EMD is utilized for nonlinear system identification.

By decreasing the clearance to 4mm, the beam undergoes vibro-impact oscillations and strongly nonlinear effects appear in the dynamics as evident in the time series and the corresponding FRF in Figure 2c. It is clear that no system identification can be performed based on the Fourier transform. On the contrary, applying EMD, we are able to decompose the data into a ‘non-smooth’ component (containing the highest frequency effects due to localized vibroimpacts) and a nearly ‘smooth’ residual containing the response of the modes due to vibro-impacts. Reduced models can then be extracted from the ‘smooth’ residual providing us with modal responses due to vibro-impact excitations and the original time series can be reconstructed, which is further discussed in the paper.

References

AN UNSTRUCTURED NODE-CENTERED FINITE VOLUME METHOD FOR COMPUTING 3D VISCOUS COMPRESSIBLE FLOWS ON HYBRID GRIDS.

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Keywords: Compressible Flow, Unstructured 3D Hybrid Grids, Node-centered Finite Volume, Navier-Stokes Equations, Turbulence Models, h-Refinement.

ABSTRACT

A conservative node-centered, finite volume discretization scheme for unstructured, hybrid, three dimensional grids was developed to simulate compressible flows (Euler or Navier–Stokes/RANS). The finite-volume discretization is implemented on three dimensional grids, utilizing tetrahedral, prismatic and pyramidal elements. The hybrid meshes can combine good viscous layer resolving capability, obtained from their prismatic elements on solid boundaries, with the geometric flexibility of unstructured meshes. An edge-based data structure is used for the computation of numerical fluxes, both inviscid and viscous, resulting in reduced memory requirements and computational effort. The algorithm utilizes Roe’s approximate Riemann solver, to compute the inviscid numerical fluxes, while second-order spatial accuracy is achieved with a MUSCL technique jointed with a limiter (Van Leer–Van Albada or Barth-Jespersen). The calculation of the necessary gradients at each node, for the implementation of MUSCL technique, is accomplished through the Green-Gauss method. For the computation of viscous fluxes, the velocity components’ gradients are needed to be evaluated at the middle of each edge; an edge-dual volume is used for this reason, composed of the neighboring cells sharing a common edge. For time integration an explicit four stage Runge–Kutta or a point-implicit Jacobi time stepping method are used. For implicit time integration a continually increasing CFL number is adopted to increase the convergence rate.

For the simulation of high Reynolds flows, three two-equation turbulence models have been incorporated, namely k-ε, k-ω and SST (Shear Stress Transport). The numerical fluxes for the turbulence models are computed in the same way as the viscous fluxes in the N-S equations. The edge-based structure is implemented for the calculation of fluxes and the edge-dual volume technique is used for the computation of the necessary gradients of turbulence variables at the middle of each edge. The solution of N-S and turbulence model PDEs are evolving simultaneously, while the interaction between them is obtained mainly via the turbulent dynamic viscosity computation. Special treatment for the source terms of turbulence model PDEs is applied to control the unphysical growth of turbulent kinetic energy at stagnation points and maintain steadiness and stability of the solution.

An automatic mesh enrichment method (h-refinement) has been implemented to increase the accuracy in regions with high gradients of the flow variables. H-refinement technique enriches the mesh by splitting existing elements into new ones. The procedure begins with the detection of desired areas for enrichment and the division of the corresponding mesh edges; the division is extended to faces and elements, following specific rules. Special treatment is needed for hybrid meshes, as those used in this work, due to the variety of element types and division ways for such elements.

The proposed algorithm has been validated against benchmark test cases and experimental data. Inviscid, viscous laminar, and viscous turbulent steady simulations around wings with NACA0012 and RAE2822 airfoils have been performed, and the corresponding results are compared with experimental data or results obtained with reference flow solvers.
COMPARING THE METABOLIC RESPONSE OF MALE AND FEMALE CEREBELLUM TO PROLONGED ADULT-ONSET HYPOTHYROIDISM IN A MOUSE MODEL USING METABOLIC PROFILING ANALYSIS

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Keywords: Gas Chromatography-Mass Spectrometry (GC-MS) metabolomics, high-throughput biomolecular analysis, metabolic network analysis, multivariate statistics.

ABSTRACT

In the systems biology era, the high-throughput “omic” technologies have enabled the holistic analysis of the various molecular levels of cellular function through the simultaneous measurement of hundreds to thousands of relevant molecular quantities. Metabolomics refers to the quantification of the (relative) concentration profile of the free small metabolites. Taking into consideration the role of the metabolites as reactants and products of the metabolic reactions, their concentration profile affects and is affected by the metabolic pathway flux distribution. Thus, the metabolic profile provides a fingerprint of the metabolic state of a biological system. Among the advantages of the metabolomic analysis is that it can be easily used to monitor transient metabolic conditions without requiring extensive knowledge of the structure and regulation of the investigated metabolic networks. This characteristic is especially advantageous for the analysis of brain metabolism, considering the anatomical, morphological and phenotypic complexity of this organ and our current shortages in understanding its metabolic mechanisms. For the effect of adult onset hypothyroidism (AOH) on brain metabolism in particular, the current knowledge remains fragmented, concerning different experimental setups and recovered from various brain regions. A holistic view of metabolism under AOH in particular brain regions is expected to significantly enhance the current knowledge about the disease. In a recent study1, which was the first metabolomic analysis of brain tissue in a prolonged AOH mouse model, multivariate statistical analysis of the metabolic profiles of the mouse cerebella indicated differences in the metabolic physiology of the tissue in the eu- compared to the hypo-thyroid animals, providing strong evidence that the mammalian cerebellum is metabolically responsive to prolonged AOH. The holistic nature of the analysis enabled the correlation between parallel occurring phenomena, some of which had previously been related to AOH effects, while others implicated new pathways designating new directions for further research. In the present work, we compared the effect of prolonged AOH on the cerebellar metabolic physiology between male and female Balb/cJ mice. The prolonged AOH was induced by a 64-day treatment with 1% potassium perchlorate in the drinking water of the animals. The raw metabolic profiles were normalized and appropriately filtered based on the methodology of Kanani and Klapa2. The normalized metabolic profiles were analyzed using the open-source TM4/MeV software (www.tm4.org/MeV) for the multivariate statistical analysis of “omic” data. The acquired results were interpreted in the context of an appropriately reconstructed metabolic network for the mouse cerebellum based on the metabolic databases, KEGG and Expasy, and a plethora of information mined from the literature. Our results enhanced the currently available “omic” dataset for the brain physiology under prolonged AOH and furthered our understanding of its effect on brain metabolism.


A NUMERICAL INVESTIGATION OF THE INFLUENCE OF ASPECT RATIO IN THREE-DIMENSIONAL, BACKWARD-FACING STEP

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Keywords: Lateral walls, 3D backward-facing step, Finite Elements, separated flows.

ABSTRACT

The influence of lateral walls in three-dimensional, numerical experiments of separated flows is studied in the case of the backward-facing step at a Reynolds number of 800. The computational domain is designed as an actual laboratory experiment. The governing equations are the steady state, isothermal and incompressible Navier Stokes equations. The expansion ratio of the computational domain is 1:2. The aspect ratio varies from 1:10 to 1:40, in order to study the influence of the lateral walls. The results of the computations focus on the spanwise variations of the length and the strength of the two eddies along the lower and the upper wall. It is shown how the flow is disturbed next to the lateral wall and how the two-dimensional attributes of the flow are recovered in the plane of symmetry depending on the magnitude of the aspect ratio. It is concluded that both numerical and laboratory experiments should be designed with an aspect ratio of at least 1:20, so that the effects of lateral walls are limited in the region close to the wall, if only the accuracy of the position of the detachment and the reattachment points matters. If the accuracy of the shear-stress distributions is also taken into account, then an aspect ratio of at least 1:30 should be chosen. This is contrary to the common practice in the field, at least from the side of laboratory experiments, where an aspect ratio of 1:10 is still considered adequate for this purpose.
BASE ISOLATION FOR BUILDINGS IN THE PRESENCE OF SOIL STRUCTURE INTERACTION: THE BASIC MODEL

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Keywords: Base isolation; Distributed parameter systems; Soil-structure-interaction; Structural dynamics

ABSTRACT

In the presence of soil-structure-interaction (SSI) phenomena, a base isolation system will perform differently as compared to the case where the structure is founded on competent soil and/or rock, for two basic reasons: (a) there is a filtering effect affecting the input ground motion signal at the base of the structure, and (b) the overall stiffness, mass and damping characteristics of the combined SSI system have changed as compared to the original structure sitting on firm ground. Thus, a base isolation design \cite{1,2} has to account for SSI \cite{3} in order to have the system fine-tuned to the particular geological conditions and the seismicity of the building site in question.

In this work, we use a distributed parameter system representation of the structure, and identify three basic response modes: flexure, shearing and torsion. The base isolation system system, comprising a sliding base and a restoring spring component, is linearized using the Bouc-Wen mechanical model. The foundation is taken as a rigid block and the soil is represented by equivalent springs. The sub-structuring type methodology employed is cast in the frequency domain, with conditions of equilibrium and compatibility enforced at the common boundaries.

The problem is looked at in three steps. First, the effectiveness of the base isolation system alone in a structure is investigated using input spectra derived from synthetic ground motions, which are calibrated against EC-8 \cite{4} prescribed design spectra. Next, the influence of soft soil on the behavior of a typical high-rise building structure located in an urban environment is examined in terms of both kinematic and inertia interaction effects. Finally, the full problem comprising both SSI in the presence of a base isolation system is gauged. The numerical study serves to reveal the interplay of material and geometric parameters that influence the final response variables, namely top story displacements and base shear forces.

References

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ABSTRACT

Today cancer treatments are based on the results of multicentre trials and studies. The main objectives of these trials and studies are to treat patients according to well-defined risk groups in order to achieve the highest cure rates, to decrease the frequency and intensity of acute and late toxicity and to minimize the cost of therapy. At the same time, response to treatment can be measured individually by tumor volume reduction and/or percentage of therapy induced necrosis at the time of surgery in the histological specimen. This might give an early individual prognostic parameter and can be used for further stratifying and more individualizing postoperative treatment in solid tumors. Together with the measurement of the in vivo response molecular biological analysis of a given tumor plays an increasing role in individualizing therapy for patients. As medicine relies on models to understand and predict the physiology and pathophysiology of biological systems these models are verified in vitro and in vivo but they can also be analyzed theoretically with in silico techniques. Advances in systems-biology-driven concepts in biomedicine enhanced by the increasing volume of molecular data and the decreasing costs of computational power have made it possible to run such large and clinically relevant simulations today. If clinicians could accurately predict which treatment will fail in a patient before it is applied, this could save lives, time and resources, and might ultimately lead to more targeted, personalized therapies. The present paper briefly outlines the computational approaches adopted in implementing a modeling and simulation framework (the Oncosimulator), as an integrated software system simulating in vivo tumor response to therapeutic modalities within the clinical trials environment aiming to support clinical decision making in individual patients. The module has been developed in the context of a number EU funded projects, such as ACGT and ContraCancrum. The development of the Oncosimulator has been based on the top-down modeling approach of the In Silico Oncology Group, as an integrated software system simulating in vivo tumor behavior and ultimately improve accuracy in the interpretation of efficacy and safety findings. To facilitate this, the above mentioned projects are pioneering the development of a modeling library and a software “framework” to enable exchangeability and interoperability of both the existing information (data and models) and future methods and applications in this area.

Keywords: In Silico Oncology, cancer modeling, model interoperability, model re-usability, model exchangeability, modeling library

COMPUTATIONAL SERVICES FOR IN SILICO ONCOLOGY: EXPERIENCES AND RESEARCH CHALLENGES

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In Silico Oncology (www.in-silico-oncology.iccs.ntua.gr) under the lead of G. Stamatakos. The top-down approach starts with the macroscopic imaging data of the tumor which is used in order to construct the spatial modeling framework. Multiscale data pertaining to lower and lower biocomplexity levels as well as (candidate) treatment scheme(s) data are integrated into the modeling framework. Following execution of the Oncosimulator a prediction of the spatiotemporal course of the tumor, eventually subject to treatment, is obtained. Such an approach tries to identify subsystems based on physiological and biological findings that are required to build a reproducible model of a specific cancer. An iterative process continues to find the highest granularity of the system in making the in silico model as accurate as possible in reflecting reality. Doing so, the model is kept under surveillance by the overall behavior of the entire system. From the mathematical standpoint discrete entity – discrete event methods serve as the basis of the Oncosimulator model development, whereas continuous mathematics plays a secondary role. Risk adapted treatment in the future is only possible by fostering translational research. Such translational research has to integrate not only latest developments in clinics and molecular genetics but also in computer science. Assembling existing information and building knowledge within the context of pharmaceutical development or clinical practice needs to be applied consistently, but currently happens inadequately owing to the complexity of integrating disease processes and drug action. Models are a convenient medium for storing knowledge. However, the modelling and simulation process typically takes place in an ad hoc manner, not allowing for potential reuse of models and analysis methods. Currently, as part of the drug development process, newly-developed models, methods, and methodologies are shared with the scientific community through publication. The availability of a public and freely available library for models would streamline the re-use and sharing of existing models and code and thus accelerate the drug development process, and ultimately improve accuracy in the interpretation of efficacy and safety findings. To facilitate this, the above mentioned projects are pioneering the development of a modeling library and a software “framework” to enable exchangeability and interoperability of both the existing information (data and models) and future methods and applications in this area.

In Silico Oncology, cancer modeling, model interoperability, model re-usability, model exchangeability, modeling library

NONLINEAR SIMULATION OF REAL-SCALE RC STRUCTURES
WITH DETAILED AND HYBRID FINITE ELEMENT MODELS

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Keywords: Reinforced Concrete, Hybrid Modeling, Natural Method.

ABSTRACT

In this paper an enhanced Hybrid Modeling (HYMOD) approach is presented which overcomes limitations regarding computational efficiency and permits the simulation and prediction of the nonlinear inelastic behavior of full-scale RC structures. The proposed approach adopts a hybrid modeling with a combination of hexahedral and beam-column finite elements where the coupling between them is achieved with kinematic constraints. With this hybrid modeling, the structural members that are mainly dominated by shear strains, such as shear walls, are discretized with 8-node hexahedral elements while the rest of the structure is discretized with Natural Beam-Column Flexibility-Based (NBCFB) elements. The NBCFB element is also enriched with the natural mode method and the fiber approach which allows the incorporation of more than one material at each beam section. In the proposed modeling the hexahedral elements treat concrete cracking with the smeared crack approach while steel reinforcement can be modeled either with 2-noded rod elements or with the NBCFB element that takes into consideration the shear and bending stiffness of the rebar. In this paper we present the NBCFB element formulation and the HYMOD approach which is based on the kinematic coupling between the 3D modeling with hexahedral elements and the 2-noded RC NBCFB beam-column elements which are used for the simulation of the RC beam and column members of the structure. The numerical results performed demonstrate the advantages of using this hybrid numerical simulation approach for the prediction of the nonlinear response of large-scale RC building structures.

REFERENCES


SURFACE MORPHOLOGICAL RESPONSE OF CRYSTALLINE SOLIDS TO MECHANICAL STRESSES AND ELECTRIC FIELD

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ABSTRACT

Surface morphological evolution driven by external fields is a fascinating topic that has attracted considerable attention over the past two decades within the materials mechanics and surface science communities. This problem has both fundamental interest in understanding field-induced nonlinear response and stability of surface morphology and technological significance over a broad range of engineering applications, from aerospace and nuclear engineering to microelectronics and nanofabrication. In this presentation, recent theoretical and computational work is reviewed on the surface morphological response of crystalline solids to mechanical stresses and electric fields. Emphasis is placed on planar surfaces of stressed elastic solids, as well as surfaces of voids in metallic thin films. A fully nonlinear, self-consistent model of driven surface morphological evolution is described and is employed in the analysis of driven surface morphological response to either electric fields or mechanical stresses acting in isolation, as well as to the combined action of the two external forces. The analysis combines self-consistent dynamical simulations with analytical theory to understand the underlying phenomena and to make quantitative predictions of the driven surface morphological evolution; the simulations employ boundary-integral methods to solve electrostatic and elastostatic boundary-value problems in conjunction with front tracking methods for monitoring mass-transport-driven surface dynamics, while the theory ranges from scaling theory to linear stability analysis. Results of the analysis are compared with experimental measurements; these comparisons include indirect ones, based on monitoring of the electrical resistance evolution in metallic thin films, and direct comparisons of predicted surface morphologies with experimentally obtained surface images. The comparisons validate the driven surface evolution model, provide interpretations to experimental findings, and are used to propose and design experimental studies in cases where experimental observations are unavailable.

Driven void surface dynamics is investigated in detail. Results are presented for the current-driven translational motion of morphologically stable voids, electromigration-induced and stress-induced morphological instabilities, void-void interactions, as well as the formation of stable surface waves and other complex oscillatory patterns. An electromechanically driven period-doubling-bifurcation route to chaos is demonstrated for voids in metallic thin films with low symmetry of surface diffusional anisotropy on the film plane [1]. Results also are presented for the current-driven morphological response of planar surfaces of stressed elastic solids; specifically, it is shown that a properly directed and sufficiently strong electric field can stabilize the planar morphology of stressed elastic solids and inhibit Asaro-Tiller/Grinfeld instabilities that lead to surface cracking [2]. In addition, the analysis has discovered a nonlinear long-wavelength rippling instability that causes the formation of a pattern of secondary ripples on the stressed conductor’s surface [3]; proper application of a sufficiently strong electric field also can inhibit this rippling instability. Finally, some future directions are discussed for further progress in the field. One such direction involves large-scale molecular-dynamics simulations for identification and analysis of dislocation mediated plastic deformation mechanisms [4] as the starting point for development of first-principles-based constitutive equations; such constitutive information will accomplish closure of solid mechanics models that are valid well beyond the linear elastic regime.

AERODYNAMIC AND STRUCTURAL INVESTIGATION OF A FULL COMPOSITE RADIO-CONTROLLED AIRCRAFT

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Keywords: Aerodynamics, CFD, Structural analysis, composite aircraft design.

ABSTRACT

A full composite aircraft has been designed, built and fly tested during the Air Cargo Challenge Competition 2007 in Lisbon, Portugal. The main purpose of this competition was the development of a radio controlled cargo aircraft able to carry the maximum payload for the given motor.

In this paper, the flow field around the main components of the aircraft (wing and fuselage) was investigated using a commercial Computational Fluid Dynamics (CFD) analysis package. The drag and lift coefficients, for a specific Reynolds number range, were estimated in order to reduce the electric power consumption of the aircraft. The numerical results were compared against analytical expressions available in literature.

The drag and lift hydrodynamic forces prediction is vital for the structural design of the wing and fuselage components. These forces applied on the structure can affect the aircraft’s structural integrity. Structural numerical models were developed separately to investigate the strength of each component.

The numerical simulations were performed using the NASTRAN/PATRAN Finite Element Analysis code. The extracted numerical results were used for the final dimensioning of each component. These dimensions were important because of their impact on the total take-off weight of the aircraft.
OPTIMIZATION OF A LARGE SCALE SIGNALING NETWORK USING AN INTEGER LINEAR PROGRAMMING FORMULATION

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Keywords: signaling pathways, signal transduction, systems biology, high-throughput proteomics, logical models

ABSTRACT

Introduction
Understanding the signaling mechanisms involved in major cellular processes is the cornerstone for addressing complex human diseases. Modeling of signal transduction pathways is often performed in a reductionist way by modeling the events triggered by a single stimulus, such as a growth factor, a cytokine, or a chemokine. In such cases, the time courses of a few downstream proteins are measured and the underlying signaling network is modeled using a mathematical formalism like Ordinary or Partial Differential Equations (ODEs or PDEs). Although ODEs can capture the detailed kinetics of signaling reactions, they are not applicable to networks numbering more than a dozen nodes. Thus, ODEs and PDEs offer little potential for a holistic view of the signaling pathway. A more viable approach to modeling large scale signaling networks comes in the form of Boolean Modeling. In such models, protein activity assumes Boolean values (ON/OFF) and the network connectivity is achieved by logic gates (AND/OR/NOT). Although Boolean modeling requires minimal number of free parameters capturing the cell’s signaling mechanisms, calibrating a large Boolean model against experimental data is far from trivial and requires highly efficient computational procedures. In this project we optimize a large scale signaling network numbering more than 500 nodes and 1000 reactions. High throughput experimental data is combined with state of the art optimization algorithms to elucidate the complex cross talks taking place in primary human hepatocytes. The optimization procedure is based on an Integer Linear Programming (ILP) formulation built on a Boolean framework.

Experimental approach
A 2-step experimental procedure is implemented. First, a library of 89 stimuli –aimed to include all major players of liver homeostasis- is screened. For each treatment, primary human hepatocytes are stimulated by a single stimulus and the activation level of 16 key phosphoproteins is measured. In the second step, the compounds found to have a significant effect on the cells, are introduced in combinations of 2 with the presence of inhibitors and the same signals are measured. The presence of inhibitors and combinations is vital for the constrain of the algorithm. By introducing inhibitors that block certain pathways leading from a receptor to downstream signals while monitoring the activation levels of all 16 signals, the algorithm infers what proteins (if any) lie downstream the blocked target. Combinations have similar ramifications.

Computational approach
First a generic pathway is constructed using online pathway databases (Ingenuity, Pathway Commons, KEGG) numbering more than 500 nodes and 1000 reactions that serves as initial conditions for the ILP algorithm. An objective function is introduced to quantify the deviation of the generic pathway from the experimental data. Then an ILP formulation prunes the generic pathway by removing reactions that contradict the dataset at hand, thus minimizing the objective function. The optimized map closely represents the signaling activity of primary human hepatocytes.

Conclusion
By applying an Integer Linear Programming formulation we are able for the first time to optimize a signaling pathway numbering more than 500 nodes and 1000 reactions according to experimental data. In contrast to reductionist techniques like ODEs and/or PDEs that emphasize on detailed modeling of small scale networks, we adopt a wider view of the signaling pathway and identify novel players of liver homeostasis.
LOCAL DAMAGE INDEX FOR SEISMIC ASSESSMENT OF GRAVITY LOAD DESIGNED R/C STRUCTURES

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Keywords: Damage Index, Finite Element, Reinforced Concrete, Gravity Load Designed, Flexure, Shear, Bond.

ABSTRACT

The vast majority of existing reinforced concrete (R/C) structures were designed and constructed in accordance with standards that do not meet current seismic code requirements. The lack of ductile detailing and capacity design principles makes these structures vulnerable to brittle types of failure in case of a major seismic event. Hence, it is important for seismic assessment of existing, ‘old-type’ R/C structures to take into account additional damage caused, apart from flexure, by shear and bond-slip mechanisms.

A great number of seismic damage indices have been proposed in the literature. The level of sophistication of the existing damage indicators varies from the simple and traditional displacement ductility to cumulative damage models which attempt to take into account damage caused by repeated cycling. Local damage indices developed so far for assessing seismic behaviour of R/C structures have been focused mostly on modeling flexural response. Structural damage induced by shear related mechanisms and anchorage bond-slip is either ignored or lumped into the same constitutive law with flexure (e.g. moment-chord rotation relationship).

In this study, a new local damage index for under-designed reinforced concrete (R/C) structures is introduced. This indicator may be considered as an extension of a previous damage index proposed by the writers [1], which considers seismic damage induced by flexure and shear in a distinct manner. In the new damage indicator, deterioration caused by all deformation mechanisms (flexure, shear, anchorage bond-slip) is treated separately. In addition, the proposed index is able to take into consideration the additive character of damage arising from the three response mechanisms as well as the increase of degradation caused by their interaction.

The proposed local damage index is applied in conjunction with a finite element model developed by the writers and described elsewhere [2,3] in order to predict the damage condition of experimental R/C column and frame specimens designed primarily for gravity loading. It is concluded that in any case and independently from the prevailing mode of failure, the new local damage index describes well the detriment state of examined specimens.

REFERENCES


SOLVING LARGE SCALE PROBLEMS IN MESHLESS EFG SIMULATIONS

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Keywords: Meshless, EFG, Large-scale problems.

ABSTRACT

Over the past decades mesh reduction techniques (meshless or meshfree methods) have emerged as a matching part to the well established finite element method (FEM), which has been applied with great success in many fields with both academic and industrial applications. One of the main limitations of finite element approximations is that they can only rely on a prearranged topological environment – the mesh, which is an artificial constraint to ensure compatibility of the finite element interpolation. This limitation leads to several obscurities such as meshing difficulties and increased manpower time in order to resolve them, discontinuous stress fields, accuracy loss in large deformation problems and special treatment of nonaligned discontinuities. On the other hand, Meshfree methods have demonstrated superior results in crack growth and propagation, strain localization and dynamic shear band propagation, projectile penetration and more. The main disadvantage of Meshfree methods is that their memory requirements and computational costs are much higher than those of the ordinary FEM. This is the reason for their limited application to academic and small-scale problems up to now. In this paper we introduce a novel approach for reducing the computational cost of Meshless Methods by employing Domain Decomposition techniques initially developed for FEM. Specifically we consider the FETI family of methods that has been successfully used with FEM in many structural engineering problems. We address the issues of dividing an overlapping Meshfree method (Element Free Galerkin Method – EFG) to several non-overlapping subdomains, and modify the required displacement compatibility conditions by a new technique and solve the problem with iterative methods. Finally, our implementation is verified with two large-scale examples.

REFERENCES


OPTIMUM SEISMIC DESIGN OF STEEL LIQUID STORAGE TANKS

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Keywords: Steel liquid storage tanks, Optimization, Seismic design, Eurocode 8

ABSTRACT

In this paper, an optimization procedure for above-ground thin-walled cylindrical steel liquid storage tanks under seismic loading is presented. Thin-walled steel tanks are very sensitive for seismic loading and their behaviour during earthquakes is very complicated. The aim of this work is the simple, fast and direct seismic optimum design of these special structures, avoiding complicated computational methods such as finite or boundary elements. This objective is achieved using software developed in-house, where the optimum seismic design is achieved satisfying the stability of these structures under extreme seismic design loads according to the Eurocode 8 provisions. Characteristic numerical examples are presented to illustrate the method and demonstrate its capabilities.

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NON-EQUILIBRIUM FLOWS THROUGH MICRO-SLITS AND MICRO-ORIFICES

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Keywords: Rarefied gas dynamics, Kinetic theory, Microflows, Knudsen number.

ABSTRACT

Non-equilibrium flows may appear in several technological fields including microfluidics, vacuum technology and high altitude aerodynamics. The degree of departure from local equilibrium is characterized by the Knudsen number, which is defined as the ratio of the mean free path over a characteristic macroscopic length of the problem. It is well known that for Knudsen numbers larger than 0.1 the typical Navier-Stokes-Fourier approach is not valid and alternative mesoscale approaches based on kinetic theory, as described by the Boltzmann equation or reliable kinetic model equations, must be implemented.

Over the years linearized kinetic equations have been extensively applied with great success to solve internal gas flow through long microchannels of various cross sections in the whole range of the Knudsen number [1,2]. The numerical solution is fully deterministic based on the discretization of the physical space by finite difference schemes and of the molecular velocity space by discrete velocity methods. Then, the discretized equations are solved in an iterative manner, while synthetic acceleration algorithms are applied in order to accelerate the slow convergence of the iteration map at the slip and hydrodynamic regimes. Overall, reliable results for low speed flows through long microchannels of any cross section may be obtained with moderate computational effort. However, when the flow becomes nonlinear, i.e. in the case of fast flows through channels of finite length, including flows through micro-slits and micro-orifices, advanced and efficient kinetic modeling is not available.

In the present work, the gas flow through a micro-slit and a micro-orifice, connecting two reservoirs held at different pressures has been tackled by introducing computationally efficient nonlinear fully deterministic algorithms. The non-linear form of BGK kinetic model equation is used, as an alternative to Direct Simulation Monte Carlo (DSMC), subject to Maxwell diffuse boundary conditions. The corresponding kinetic equations have been solved numerically, applying in the physical space a second-order finite volume scheme and in the molecular velocity space, the discrete velocity method. Moreover, in an effort to decrease the computational effort an enhanced algorithm is proposed by applying certain computational techniques, to overcome the limitations associated with the multi-dimensional nature of the problem. In particular, the total number of iterations is significantly reduced by applying Wynn-epsilon acceleration and a gradual grid refinement method to speed-up the well known slow convergence of the iterative map in the slip and hydrodynamic regimes [3]. Moreover, the code is parallelized in the molecular velocity space and memory demands are reduced by proper handling of the allocated arrays. Results for the flow rates as well as the macroscopic quantities are presented in the whole range of the rarefaction for various values of the pressure ratio between the two reservoirs. Comparison with previously reported corresponding DSMC results indicates very good agreement. The effect of the various geometric and flow parameters on the flow field is examined.

REFERENCES

CAPILLARY EFFECTS IN EXTRUDATE SWELL COMPUTATIONS: ARE THE PRESSURE AFFECTED?

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**Keywords:** Capillary Effects, Free-Surface Flows, Extrudate Swell, Finite-Element Method.

**ABSTRACT**

Extrudate swell is a phenomenon present in exit flow of all viscous fluids from tubes or slits. For Newtonian fluids, the effects of inertia, gravity, compressibility, temperature- and pressure-dependent viscosity, and slip at the wall are well known and do not present major difficulties. The effect of surface tension (capillary number, \( \text{Ca} \)) on the free surface was a major undertaking in the 80’s, and the problem of extrudate swell was more or less settled with a clever integration by parts of the curvature terms due to Ruschak \cite{Ruschak1980}. However, the excess pressure losses in the system, giving rise to the exit correction, have never been reported. The current simulations have used the Newton-Raphson (N-R) and the Picard (P) iterative schemes, the ordinary and singular Finite Element Methods (FEM), and the kinematic boundary condition (KBC) and normal stress boundary condition (NSBC) for locating the free surface. Correct results are obtained only with the ordinary FEM with N-R and the KBC, or, alternatively, with P and the KBC for \( \text{Ca}>1 \) and the NSBC for \( \text{Ca}<1 \). The pressure correction remains almost constant either for planar (slits) or axisymmetric (tubes) geometries. All other methods give an erroneous rapid decrease in pressure, due to a deterioration of the numerical results around the exit singularity as \( \text{Ca} \to 0 \).

FREE (OPEN) BOUNDARY CONDITION REVISITED: SUITABLE AND UNSUITABLE APPLICATIONS

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ABSTRACT

The Open (or Free) Boundary Condition (OBC) was proposed in 1992 to correctly impose outlet boundary conditions in arbitrarily truncated domains. In two benchmark problems of the early 90’s, the OBC was found to give excellent results when compared with solutions from long untruncated domains. In the present work, the OBC is re-examined in the extrudate-swell problem, a simple benchmark problem with a free surface. The OBC was found to work beautifully for Newtonian fluids under the effects of inertia, compressibility, temperature- and pressure-dependent viscosity, and slip at the wall. However, for gravity flows (St number) or surface tension effects (Ca number), the results did not match those from long domains at the truncated synthetic outflow boundary. These findings are apparently due to the gravity body force, which always contributes an extra force on a given domain, and to the exit boundary conditions, which are present at the outflow in capillary flows.

MECHANIC-STOCHASTIC MODEL FOR THE SIMULATION OF ELASTIC MATERIAL RESPONSE IN THIN METALLIC POLYCRYSTALS

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Keywords: Elasticity, FEM, Texture, Stochastic, Micro-components

ABSTRACT

The miniaturization of mechanical and electronic devices demands an adaption to the production techniques to scales under the standard working range. For the production of modern components, very often thin metal pieces must be cold formed. This simple task in the usual scales can produce a series of problems in thin metal components of small scale, as there are only few material grains constituting the complete piece.

The main modeling and computational challenges arise from the fact that the small scales invalidate the usual assumptions of homogeneous material, as the variations in the mechanical properties for the diverse grains constituting the piece cannot be neglected. One common approach is to model the metal pieces as polycrystals, with each crystal having slightly different material properties.

For the thin metallic polycrystals, the complete material anisotropies must be considered. On the one hand, the thin metal sheets are produced by a rolling machine and present a texture, and, on the other hand, there are small variations in the mechanical properties of the different grains.

In this work, we present the main ideas for a coupled mechanic and stochastic model, the algorithm for its computation and the resulting distributions of the strain and stress tensors components on representative volume elements (RVE). Key parts of the algorithm are the construction of semi-periodic RVEs and the splitting of the elastic response in six basic modes. Computation of material responses in the RVE scale produces a material library where the effects in the polycrystal scale are captured.

This material library is later used to predict the variations in the mechanical responses of a large piece of material for which a simulation with resolution in the grain scale would be unpractical or even impossible.

Although our method presented here is of elastic nature, some initial ideas for its extension to plastic deformations will also be presented.
FUZZY CONTROL OF A SMART ELASTIC PLATE

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Keywords: smart structure, elastic plate, vibration suppression, time-dependent spectral method, Newmark-beta scheme, fuzzy control.

ABSTRACT

A dynamic problem of vibrations of a smart plate with active control is considered. The mathematical model is a dynamic linear partial differential equation of hyperbolic type. It describes deflections of a thin elastic rectangular plate which is subjected to external disturbance forces and generalized control forces, produced for instance by electromechanical coupling effects. A nonlinear controller has been designed, based on fuzzy inference. The initial and boundary conditions are set up for the equation. The initial-boundary value problem is spatially discretized by means of the time-dependent Fourier spectral method. The direct numerical integration technique, namely, the implicit Newmark-beta method, is employed for the numerical solution of the problem. The method has been implemented within MATLAB and the Fuzzy Logic Toolbox has been used for the realization of the fuzzy controller.
SIMULATION OF TRANSIENT FILTRATION PROCESSES IN POROELASTIC MEDIA WITH PHYSICAL NONLINEARITIES

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Keywords: Coupled Problems, Poroelasticity, Thermoelasticity, Nonlinear Transient Problem, Finite Element Method, Methane Extraction, Fluid Pressure.

ABSTRACT

The paper considers filtration and coupled poroelastic problems in order to describe degassing processes which take place under hydrodynamic influence on coal beds containing methane. A coal seam is represented by heterogeneous physically nonlinear porous media where injected fluid moves under filtration through porous space. Well-known analogy between filtration and thermal conductivity equations and between poroelastic and thermoelastic equations is applied in order to solve the above problems in ANSYS finite element program.

Numerical simulation is carried for a three-layer coal seam in the Krasnodonetsk coalfield of the Eastern Donbass Basin consisting of coal layer and two layers of associated rocks which have different mechanical and filtration properties. The key characteristic of the hydrofracturing process is nonlinear dependence of the filtration coefficients of the coal layer on the pore pressure.

The first stage of the modeling considers pure filtration problem for non-deformable porous medium. The initial boundary value problem is set in axisymmetric and 3D settings. An analogy between filtration and thermal conductivity equations enables to solve transient nonlinear filtration problem as thermal conductivity problem with the help of ANSYS finite element program. Numerical results allow obtaining pictures of pore pressure distribution in the coal seam and estimating the size of degassing zone. 3D case is studied in order to simulate more complex geometry of the coal seam intersected by the layer of the fluidization zone.

The next stage of the modeling considers the process of fluid filtration in porous medium together with deformation of porous skeleton. In this case the coal seam is represented by saturated two-phase porous medium in a coupled-field axisymmetric problem setting. The well-known analogy between poroelastic and thermoelastic equations allowed to treat the poroelastic problem as a thermoelastic problem and therefore to apply thermal-stress analysis modules for numerical simulation in ANSYS finite element program. Because of the large spread in the orders of the material modules a transfer to dimensionless variables was performed. Numerical results for fully coupled and uncoupled problems were compared in order to analyze the effect of the stresses. Various input data variations were carried out in order to estimate the influence of different input parameters on the pore pressure distribution. The results of this analysis allowed choosing an effective type of hydrodynamic influence subject to the parameters of the problem.

In order to study fracture processes in the coal seam under hydrodynamic influence more complicated coupled poroelastic model of three-layer coal seam with a circular inner crack in the coal layer was considered. In order to model the singularities of the stresses in the vicinity of the crack tip and to insure necessary asymptotic of the displacements field the finite element mesh was condensed in the vicinity of the crack vertex and to displace middle nodes of finite elements surrounding the crack vertex for a quarter towards the vertex. Numerical results enabled to analyze stress concentration, compute stress intensity factors and evaluate the influence of the crack on the size of the borehole degassing zone.
ANALYSIS OF INHOMOGENEOUS ANISOTROPIC PLANE VISCOELASTIC BODIES WITH FRACTIONAL DERIVATIVE MODELS

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Keywords: viscoelasticity, inhomogeneous anisotropic bodies, generalized fractional derivative models, boundary element method, analog equation method.

ABSTRACT
The response of inhomogeneous anisotropic plane bodies made of linear viscoelastic materials is investigated. The employed viscoelastic material is described with generalized multi-term differential models of fractional order. Many researchers have shown recently that fractional derivative models describe accurately the response of many viscoelastic materials with much less parameters than integer order derivative models. The governing equations are derived by considering the equilibrium of the plane body element. Then introducing the viscoelastic constitutive relations, two coupled second order linear fractional partial differential equations in terms of the displacement components are derived. Using the concept of the analog equation [1] these equations are transformed into two uncoupled Poisson’s equations. Subsequent application of the BEM enables the spatial discretization yielding thus the semi-discrete equations, which constitute a system of two-term ordinary fractional differential equations (FDEs) of evolution type for the fictitious sources. Their solution is obtained using the numerical method for FDEs developed recently by Katsikadelis [2]. Once the fictitious sources are established the displacements are evaluated from the integral representations of the solution of the substitute problems. Numerical examples are presented, which not only demonstrate the efficiency of the solution procedure and validate its accuracy, but also give a better insight into this complicated structural plane body response.

References
NUMERICAL STUDY OF THE EFFECT OF SPEAR VALVE DESIGN ON THE FREE JET FLOW CHARACTERISTICS IN IMPULSE HYDROTURBINES

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Keywords: Pseudo-compressibility, free-surface jet, nozzle flow, impulse hydroturbine, spear valve, numerical simulation

ABSTRACT

Impulse turbines are generally used for conversion of hydraulic energy into electricity in areas where the hydraulic head of the water resources is quite high. The main parts of these turbines are the injectors, which transform the hydraulic energy into kinetic energy, and the runner. The free-surface jet which comes out from the injector interacts with the buckets of the runner and causes its rotation. The turbine efficiency is primarily affected by the buckets design and the jet characteristics. The latter are depended on the design of the nozzles of the turbine injectors. This paper investigates numerically the effect of different values of a nozzle spear valve angle on the characteristics of the free jet flow, as well as on the energy losses at the nozzle area.

The numerical simulation of a free-surface jet is a demanding task, since it comprises a two-phase flow and the jet geometry is not known in advance. In this case, a numerical algorithm which allows the determination of the geometry of a free-surface jet has been developed based on the method of pseudo-compressibility. This algorithm is based on the finite volume method and its main feature is that it solves only the liquid-phase flow, without taking into account two-phase flow as Volume of Fluid and other models do. The equations governing this type of flow are the continuity and Navier-Stokes equations. The addition of the temporal derivative of pressure in the continuity equation (pseudo-compressibility method) allows the simulation of the flow, while the initial variables of the problem are velocity and pressure. For the simulation of turbulence the standard k-ε model is used. The geometry of the free-surface jet is determined with the following procedure. At first it is approximated with the help of a Bezier curve and the flow is computed. At the end of the simulation, the velocity normal to the surface of the jet boundary cells is computed. If its value is not close to zero, the grid is reconstructed by displacing its nodes and the flow is simulated again. The whole procedure is repeated until the computed velocity normal to the surface of the jet boundary cells is practically equal to zero.

The flow of the free-surface jet has been considered to be an axisymmetric problem. At first, a nozzle geometry identical with that of a Pelton turbine model, which is installed in the NTUA’s Laboratory of Hydraulic Turbomachines, was examined. The numerical simulation was carried out for various nozzle openings and the computed discharge was in good agreement with existing experimental results. Next, the jet flow was simulated for various different values of the spear valve angle and also for a different nozzle outlet angle. From the comparison of the flow simulation results for the various nozzle geometries, it is assumed that the jet characteristics are primarily affected by the value of the spear valve angle, whereas the effect of the outlet angle value is negligible. As far as the nozzle efficiency is concerned, the reduction of the nozzle outlet angle leads to higher losses. The effect of the alteration of the spear valve angle is related to the value of the nozzle opening.
STEADY SOLUTIONS OF INERTIAL FILM FLOW ALONG STRONGLY UNDULATED SUBSTRATES

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Keywords: Steep corrugation, subcritical or supercritical flow, capillary or gravity regime, separation eddy, multiple solution, flow oscillation.

ABSTRACT

Steady flow of a liquid film along sinusoidal, steeply corrugated walls is investigated by finite-element simulation of the 2D Navier-Stokes equations. Resonance between the wall and capillary-gravity waves travelling against the flow defines a critical Re and separates the flow into a subcritical and a supercritical regime. Steep corrugations trigger extensive flow separation in both regimes. However, the separation characteristics -most notably the limiting behavior for very thin and very thick films-vary because of the different significance of capillary forces in the two regimes. For very steep corrugations, two intersecting solution branches co-exist. The present computational predictions are compared favorably with independent experimental observations.
TRACER MOVEMENTS IN OPPOSITE FLOW DIRECTION UNDER SATURATED CONDITIONS. A NOVAL FINDING IN DISPERSION OPERATIONS BY USING SCHEIDEGGER-BEAR’S FORMULA

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Keywords: Dispersion Parameter, Counter Flow Direction, Computational Method, Scheidegger-Bear.

ABSTRACT

This manuscript is concerned with the dispersion of a tracer fluid flowing through a porous medium. Nowadays, computer codes use dispersion parameters derived from advection dispersion analysis to estimate the behavior of contaminants inside an aquifer. In most cases, the basic of these codes is the powerful Scheidegger-Bear formula applying numerical dispersion coefficients. Earlier research studies largely dealt with issues concerning downstream movements from a contamination hotspot. Our research project on hydrodynamic dispersion was focused on the upstream movement. The target was to simulate the hydrodynamic dispersion by using a dyes tracer and to analyze the results using our numerical modeling program. Nevertheless, the experimental results of the upstream tracer flow did not fit the actual simulation of the modeling program. For further understanding several other simulations have been done to find a solution for this problem. However, the changes in velocity and the longitudinal dispersivity coefficient had no effect on the results. The spreading in the opposite direction still occurred after long time intervals. Even simulations with the MODFLOW program showed identical results. To date, we have not found a concrete mathematical solution for this phenomenon.
THE EFFECT OF GRAVITY LOADS ON SEISMIC PERFORMANCE OF SPECIAL MOMENT RESISTING STEEL FRAMES

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Keywords: Steel Moment Resisting Frame, Performance Evaluation, Distributed Plasticity, Nonlinear Dynamic Analysis.

ABSTRACT

In order to investigate the effects of gravity loads on the seismic performance of Special Moment Resisting Frames (SMRFs) gravity loads are increased while the seismic effective mass is kept constant by adjusting the ratio of dead to live loads. The effects of span arrangements are also examined by changing the number of spans while the total floor area is kept constant. To this aim, 3 five-story buildings are designed according to the relevant Turkish Codes by allowable stress design philosophy. Special attention is given to the optimization of the frames in order to avoid arbitrary amount of overstrength which would affect the global performance favorably. The lateral load resisting system consists of two perimeter special concentrically braced steel frames (SCBFs) in “Y” direction in the plan and two SMRFs in “X” direction. Total plan area is the same for all of the model buildings while the number of spans and span lengths differ in “X” direction. With the chosen geometric properties design earthquake load and seismic effective mass is kept constant for these buildings. The frames are modeled by displacement based beam-column elements considering the distributed plasticity in an open source computer program, OPENSEES. Geometric nonlinearity is taken into consideration by co-rotational transformation. Number of 15 ground motions are simulated by the computer program SIMQKE-II, whose mean spectrum matches to 1.5 times the design spectrum resulting in 2% probability of exceedance in 50 years. Nonlinear dynamic analyses are performed for the designed frames under the simulated ground motions. Beam, beam-to-column connection and column rotations are determined according to the definitions of SAC Steel Project Phase II. Results indicate that for a 23% increase in gravity loads the increase in the plastic rotation of beams and beam to column connections can reach to 27% and 10%, respectively. Regarding the span arrangements the plastic rotation of beam to column connections increase with increasing number of spans.
AN ENERGETIC APPROACH TO FRICTIONLESS CONTACT PROBLEMS USING THE DIRECT COLLOCATION BEM

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Keywords: Boundary Element Method, Signorini Conditions, Receding Contact, Advancing Contact, Potential Energy, Minimization Procedures.

ABSTRACT

Most of the procedures using boundary integral equations method to solve elastic problems with contact are based on strong imposition of compatibility and equilibrium along the contact zones. In this work a novel approach using energy principles and the direct collocation boundary element method (BEM) is introduced. The approach is able to solve general frictionless contact problems of multiple elastic bodies. Both conforming and non-conforming boundary discretizations of contact zones are included. After introducing some theoretical background, the numerical formulation of the approach is presented. Some considerations on the computation of strain energy by the collocation BEM are also given. In the last part of this work, examples of classical contact problems are solved by the developed and implemented computational algorithm in order to assess its performance.
A NEW MATHEMATICAL TECHNQUE IN CONSTRUCTING THE GENERAL PARAMETRIC SOLUTION OF THE NONLINEAR ODES OF THE TYPE 
\[ y'''' = f''''(x) y'''(y'_x)^l. \] APPLICATION TO THE WHITE-DWARF RELATIVISTIC EQUATION

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Keywords: White-Dwarf, Emden-Fowler, General Solution.

ABSTRACT

In this paper we develop a successful new mathematical technique leading to the construction of general solutions in parametric form of the nonlinear differential equations (ODEs) of the type 
\[ y'''' = f''''(x) y'''(y'_x)^l \] 
\( (n, m, l) \) arbitrary parameters), and thus of the types of the generalized Emden-Fowler or the normal Emden-Fowler (ODEs) \( y'''' = x^m y''(y'_x)^l \) and \( y'''' = x^m y'' \) respectively \([1,2]\). Here the notation \( y'_x = dy/dx \), \( y''_x = d^2y/dx^2 \),... is used for the total derivatives. This method is based on convenient substitutions and on successful functional transformations.

Several basic practical nonlinear (ODEs) of the second order in mathematical physics and nonlinear mechanics \([3]\) are reduced to equivalent equations of the examined type of nonlinear ODEs, by means of various convenient substitutions and admissible functional transformations \([1,2,4]\), such as the White-Dwarf in relativistic mechanics \([3,6,7]\), the “elastica” equation for bars under distributed axial load in large geometrical elasticity \([5]\), the dimensional axisymmetric Schrödinger equation \([16]\) in mathematical physics, etc. The resulting new equivalent equations are of the same type to the examined here problems (ODE) and they do not admit general solutions in terms of known (tabulated) functions, since only very special forms of them can be analytically solved \([2,4]\).

The application here concerns the White-Dwarf equation in stellar structure \([3,7]\) that concerns curvature term and the parametric solutions are obtained in exact form.

REFERENCES

A NEW MODEL FOR SHAPE MEMORY ALLOY MATERIALS UNDER GENERAL STATES OF DEFORMATION AND TEMPERATURE CONDITIONS

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ABSTRACT

In this work we provide a general geometrical framework, which constitutes a basis for the derivation of constitutive models for materials undergoing phase transformations. This framework is presented abstractly in its most general form and it leaves the number and the kind of the internal variables and the kinematics of the deformation entirely unspecified. Large deformation generalized plasticity is presented in this geometrical framework and is suitable for the derivation of three–dimensional thermomechanical constitutive laws for shape memory materials. Then, we derive a finite strain constitutive model for these materials. The ability of the derived model in simulating several patterns of the extremely complex behavior of those materials, under isothermal and non–isothermal loadings, is assessed by representative numerical examples.
THE EFFECT OF THE GEOMETRIC IMPERFECTIONS ON THE ROTATIONAL CAPACITY OF STEEL BEAMS AT ELEVATED TEMPERATURES

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Keywords: rotational capacity, numerical modeling, geometric imperfections, elevated temperatures

ABSTRACT

The main objective of this paper is to propose advanced three-dimensional models based on the use of shell elements that can be used for the simulation of the structural steel behaviour under fire conditions. The problem is handled through coupled thermo-mechanical analysis in the context of the finite element method. The basic target is to ensure that the developed numerical models can describe adequately the complex behaviour of structural steel in elevated temperatures. For this purpose, an experimental study, available in the literature, is used for comparison. The three – dimensional numerical model that is proposed in the current study, is developed using the non-linear finite element code MSC Marc. The first step is to simulate the behaviour of steel I-beams studied experimentally in [1] and compare the test results with the corresponding values from the numerical analysis.

Based on the proposed numerical models, which are verified through the results contained in the literature, moment – rotation curves for various members in elevated temperatures are obtained. These functions can be used for the analysis of frame structures under fire conditions through simpler software packages, utilizing beam finite elements with concentrated nonlinear behaviour.

ADAPTIVE FUZZY CONTROL OF SMART STRUCTURES - ANFIS

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Keywords: smart structures, fuzzy control, adaptive fuzzy inference (ANFIS).

ABSTRACT

Smart structures incorporate sensors and actuators, as well as control mechanisms that provide the smart (intelligent) behaviour. The control system is, therefore, an important part of the system. Linear feedback of linear systems can be studied by using classical methods of control. Nonlinearity in the system or in the controller makes the problem much more complicated. Fuzzy and hybrid neuro-fuzzy controllers can be used in this case.

In previous investigations (Tairidis et al. 2007) a fuzzy controller has been proposed and tested numerically on a smart beam composed of piezoelectric sensors and actuators. Manual tuning of the fuzzy controller can not lead to optimal performance. Among others, the controller has worse performance in terms of velocities and accelerations, as it can be expected due to it’s nonlinear feedback, that would lead to fatigue problems in the involved components. Previous attempts of our group to alleviate this problem have been based on the automatic tuning of the controller by means of a genuine global optimizer, namely the particle swarm optimization (Marinaki et al. 2010). In this paper an adaptive fuzzy controller based on the well-known ANFIS system has been tested.

The proposed method is based on the following steps:

i. A detailed mechanical model of the smart system is constructed
ii. The dynamics of the system with a preliminary controller are studied and saved
iii. An adaptive fuzzy controller is optimized by using the ANFIS method
iv. The trained controller replaces the initial one

Extended numerical results and parametric investigation of the proposed system on a smart beam with piezoelectric sensors and actuators which have been modeled within MATLAB/SIMULINK demonstrate the applicability of the method.

References


PARTICLE METHODS AND COUPLED PROBLEMS IN ROTORCRAFT AEROMECHANICS

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Keywords: vortex methods, particle mesh method, Hamilton Jacobi equation, helicopters

ABSTRACT

Performance analysis and design of rotorcrafts is directly connected to the solution of coupled problems. Taking the ordinary helicopter as a typical example, several couplings and interactions take place. There is strong vortex to solid surface interaction over the main rotor, also known as BVI; the tail rotor is necessarily operating in the wake of the main rotor; BVI encounters will generate intense noise generation; the blades are flexible and so there is non-linear aeroelastic coupling involving large displacements and rotations which cause significant vibrations; finally in order to comply with flight requirements, noise regulations and passenger comfort, there is control of the main and tail rotor. So all in all, rotorcraft aeromechanics deals with servo-aero-elastic problems and aero-acoustic analysis.

Due to the very different scales involved, a fully coupled simulation of the complete rotorcraft is extremely expensive. One possible way to render the simulations affordable is to suppress one or more of the interacting components leading to purely aerodynamic analysis in which case the flow can be resolved quite accurately or comprehensive aeroelastic analysis giving emphasis to the structural vibrations etc. Another approach is to keep all mechanisms in the simulation and tailor in the best possible way the methods of approximation. To this end,

- Controls, dynamics and structural mechanics are best described in the context of Hamiltonian mechanics. In this case the description is Lagrangian and the usual approximation made, is the finite element method. Due to their high slenderness, the blades can be accurately described by non-linear beam theory while the fuselage is in many cases taken rigid – in other cases a finite element description is needed either in full form or in some equivalent definition.

- The fluid flow is represented by means of particles. The main advantage of such an approach is that the description of the flow is also Lagrangian and therefore fully compatible with the solid part. Another advantage is that there is no need for a grid. However, particle methods are known to have difficulties with boundary conditions. In order to bypass this difficulty, the otherwise particle method is coupled with a grid based method, which is restricted close to the solid boundaries referred to as near region. It the flow is potential, the near region is reduced to a surface grid and the equations to be solved are surface integral equations. Then the particles will be carrying vorticity and for this reason the underlying method is a vortex particle method. In certain cases however compressibility cannot be neglected. Then in the near region, one should solve the Euler equations and particles should not only carry vorticity but also mass.

Following the above outline a simulation environment has started to develop in mid 90’s at NTUA aiming at performing fully coupled simulations. Besides choosing the main approximation tools, the whole development required the implementation of several acceleration techniques, like tree-algorithms, fast Poisson solvers connected to the Particle Mesh technique. In the present paper, results from fully coupled simulations will be presented and comparisons with wind tunnel measurements of a complete helicopter will be made. It concerns a scaled BO105 model which was operated as a real helicopter except for the fuselage which was rigid. The discussion will focus on the latest developments and in particular on the computational characteristics and the procedures for cost reduction.
SOME CASE STUDIES OF MONTE CARLO AND MOLECULAR DYNAMICS SIMULATIONS

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Keywords: molecular simulation, Molecular Dynamics, Monte Carlo, clathrate hydrates, pore size distribution, carbon characterization.

ABSTRACT

In the very early stages of computer simulation in 50s, the study of even the simplest system required computational facilities like MANIAC (the first computer to be used for molecular simulations, in Los Alamos Laboratory), that involved very high cost and occupied a lot of space. After 60 years of application and constant development, molecular simulation has already become an essential part of Materials Science, and has proven to be a valuable and very reliable approach for the study of huge variety of systems and natural phenomena. This rapid expansion and recognition of computer simulation can be attributed to two coexisting reasons. The first and most obvious reason is the sharp increase in the available computational power over the last two decades. Contrary to the unaffordable systems of 50s, modern home-use computers can be used to simulate quite complex systems. The second reason is the inherent trend of researchers to advance to more and more complicated systems where larger amounts of information should be processed and higher accuracy is required. These requirements render a real experiment a very difficult and demanding task. For this reason, computer experiments have started to partly substitute real experiments, though the complete substitution is beyond the limits of physical sciences. In contemporary Materials Science, computer simulation comprises the third major methodology along with theory and experiment.

In this work, we present three case studies to illustrate some ways to utilize molecular simulations in the study of materials. In the first case, the composition of clathrate hydrates of several gases at various conditions is determined by Monte Carlo (MC) simulations, and the results are found to be in good agreement with the experimental data. In the second case, Molecular Dynamics (MD) simulations are used to predict the structural properties of some molecules that appear in biological tissues. Both of these studies would not be feasible if they were carried out exclusively by experimental means since the cost and the requirements of a single experimental measurement (just at one specified set of conditions) is extremely high. In the third case, another functionality of molecular simulation is illustrated: the interpretation of experimental data. To this purpose, gas sorption data are combined with MC simulations towards the characterization of nanoporous carbon materials.
DESIGN AND COMPUTATIONAL EVALUATION OF S-DUCT INTAKES FOR UAV APPLICATIONS

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Keywords: Computational Fluid Dynamics, S-duct intakes, Unmanned Aerial Vehicles.

ABSTRACT

The design of intakes for high performance Unmanned Aerial Vehicles (UAVs) is not a trivial task, as those vehicles combine characteristics of high performance agile aircrafts on one hand, and missiles with air-breathing propulsion on the other. Several conflicting targets have to be accomplished, such as good efficiency, in terms of high pressure recovery and low pressure distortion, low drag, and high margins of stability. The aforementioned characteristics should be maintained throughout a wide range of operating conditions, such as flight Mach numbers, angles of incidence, sideslip, and engine thrust, while, at the same time, weight, cost and complexity should be maintained as low as possible. Although only subsonic flight is considered in this work, a Mach number range from zero to plus 1.0, a range of incidence between -5° and +30°, a sideslip variation of about 10° and a range of engine airflows from idle to maximum may be required. Taking into account the S-type shape of the intakes, separated flow and complex shock-boundary layer interactions, sometimes unsteady, will be present over a wide range of flight conditions. Moreover, all of the above should be considered within the framework of fuselage – wing – intake – engine interaction.

In this work, a numerical study is performed in order to design an S-Duct intake for UAV applications with good efficiency in a wide range of operating conditions. Initially, a fully-parametric 3-D CAD model of the intake was constructed. By adjusting the corresponding geometric parameters, various different geometries can be easily produced. In this way scaling the geometry or fitting the intake in a different aircraft configuration become easy tasks. The CAD-model was used in order to produce different intake configurations, within specific geometric constraints, and study the influence of geometry variation on efficiency.

O-type blocking methodology was used in order to construct the block-structured mesh of hexahedral elements, used in our simulations. The adopted blocking strategy consists of making blocks for the primitive and general geometrical features and continuing to the most detailed and smaller parts of the geometry. A complicated block-structured topology was used for the grid construction, resulting in 39 different blocks. The adopted topology enabled the construction of a fine mesh near the engine bullet wall at the engine inlet region. Appropriate associations were applied between the blocks and the corresponding geometry surfaces or curves in order to keep the surface representation and the mesh density variation as smooth as possible. The number of elements in each cross section of the duct was kept almost constant in all cases (different duct geometries), with the number of elements in the longitudinal direction varying with the axial length of the duct.

The commercial CFD code ANSYS-CFX was used to compute the flow field inside the flow domain of each case considered. The Reynolds averaged Navier-Stokes (RANS) equations are discretized using an implicit, vertex-based finite volume method, combined with the shear stress transport (SST) two-equation turbulence model and an automatic wall treatment. SST was used as it provides good predictions in adverse pressure gradient boundary layers, as those found in this study. The simulations were carried out in a steady mode, using 2 maximum continuity loops, high resolution advection scheme and a physical time step. The computation results for the different S-duct geometries were used in order to guide the design process and select a configuration with superior performance.
UNDERSTANDING TSUNAMI WAVES THROUGH NUMERICAL SIMULATIONS: THE CASE OF MINOAN TSUNAMI, 17TH CENTURY BC

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ABSTRACT

Tsunamis are gravity waves caused by submarine earthquakes and volcanic eruptions. Tsunami waves are also locally generated by coastal and submarine earth slumps. Assessing hazards associated with tsunamis requires a good understanding of their generation mechanisms, propagation in the open sea and inundation in coastal segments. One of the most powerful advanced tools to perform such studies is the numerical simulation of tsunamis. In the Mediterranean Sea region, the largest tsunamis were reported to generate along the Hellenic Arc and Trench which is the most active seismotectonic structure in the region. Historically such tsunamis that propagated in extensive areas of the eastern Mediterranean basin were reported on AD 365, 1303 and 1956. The giant Late Bronze Age eruption of Thera (Santorini) volcano in the 17th century BC was one of the most important ever experienced by humanity. One of the distinct geophysical phenomena associated with the LBA Thera eruption was the large Minoan tsunami which is documented in publications reporting coastal and sea-bottom tsunami sediment deposits left in several localities of the East and Central Mediterranean. The elevation of the coastal tsunami sediment deposits ranges from -1.6 m to +9 m in relation to the mean sea level (msl). Calibrating against a msl rise of about 1.5 m, which occurred in the Mediterranean in the last 4000 years, it comes out that the elevation of the LBA tsunami deposit localities at the time of deposition ranged from 0 to +10.5 m. Maximum elevation was observed in NE Crete. We simulated the tsunami with two scenario mechanisms, caldera collapse and pyroclastic flows. For the wave propagation fully non-linear Boussinesq equations were adopted. Synthetic tsunami waveforms were produced in virtual tide-gauges situated at shallow water depths of about 20 m to reduce uncertainties due to shallow depth bathymetry. Caldera collapse produced one-peak wave amplitudes which fit well enough the elevations of deposit localities. For caldera collapse scenarios of 19 km³ and 34 km³ in volume, wave amplitudes of ~2.5 m and 7.5 m were found offshore NE Crete. Due to the strong energy directivity associated with the pyroclastic flow, tsunami amplitudes are consistent with deposit elevations only for localities where the wave energy is directed to. For pyroclastic flow of 55 m in thickness penetrating the sea at azimuth of 200°, that is towards NE Crete, wave amplitude of ~9 m was found. The pyroclastic flow mechanism may account for small and moderate tsunami waves produced during the entire eruptive activity. Due to the energy directivity effect, however, the mechanism is considered incapable to produce the minimum tsunami amplitudes required to deposit sediments in many different azimuths with respect to a preferred direction of penetration. On the contrary, the caldera collapse scenario may account for significant wave amplitudes in different directions from the tsunami source. The simulation results of the extreme case of Minoan tsunami are useful not only to study the particular wave but also for the assessment of hazards that may be produced from future large tsunamis in the Mediterranean basin.
RELIABILITY ANALYSIS USING SUBSET SIMULATION AND NEURAL NETWORKS

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Keywords: Subset Simulation, Neural Networks, Markov Chain, Metropolis-Hastings, Reliability Analysis

ABSTRACT

This paper examines a methodology for computing the probability of structural failure by combining neural networks (NN) [1] and Subset Simulation (SS) [2]. SS is a powerful tool, simple to implement and capable of solving a broad range of reliability problems. In many cases however, SS leads to reliability predictions that exhibit a large variability due to the fact that the robustness of the SS prediction depends on the selection of an adequate width of the proposal distribution when applying the modified Metropolis algorithm. In this work a methodology is proposed for reducing the inherent variability of the SS estimation using a Neural Network-based Subset Simulation methodology (SS-NN). This approach takes advantage of special characteristics of the SS procedure in order to exploit the capability of NN to accurately approximate limit state performance of structural systems. The main challenge lies in the ability of a NN to approximate accurately complex structural response when properly trained in the ranges defined by the progress of the SS for each random variable. In the numerical examples considered, it is demonstrated that robust and computationally efficient estimations of the failure probability are obtained using the proposed procedure by enhancing the computational performance of the SS method.

2.3 References


A NUMERICAL METHOD FOR PREDICTING ACOUSTICAL WAVE PROPAGATION IN OPEN SPACES*

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Keywords: aeroacoustics, compact differencing, spatial filtering, benchmark problems, absorbing boundary conditions, perfectly matched layers, Kirchhoff vortex, acoustic analogy.

ABSTRACT

Wave propagation phenomena play an important role in many engineering fields such as aeroacoustics, blood flow in arteries, phonation, electromagnetism, quantum mechanics and seismology. Knowing a priori the mechanism waves are generated, propagated, scattered, reflected and/or dispersed in some medium allows engineers to take decisions about the topological placement of devices (antennas), the construction of safe buildings and the optimal acoustic design of rooms/halls.

In the present work we present a numerical methodology for evaluating wave propagation phenomena in two dimensions in the time domain with focus on the linear acoustic second order wave equation. An outline of the higher order compact discretization schemes followed by the time discretization technique is first presented. As high order schemes are non dissipative they’re prone to develop spurious oscillations, which may grow during the integration process and contaminate the solution. Therefore the method is completed with the addition of spatial filtering based on the same compact schemes’ principles.

The important role of boundary conditions is subsequently addressed. In order to be able to predict radiation in the far field, one must truncate the computational domain in the near field by proper and physical means without sacrificing the accuracy of the numerical solution or introducing significant artifacts into the computation. Two popular ways used by several analysts are presented and compared here: First the formulation of ‘absorbing conditions’ in the form of partial differential equations especially for the origin of the domain, and second the construction of an absorbing layer surrounding the domain, in which waves (after they’ve exited the domain) are attenuated and decayed exponentially. This idea first presented for the Maxwell equations in electromagnetism and later readopted under several variants, is recalled and reformulated here for the case of a 2D domain but without having to split the 2nd order wave equation into a 1st order hyperbolic system and thus introducing more unknowns and increasing the computational effort/memory.

Subsequently the method is assessed by recalling three benchmark problems. In the first where a Gaussian pulse is generated and propagated in a 2D rectangular domain, the accuracy and absorbability of the boundary conditions are compared. In the second a similar situation is investigated but under curvilinear coordinates and under the presence of a solid body which scatters the pulse. Finally the sound field inducted by the flow of corotating vortex pair is calculated and compared with the corresponding analytical solution. Results are presented and discussed so as to thoroughly demonstrate the behavior of the method.

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FREQUENCY-DEPENDENT MODAL DAMPING RATIOS IN LINEAR NON-CLASSICALLY DAMPED SEISMICALLY EXCITED FRAMES

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Keywords: Modal damping ratios, frequency domain, linear structure, seismic excitation.

ABSTRACT

Frequency-dependent modal damping ratios are provided in order to approximately calculate the seismic response of linear non-classically damped frames using modal superposition in its classical form (normal mode shapes that diagonalize the damping matrix). These frequency-dependent modal damping ratios are obtained by solving a set of non-linear algebraic equations coming from a modal identification model of a structure that involves its real mode shapes as well as the modulus of the complex roof-to-basement frequency response transfer function of the frame. The solution of these equations is performed for various frequencies that cover the significant frequency range of the frame as well as that of the seismic excitation. Therefore, curves that provide modal damping ratios as function of frequency are constructed and bounds for their values are obtained. It is shown that the seismic response of a non-classically damped frame can be approximately found by using the bounds for modal damping ratios from these curves in conjunction with the normal mode shapes of the frame. Moreover, it is discussed how these curves can provide indications to the seismic design of the frame.
AN ALGORITHM FOR CREATING TRIANGULAR $C^1$ FINITE ELEMENTS WITH POLYNOMIAL INTERPOLATION

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Keywords: Triangular finite elements, $C^1$ continuity, Gradient elasticity.

ABSTRACT

Various finite elements providing a $C^1$ continuous interpolation of the displacements were developed in the 1970s, to be used in problems of thin-plate bending, where the underlying partial differential equation is of the fourth order. More recently, interest in this kind of elements was renewed in connection with their use with strain-gradient theories, which similarly involve a fourth-order partial differential equation [1].

One such element with 21 degrees of freedom was initially proposed by Argyris et al. [2] (and, independently, by other researchers), while a simpler element with 18 degrees of freedom was also derived starting from the initial element. In a recent paper [3], we have presented an algorithm which allows the creation of the simpler element without needing to first formulate the more complex one. This algorithm was presented in such a way that it allows the creation of other similar elements, with different orders of the interpolating polynomial.

In this paper, we present in more detail the relevant algorithm and the resulting finite elements obtained through it. Since in these elements the type of degrees of freedom is determined beforehand, a specific class of elements is obtained based on the required interpolation order. Based on these results, however, we can then proceed to generalize the proposed algorithm to consider additional arbitrary types of degrees of freedom. The details of this generalized algorithm are therefore presented, together with some additional $C^1$ elements which are thus derived. Since the basic characteristic of all elements being considered is that they employ a polynomial interpolation, the issue of whether the proposed algorithm is exhaustive, i.e. it can produce all such elements, is also discussed.

The numerical behavior of the different elements presented in this paper is tested through some simple benchmark problems of gradient elasticity. This testing provides strong indications concerning the accuracy, stability and relative performance of the different elements.

REFERENCES


TRANSIENT DYNAMIC ANALYSIS OF A FLUID–SATURATED POROUS GRADIENT ELASTIC COLUMN

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Keywords: Poroelasticity, Gradient elasticity, Dynamic response, Column problem

ABSTRACT

The dynamic response of a fluid-saturated porous gradient elastic column to a transient disturbance is determined analytically-numerically. The basic dynamic theory of a fluid-saturated poroelastic medium due to Biot is modified by replacing the classical linear elastic model of the solid skeleton by the simple gradient elastic model of Mindlin with just one elastic constant (internal length scale) in addition to the classical ones. Thus, the new theory, which is presently restricted to the one-dimensional case, can take into account the microstructural effects of the solid skeleton. After the establishment of appropriate boundary and initial conditions, the one-dimensional dynamic column problem is solved analytically with the aid of the Laplace transform with respect to time. The time domain response is finally obtained by a numerical inversion of the transformed solution. The effect of the solid microstructure on the response is assessed and discussed.
We will present a Lagrangian computational methodology that allows the calculation of turbulent heat and mass transport behavior in the case of wall turbulence. The methodology is a particle method, in which the trajectories of heat or mass markers are monitored in time and space in a turbulent flow field. Statistical information about the behavior of these markers is collected, and is used to determine the temperature or concentration profile in the channel and to determine turbulent transport quantities, like eddy diffusivity and the turbulent Prandtl number. We call this methodology the Lagrangian scalar tracking method (LST).

The study utilizes a direct numerical simulation (DNS) of turbulent flow in an infinite channel and in plane Couette flow to generate the flow field. The computational box dimensions are $4\pi h \times 2h \times 2\pi h$ in $x$, $y$, $z$ for Poiseuille flow and $8\pi h \times 2h \times 2\pi h$ for Couette flow (where $h$ is the half channel height, and $h = 150$). LST involves the tracking of the trajectories of scalar markers in the flow generated by the DNS. The effects of convection are simulated by moving the markers under the assumption that they follow the velocity field. The diffusion effect is simulated by adding a 3D random walk on the marker motion that follows a normal distribution with a standard deviation dependent on the Prandtl number, $Pr$, of the fluid [1]. The range of $Pr$ covers 4 orders of magnitude, between 0.1 and 1000. The trajectories of about 150,000 heat markers are calculated for each case.

The turbulent transport quantities that can be calculated using this methodology include the mean temperature profile as a function of the $Pr$, and the eddy viscosity and the eddy conductivity in convective turbulent flow. These values are then used to determine the turbulent Prandtl number, $Pr_t$, which is necessary to close the system of equations for heat transfer, when eddy viscosity based models (such as $\kappa$-models) are utilized. Most of prior studies have reported that $Pr_t$ strongly depends on the molecular Prandtl number. In addition, for cases of wall turbulence, the $Pr_t$ has shown strong dependence on the distance from the walls, which will be discussed in our analysis.

The presentation will discuss the numerical methodology and results will be compared with available data from earlier DNS works [2]. Finally, the effects of the molecular $Pr$ in turbulent heat transfer for both the channel Poiseuille and Couette flow cases will be discussed.

References


NUMERICAL IMPLEMENTATION OF $J_2$ NON-ASSOCIATIVE FLOW PLASTICITY MODELS FOR SHELL BUCKLING IN THE INELASTIC RANGE

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Keywords: Bifurcation, Buckling, Plasticity, Numerical integration, Finite elements.

ABSTRACT

In the present paper, a special-purpose numerical technique is employed to examine the structural stability of cylindrical shells under axial compression, which buckle in the plastic range. It is an in-house finite element technique for the nonlinear analysis of cylindrical shells, through a “tube-element” discretization, which has been used successfully in the past for nonlinear modeling of tubular beam-columns.

A key issue of this technique concerns the use of an appropriate plasticity model. Analytical and numerical predictions of structural buckling in the inelastic range have been shown to be in closer agreement when the deformation plasticity theory moduli are employed, instead of the moduli of the widely accepted flow plasticity theory. This result has been very important towards bifurcation prediction from an elastic-plastic prebuckling (fundamental) solution. The better predictions of deformation theory in terms of the flow theory have been attributed to the formation of a “vertex” or “corner-like shape” on the yield surface at the point of loading when the deformation theory is employed. This “vertex” is in accordance with experimental evidence, which indicate a high curvature region on the yield surface at the point of loading. On the other hand, the flow theory assumes always a smooth yield surface, resulting in stiffer material moduli, especially in directions that deviate from the fundamental stress path. It is noted that, at the onset of buckling, an abrupt change of the stress direction occurs with respect to the fundamental state, which may not be accurately predicted by the “stiff” moduli of the flow theory. Towards this purpose, a non-associative plasticity model is developed, which describes accurately material behavior in the buckling stage, where an abrupt change in the direction of stresses occurs.

The present paper describes the numerical implementation of two plasticity models. The first employs the von Mises yield surface ($J_2$ plasticity) and the rate form of $J_2$ deformation theory, leading to a non-associated flow rule. The second constitutive model is a large-strain enhancement of the model proposed by Hughes and Shakib for small strains; this is a modified $J_2$ flow theory model with elastoplastic modulus depending on the direction of strain increment with respect to the outward normal to the yield surface. The numerical implementation is conducted through both the classical Euler-backward and Euler-forward substitution numerical schemes for elastic-plastic shell analysis, where stress and strain tensors are described in curvilinear coordinates, with the extra constraint of zero normal stress through the shell thickness. The above technique will be employed to identify first wrinkling and determine post-wrinkling behavior of the steel cylinder subjected to uniform axial compression. In particular, the ability of the steel cylinder to deform beyond initial wrinkling will be examined, so that the post-buckling reserves of the pipe component are determined. The numerical results will be compared with available experimental data.
AN IMPROVED AUGMENTED LAGRANGIAN TECHNIQUE FOR FREE SURFACE VISCOPLASTIC FLOWS

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Keywords: Augmented Lagrangian Method, Non-Linear Conjugate, Herschel-Bulkley Fluids, Free Surface Flows

ABSTRACT

Viscoplastic materials behave either as a rigid solid if the yield stress is not exceeded in the fluid or as a generalised Newtonian fluid beyond this critical value [1]. Their rheological behaviour can be described by the discontinuous Herschel-Bulkley constitutive model which takes into account the shear-thinning nature of the fluid. This enables the exact description of solid and liquid regions as required by the existence of discrete regions of zero and nonzero shear. The accurate determination of these regions is achieved by introducing a Lagrange multiplier in the constitutive equation, this is the so-called augmented Lagrangian technique [2,3]. Thus, the nonlinear optimization problem, namely the problem of minimizing the rate-of-strain is reduced to a saddle point problem which is solved iteratively via a Picard-type coupling of the flow and mesh sub-problems. Actually, it is an iterative method which converges rather slowly and its convergence rate depends strongly on the value of the augmentation parameters. Here, we propose a new method for adjusting these parameters following the non-linear conjugate method. Three different approximations, the Fletcher-Reeves, Polak-Ribiere and Hestenes-Stiefel formulas, are tested on the simulation of the motion of a rising bubble in a Bingham plastic. Results demonstrate the accuracy of the improved method in the calculation of the yield surfaces. Moreover, the method enables us to determine precisely the shape of the bubble, the speed and shape of the yield surface for a wide range of viscoplastic materials. The increase of Bingham number leads to a reduction in the rise velocity of the bubble while the yield surface at the equator plane and away from the bubble grow until it is trapped. In case of slightly deformable bubbles, our results were compared with the continuous Papanastasiou approximation for Herschel-Bulkley fluids [4].

REFERENCES

PARAMETRIC STABILITY AND SIMULATIONS OF INSONATED CONTRAST AGENTS—EFFECT OF THE CONSTITUTIVE LAW

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Keywords: Microbubbles, lipid coating, constitutive law, ultrasound, parametric stability, boundary elements

ABSTRACT

Contrast agents are microbubbles encapsulated by a lipid or polymeric shell that is used in order to stabilize them against dissolution. Once injected in the human body they scatter sound in a nonlinear fashion acting as contrast enhancers against nearby tissue in modern diagnostic modalities, or as drug delivery vectors in therapeutic treatments involving ultrasound.

They are known to exhibit dynamic patterns such as thresholding, compression only behavior, diffusion and deflation, shape deformation, buckling, jetting and break-up, not all of which can be adequately predicted based on a single model describing the mechanics of the coating. The effect of shell elasticity and viscosity as well as their nonlinear evolution with varying amplitude and frequency of the acoustic disturbance, is studied against the above patterns, first in the context of spherosymmetric pulsations. The superiority of strain softening models is discussed and the relevance of strain hardening models is presented in the context of the “compression only” behavior of lipid coated microbubbles. The latter is associated with a folding instability that occurs dynamically in the form of buckling and that is accelerated in the presence of prestress.

Next the dynamics of axisymmetric deformations is studied subject to different constitutive laws for the coating and the possibility for parametric mode excitation and resonance is investigated. The boundary element methodology is adopted for simulating free pulsations of a contrast agent subject to acoustic disturbances and it is seen that strain softening shells exhibit saturated pulsations in the region where linear stability analysis predicts unstable growth of shape modes via harmonic and subharmonic resonance. The onset of static and dynamic buckling is also studied and possibilities for break-up and jet formation are discussed.
AN INTRODUCTION TO COMSOL MULTIPHYSICS: THE INDUSTRY-LEADING MULTIPHYSICS MODELING AND SIMULATION ENVIRONMENT

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ABSTRACT

COMSOL Multiphysics is a flexible simulation platform that allows scientists and engineers to model all relevant physical aspects of their designs. COMSOL environment facilitates all steps in the modeling process – geometry definition, meshing, physics specification, solving, and results visualization. Model set-up is quick, thanks to a number of predefined physics interfaces for applications ranging from fluid flow and heat transfer to structural mechanics and electromagnetic analyses. Material properties, source terms and boundary conditions can all be arbitrary functions of the dependent variables. Predefined multiphysics - application templates solve many common problem types. There is also the option of choosing different physics and defining custom interdependencies, or specifying custom partial differential equations (PDEs) and link them with other equations and physics. The flexible nature of the COMSOL environment facilitates further analysis by making “what-if” cases easy to set up and run. Production level simulations can be achieved by optimizing any aspect of the model. Parameter sweeps and target functions can be executed right in the user interface. From start to finish, COMSOL is a complete problem-solving tool providing the confidence to build models with real-world precision.
MODELLING OF PARTICLE INERTIAL EFFECTS: AEROSOL DEPOSITION IN A 90° BEND

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Keywords: Inertial effects, Bend deposition, CFD modelling, Eulerian-Eulerian method

ABSTRACT

Simultaneous calculation of diffusion and inertia is important because these two mechanisms occur simultaneously in many aerosol processes. Effects due to particle inertia in aerosol flows are optimally modelled using a Lagrangian formulation, according to which the particle equations of motion are solved. However, incorporation of particle Brownian diffusion in such a description increases computational difficulties due to the stochastic nature of the phenomenon. Thus, scientific interest is directed towards a coupled Eulerian modelling encompassing both inertial and diffusional transport.

A numerical model for the simulation of aerosol flows via an Eulerian-Eulerian, one-way coupled, two-phase flow description is presented. A noncommercial computational fluid dynamics code [1], which utilizes the finite volume method and incorporates high order discretisation schemes, is used to obtain the velocity and pressure fields of the gaseous (continuous) phase. A modified convective diffusion equation models particle transport.

In order to explicitly consider the effect of inertia on Brownian diffusion in isothermal aerosol flows under steady state conditions, a low Stokes number expansion of the average momentum equation was used [2]. As a result, a first-order correction to the particle velocity field \( \tilde{v}_p \) due to particle inertia was obtained:

\[
\tilde{v}_p = \tilde{u} - D \ln c - \tau_p \left( \tilde{u} \cdot \nabla \right) \tilde{u} + O(\tau_p^2),
\]

where \( \tilde{u} \) is the carrier gas velocity, \( c \) the particle size distribution, \( D \) the Brownian diffusion coefficient and \( \tau_p \) the particle relaxation time. In this case, the equation that describes the particle size distribution \( c \) and its variation in space and time takes the form:

\[
\frac{\partial c}{\partial t} + \nabla \cdot (c \tilde{u}) - \tau_p \nabla \left[ c \left( \tilde{u} \cdot \nabla \right) \tilde{u} \right] = \nabla \cdot D \nabla c.
\]

This modified convective diffusion equation, which includes inertial and diffusive particle transport, is solved by the use of computational fluid dynamics techniques for the steady state case. The model is validated by comparing the calculated laminar fluid flow and particle deposition fractions with analytical and experimental studies of aerosol flows in a laminar-flow 90° bend of circular cross-section. Model predictions are also compared to numerical predictions of Eulerian-Lagrangian models. The numerical results of the proposed methodology are compared with benchmark solutions available in literature.

REFERENCES
COMPUTATIONAL ACOUSTICAL STUDY OF A CONCERT AND A CONFERENCE HALL

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Keywords: Concert hall, conference hall, acoustics, computational analysis, frequency response, sound absorption.

ABSTRACT

A concert and a conference hall have been considered and their frequency response has been calculated. The material plays an important role in the acoustics of enclosed spaces. It has been modeled either as rigid and thus with no losses or using an impedance approach in order to include damping. The way the mean and the standard deviation of the sound pressure level are influenced by damping has been analyzed for boundaries with and without losses. Moreover, the diffuse field of the halls as well as the sound that reaches the listeners of different rows of seats have been studied.

Figure 1. Sound pressure level inside the concert hall at 700 Hz with rigid boundaries and the source placed in the middle of the stage at (3, 5.75, 2.4)

REFERENCES

ON THE DECREASING OF THE BURNOUT TIME FOR A GAS-AIR MIXTURE IN A CLOSED VOLUME

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Keywords: Large-particle method, Combustion, Explosions, Fluid dynamics.

ABSTRACT

The problem is solved with the aid of a model describing in a differential form the fundamental conservation laws applied to gas medium where a flame front was spreading. The numerical solution of simultaneous equations is based on a modified method of large particles (Davydov’s method), at the same time there are introduced some simplifications allowing obtaining, nevertheless, a combustion situation adequate enough in an area with complex boundaries. The problem solution and computer model construction required computer resources in an acceptable amount.

In the model were included the following suppositions regarding the mixture:
- the mixture is an ideal gas, homogeneous and stoichiometric;
- difference in thermo-dynamic properties of a starting mixture and combustion materials;
- a combustion front represents a boundary of two media – a starting mixture and combustion materials.

Taking into consideration these assumptions the problem of combustion modeling is reduced to spreading the values of an additional grid parameter – a mass part of combustion materials. The inclusion of this parameter in the computation scheme of the large particle method is carried out in a natural way. Besides, in the model there are taken into account experimental data obtained by the authors at the estimate of heat loss through the area walls in the course of burnout.

It is shown by an area in the form of cylinder (mixture ignition occurs at the left of a butt-end), that partition installation (\(f = F_\Pi / F_0\), where \(F_\Pi\) is the area of cylinder cross-section) affects mixture burnout time, at the same time the influence is evident already at \(f < 0.9\) and reaches minimum with the partition position at a stretch of \(0.3 < 1 < 0.65\), where \(l = L / L_0\), \(L\) – the coordinate of partition place, \(L_0\) – the cylinder length. The period gas mixture burnout in a closed area can be decreased by a factor of 2-2.5 at the expense of the partition.

By a physical experiment was proved a burnout reduction within the same limits, but the stretch where it occurs turned out to be shorter, namely: \(0.3 < 1 < 0.5\). This result divergence did not find any explanation for the time being.

The work is carried out at the support of the Russian Fund for Fundamental Researches.
INVESTIGATING THE MICROSTRUCTURE AND TRANSPORT PROPERTIES RELATIONSHIP OF RANDOM HETEROGENEOUS MATERIALS USING SIMULATED ANNEALING TECHNIQUES

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Keywords: Porous materials, stochastic reconstruction, simulated annealing, transport phenomena.

ABSTRACT

The study of structural and transport properties of random heterogeneous materials, such as porous or composite solids, is a subject of great importance in the design of these materials for various industrial applications in fluid separations by adsorption or membranes, catalysis and in the understanding of the mechanisms of various processes involving porous media that include oil and gas production from petroleum bearing reservoirs, transport of contaminants in soils and aquifers and drying processes.

Understanding the relationship between microstructure and transport properties is a general problem that has received considerable attention, particularly for porous materials, through various theoretical approaches since the early 50’s. However, the direct interpretation of experimental transport data from real porous materials in relation to the underlying microstructure is cumbersome due to the complexity of the porous matrix.

In the present work we develop computational methods for the accurate representation of porous materials based primarily on image processing information, with a view to describe the fine architecture of the porous matrix. This is accomplished through the development of stochastic reconstruction methods based on simulated annealing techniques that can generate realistic 3-D replicas of porous media, utilizing statistical information obtained from a few 2-D images of SEM or TEM micrographs measured on the actual materials. The generated 3D structures are further explored in terms of structural characterization and prediction of transport properties for an in-depth understanding of the complex structure-property relation that can help us design porous or composite materials for improved process performance.

References

GLOBAL VERSUS LOCAL INTERPOLATION IN THE FEM FREE VIBRATION ANALYSIS OF PRISMATIC BARS

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Keywords: Finite elements, Lagrangian polynomials, p-Version, B-splines, Static and Dynamic analysis, Bars.

ABSTRACT

This paper compares the conventional finite element (Galerkin/Ritz local interpolation) with global interpolation methods for the eigenvalue analysis of prismatic bars. In this work, global interpolation consists of either the use of Lagrangian polynomials or B-splines. While in the first case the degrees of freedom are axial displacements associated to the well known nodal points, the use of B-splines involves generalized variables. It is shown that the p-Version formulation is equivalent with both Lagrangian polynomials and Bézier curves (Bernstein polynomials). In contrast, for a similar discretization, B-splines (natural or non-natural) lead to slightly different results.
SOME ISSUES ON CAD/CAE INTEGRATION: GLOBAL INTERPOLATION USING ISOPARAMETRIC AND ISOGEOGRAPHIC TECHNIQUES

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Keywords: Finite macroelements, Gordon-Coons, Bézier, B-splines, NURBS, Static and Dynamic analysis.

ABSTRACT

This paper discusses several possible attempts to cover the gap between computer-aided design (CAD: geometric model) and computer-aided engineering (CAE: finite elements, boundary elements, etc.). After a short review of CAD surfaces (Gordon-Coons, Bézier, B-splines, NURBS), the systematic formulation of creating several types of macroelements is presented. Gordon-Coons is applied in conjunction with piecewise linear, Lagrange polynomials and natural B-splines. Also, ‘Bézierian’ elements are introduced for the first time. The previously used (by the author) natural B-splines are here replaced by general ones; difficulties related to the implementation of the boundary conditions are commented. Aspects of NURBS isogeometric formulation are given. Application in conjunction with the Boundary Element Method is mentioned. Numerical examples include 2D and 3D elastic structures as well as acoustical cavities using Galerkin-Ritz and collocation procedures.
B-SPLINES COLLOCATION EIGENVALUE ANALYSIS OF 1-D PROBLEMS

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Keywords: Collocation, Hermite polynomials, B-splines, Eigenvalues, Beams, Acoustic pipes.

ABSTRACT

This paper investigates the performance of the B-splines collocation method in the eigenvalue extraction of one-dimensional problems such as elastic bars and acoustic pipes. First, the entire domain was idealized using a certain number of breakpoints. It was found that using two knots per breakpoint, it is sufficient to use two collocation points between successive breakpoints; thus the number of unknowns becomes equal to the number of equations, being twice the number of breakpoints. In analogy to the finite element method, mass and stiffness matrices were produced. Second, the piecewise Hermite collocation was applied. In the first case particular attention was paid to the handling of the Neumann boundary conditions. In three numerical examples, the quality of the solution was found to be excellent. It was also found that B-splines collocation leads to identical results with those obtained using the piecewise Hermite collocation.
SIMULATING THE DYNAMIC DISTRESS OF PILE FOUNDATIONS

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Keywords: pile foundations, dynamic distress, finite element simulations, soil-pile interaction, p-y curves.

ABSTRACT

The response of a piled foundation under lateral loading is a complicated soil-structure interaction problem, especially when dynamic loading is involved (i.e., wind or seismic). Various methods can be found in the literature for the assessment of this response. Many efforts have been focused on analytical solutions of the problem, while various experimental tests have been performed worldwide. The numerical simulation of the problem is not an easy task as the behavior of the system depends on the ability of the engineer to incorporate phenomena related to material non-linearity (e.g., the non-linear response of the soil or the piles) and/or geometrical nonlinearity (e.g., sliding at the soil-pile interface). The present study tries to illustrate certain critical issues related to static and dynamic response of pile foundations under lateral loading. As a characteristic case the current investigation is examining the response of monopile foundations of wind turbines, which is one of the most popular foundation methods especially for offshore wind turbines. To highlight the most important aspects of pile design under lateral loading, the problem stated above is examined by utilizing two different methodologies: (a) a Winkler foundation model, and (b) a 3-D continuous finite element model, while the results are compared with experimental data from the literature. It is shown that the use of the Winkler approach, along with the provisions of the norms for the generation of p-y curves, leads to an overestimation of the soil-pile system stiffness. In contrast, 3-D finite element modeling has been proven capable of predicting more accurately the soil-pile stiffness given that the mechanical properties of the soil have been accurately assessed. It is highlighted that extra attention should be paid in the simulation of the soil-pile interface to take into account phenomena such as soil-pile separation, drag forces, gap closure, etc. Moreover, an appropriate constitutive law should be used for the soil, as the ones like Mohr-Coulomb are unable to predict accurately the ultimate soil resistance due to the significant hardening they exhibit.

References

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A SYSTEMATIC APPROACH FOR THE COARSE-GRAINED BIFURCATION ANALYSIS OF THE EFFECT OF SOCIAL NETWORK STRUCTURE ON THE EMERGENT DYNAMICS OF INDIVIDUAL-BASED STOCHASTIC MODELS

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Keywords: complex systems, nonlinear dynamics, social networks, bifurcation analysis, epidemic models.

ABSTRACT

The dynamic effects of network heterogeneity are central to fundamental public-health measures and policies in order to control the outbreak of a disease in an efficient way through vaccination, quarantine, or use of antiviral drugs on targeted parts of the population. Poor understanding of the evolving macroscopic dynamics as these emerge due to contact interactions through the social network may result to negative consequences in a real outbreak.

For a systematic analysis, while one can resort to the use of statistical mechanics in order to extract coarse-grained continuum equations for homogeneous networks, major barriers arise in trying to find good closures when dealing with complex heterogeneous networks that approximate in a better way the real world. In the absence of accurate macroscopic model what is usually done is brute-force simulation: different population sizes along with different network structures and different values of the model parameters are tested in order to investigate their influence to the emergent dynamics.

We show how one can construct in a systematic way bifurcation diagrams of the coarse-grained dynamics of individual-based stochastic epidemic models evolving on complex networks with respect to their topological characteristics. More specifically we have developed algorithms that allow the continuation of the solution branches with respect to topological network parameters such as the clustering coefficient and the mean-path length. For our illustrations we chose an important representative of complex behavior: the majority-rule model. Majority-rule models have been extensively used to simulate and gain a better understanding on the behavior of many complex systems ranging from epidemic spread dynamics [1] to the spread of information [2] and neuroscience [3].

The coarse-grained bifurcation diagrams are constructed exploiting the Equation-Free approach [4] for multiscale computations. To our knowledge this is the first time that such an analysis is performed in an explicit manner for detailed models evolving on heterogeneous networks with respect to the topology characteristics.

REFERENCES


ELASTOPLASTIC FRAME ANALYSIS WITH SOFTENING IN THE FORM OF MIXED COMPLEMENTARITY PROBLEM

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Keywords: Strain softening, Elastoplastic Analysis, Holonomic, Non holonomic, Complementarity problem, Lemke Algorithm

ABSTRACT

In this work the elastoplastic analysis of frame structures that exhibit local strain softening behavior is presented. In particular, a non holonomic (path dependent) problem is formulated in the context of mathematical programming theory in the form of a mixed complementarity problem (MCP). The effects of combined bending and axial force are included through a (hexagonal) piecewise linear yield criterion that can accommodate either perfectly plastic behavior or isotropic softening. The solution is established on the basis of Lemke pivoting algorithm through an iteration process that examines all possible alternatives. Numerical examples are presented to validate the proposed non-holonomic solution scheme that traces all equilibrium paths, keeping track of the influence of softening at the overall structural response and assesses the influence of combined stresses. In addition, special attention is paid to the comparison of the existing solutions that are based on different solution algorithms. In addition, geometric non-linearities are introduced incorporating a suitable geometric stiffness matrix and additional iterations to establish the required accuracy. The same examples are analyzed and the effect of geometric nonlinearity in the elastoplastic analysis of softening frames is demonstrated.
THE EFFECT OF ARTERIAL GEOMETRY AND STENOSIS ON LDL ACCUMULATION IN ARTERIES

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Keywords: Atherosclerosis, Plaque rupture, LDL transport, finite elements

ABSTRACT

Cardiovascular diseases and atherosclerosis are the most common causes of mortality in western societies. Atherosclerotic plaque development is affected by diet high in low density lipoprotein (LDL). Furthermore, blood flow dynamics influence the arterial wall and it is found that plaque is formed at regions with slow flow rates and low wall shear stress (WSS), such as at bifurcations or curves. In this work, we study the influence of already developed atherosclerotic plaques to LDL transport in coronary arteries. In particular, two arterial models are used. The first one is an atherosclerotic artery segment, while the second one is the same segment widened, with a stent, positioned at the region of the largest stenosis. We investigate where the LDL is accumulated and subsequently how the arterial wall morphology affects the plaque formation. Blood flow is modelled using the Navier-Stokes equations and LDL transport is modelled using the diffusion-convection equation. Kedem-Katchalsky equations are used to describe the endothelial permeability. We assume pulsatile flow applying real patient-specific flow rate data as boundary conditions. The observed results show a correlation of WSS with LDL accumulation. Especially, in the case of the atherosclerotic artery, increased LDL concentration is found at regions of low wall shear stress (0-1.2 Pa). Average WSS is about 3.1Pa over the cardiac cycle, while the average normalized concentration of LDL is 1.04 Pa at the regions of low WSS. At the region of the plaque, increased WSS is observed at distal and proximal region, but very low WSS between these sites. That leads to subsequent plaque development. On the other hand, in the widened artery, the average WSS is increased by a factor of 12%. The blood velocity is increased due to dilation of the artery after the stent positioning. This leads to more normalized accumulation of the LDL, while we do not observe sites possible for plaque development in this region.
PLASTIC ZONE SCALING OF HYDRAULIC FRACTURES IN COHESIVE POROELASTOPLASTIC CONTINUUM

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Keywords: Hydraulic fracturing, Cohesive zone, Poroelastoplasticity, Fracture propagation, Finite elements.

ABSTRACT

We will present numerical results of a propagating fluid driven fracture in a poroelastoplastic continuum to simulate hydraulic fracturing in weak rock formations. Numerous applications of HF can be found in petroleum, mining, geotechnical and environmental engineering. The main focus of this research work is to determine the influence of the stress anisotropy on rock deformation and its implications on fracturing pressure and fracture dimensions. It has been previously shown that rock dilation and plastic yielding create shielding of the fracture tip and hence larger pressures are needed to propagate the fractures and the fractures are shorter and wider [1, 2].

We extend these studies to investigate the combined influence of the pore pressure and stress anisotropy which has been previously ignored. The numerical model considers the propagation in a porous plastic solid under plain strain and mode-I loading conditions. The fracture is driven by pumping of an incompressible viscous fluid with Newtonian rheology at the fracture inlet. The fracturing fluid leak-off in the host rock formation is also considered. For propagation criterion we used a Cohesive Zone Model (CZM) which appears to be appropriate for a non-linear analysis and it is easily implemented in interface finite elements [3].

The analysis was performed for an elastoplastic Mohr-Coulomb model with a set of CZ models in which the traction separation constitutive relation is described by an elastic-softening behavior. Computations were performed for different cases of stress fields investigating the stress anisotropy of the insitu stress field for constant pumping rate.

In summary, we found that highly anisotropic stress field increases the plastic yielding in a rock formation demanding higher net-pressures for propagating a fracture and the width of the created fracture is larger. This non-linear behavior may explain partially the differences observed in net-pressures between field measurements and conventional model predictions.

References

BIOMECHANICAL MODELLING OF SOFT TISSUES USING THE FINITE ELEMENT METHOD

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Keywords: Soft Tissues, Breast model, FEM, Discontinuous Galerkin.

ABSTRACT

One of the main challenges of biomechanics is the modelling of soft tissues, and one important clinical application is predicting breast deformations. Breast cancer is one of the main killers in the world and early diagnosis is currently thought to be the best strategy to give the patient the best chance of full recovery or a better prognosis. In the process of diagnosing cancer, a clinician may use different imaging techniques to locate the tumour. For each of these techniques, the breast is in a different position making it difficult to compare these images. An accurate biomechanical model, coupled with an accurate solution of the governing differential equations, would be useful for the registration of the images from the different modalities and for image guided interventions. Because of the large deformations and the behaviour of the breast tissue, incompressible nonlinear elasticity is required. But there is no agreed best method for solving these equations. The Finite Element Method (FEM) is a very good candidate based on its ability to handle irregular geometries, derivative (Neumann) boundary conditions and nonlinear materials.

In this paper we investigate which FEM is most suitable for soft tissue modelling generally, and breast tissue specifically. We are testing the Continuous Galerkin FEM (CGFEM) and the Discontinuous Galerkin FEM (DGFEM) (formulation as in Whiteley [1]). The DGFEM, can result in more degrees of freedom than CGFEM and be more difficult to implement, but it has some attractive advantages, one of which is very relevant to soft tissue modelling, it is robust with respect to nearly incompressible materials (no locking). First we use the linear compressible and incompressible theory with CGFEM since, even though soft tissues are clearly nonlinear incompressible materials, many researchers use compressible linear elasticity to model them. After showing the limitations of linear elasticity in the case of nearly incompressible materials we use the nonlinear incompressible theory with both CGFEM and DGFEM for the forward problem. The same finite element techniques are used to solve the backwards problem (as presented in Whiteley [2]) of finding the undeformed, unloaded shape of the breast starting from the known deformed shape.

The methods are tested and the implementation is validated through 2D-3D simple model problems. The results show that for nearly incompressible materials we need to use the full incompressible elasticity with different approximations for displacement and pressure. When modelling incompressibility using a Poisson ratio close to 0.5, compressible linear elasticity with linear elements suffers from locking and with quadratic elements the solution is not accurate. For nonlinear materials undergoing large displacements only nonlinear elasticity is appropriate. Between CGFEM and DGFEM the results show similar behaviour. For each element the convergence is exponential with respect to the element size, \( h \sim (h^{p+1}) \) (p: polynomial degree of approximation). Appropriate approximations for incompressible elasticity are quadratic and linear basis functions for the displacement and the pressure respectively for CGFEM and linear and constant basis functions for the displacement and pressure respectively for DGFEM. The advantage of DGFEM is that it allows for lower order elements to be used and the disadvantage is that it results in comparable degrees of freedom. The results of using DGFEM show that the method is not very sensitive to the choice of the penalty parameter, as long as it is sufficiently large. When it comes to the element choice, different elements (triangular in different layouts and quadrilaterals) give different accuracy but converge with the same rate for the same polynomial degree of the approximation. Using DGFEM and 3D elements we construct a model of the breast during X-ray mammography and MRI. We follow the clinically relevant approach of considering the known deformed configuration of the breast from MRI, then solve the backwards problem to get the truly unloaded state and then solve the forwards problem for X-ray mammography.

REFERENCES
PROPAGATION OF A PLANE WAVE TO A MATERIALLY UNIFORM BUT INHOMOGENEOUS BODY

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Keywords: Small deformations upon large; materially uniform bodies; inhomogenous bodies; plane progressive waves; secular equation.

ABSTRACT

We report results related with the propagation of a plane wave to a materially uniform but inhomogenous body; namely, a body with a frozen field of dislocations. After producing the equations of small deformations superimposed upon large for these kind of bodies, we specialize to a homogeneous finite elastic deformation of an isotropic body. By assuming the small deformation to be a plane wave we produce a set of equations for the amplitude of the wave which is accompanied by an additional set of conditions. By requiring a non-trivial solution for the amplitude we obtain the secular equation and from it a set of necessary and sufficient conditions for having a real wave speed. The second set of conditions that has to be satisfied is due to materials inhomogeneity-the presence of the defects. Essentially, the present analysis enhances the approach of Hayes-Rivlin for materially uniform but inhomogeneous bodies. The outcome is that for such bodies the restriction on the constitutive law for having real wave speeds for an isotropic material subjected to a pure homogeneous deformation involves the field of the inhomogeneity-dislocations as well.
ELECTROMIGRATION-DRIVEN SURFACE MORPHOLOGICAL EVOLUTION OF HETEROEPITAXIAL THIN FILMS ON VARIOUS TYPES OF DEFORMABLE SUBSTRATES

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Keywords: Coupled Fields, Electromigration, Surface Morphological Stabilization, Epitaxial Thin Films.

ABSTRACT

A heteroepitaxial thin film is subjected to a misfit strain due to the lattice mismatch between the two constituents of the heteroepitaxial system, i.e., the substrate and the film. The competition between the elastic strain energy stored in the epitaxial film and the film’s surface energy may lead to surface morphological instabilities in the film, such as the Asaro-Tiller or Grinfeld (ATG) instability, which is known to cause surface cracking of stressed elastic solids. Another very important surface morphological instability is the Stranski-Krastanow (SK) growth instability, which causes the formation of three-dimensional islands to follow the two-dimensional (layer-by-layer) growth of several monolayers of epitaxial film; the SK instability has been studied extensively both experimentally and theoretically.

Controlling the onset of island formation on heteroepitaxial thin films through the action of a properly applied external field, such as an electric field, would have significant impact on the synthesis of semiconductor quantum dots and their wide range of technological applications. Nevertheless, the role of surface electromigration in stabilizing the surface morphology of technologically important stressed solid materials, such as coherently strained epitaxial films, remains unexplored. In this study, we develop a three-dimensional model for the current-driven surface morphological evolution of a coherently strained epitaxial thin film on various types of substrates, which include: (a) a practically infinitely thick substrate; (b) a finite-thickness substrate clamped at its base on a holder; and (c) a finite-sized and compliant substrate. Based on this model, we carry out a linear stability analysis of the epitaxial film’s planar surface morphology.

We find that surface electromigration due to a properly applied and sufficiently strong electric field can stabilize the planar surface morphology of stressed elastic thin films. The critical electric-field strength required for surface stabilization is calculated as a function of material properties, misfit strain, and the thicknesses of the heteroepitaxial system’s constituents. More importantly, our analysis demonstrates that simultaneous action of an external field in conjunction with substrate engineering in heteroepitaxy (such as the use of clamped thin substrates or compliant substrates) can be employed in order to optimize the field-strength requirement and maximize the field-driven surface stabilizing effect. The optimal direction of the applied electric field also is determined so as to maximize the surface stabilization effect. Our results provide hypotheses that can be tested experimentally and motivate experimental measurements in heteroepitaxial film/substrate systems that can be compared directly with the theoretical predictions.
DESIGN OF A HYDROMATRIX TURBINE RUNNER USING AN ASYNCHRONOUS EVOLUTIONARY ALGORITHM ON A MULTI-PROCESSOR PLATFORM

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Keywords: multi-objective constrained optimization, asynchronous evolutionary algorithm, parallelization, hydraulic machines.

ABSTRACT

In this paper, the design-optimization of a hydrodynamic shape, namely a Hydromatrix® turbine runner, using an asynchronous evolutionary algorithm (AEA), is demonstrated. Overall, this is a computationally demanding design process, due to the cost of evaluating candidate runner geometries on a CFD code. The design is subject to several constraints, so the use of a stochastic population-based search method is strongly recommended for locating the global optimal solution. Over and above, using an asynchronous, rather than a conventional (synchronous or generation-based) EA was dictated by the need to maximize the performance of the design process on the available parallel system with heterogeneous processors.

A Matrix turbine⁰ utilizes a factory assembled grid of small unregulated turbine-generator units, see figure. With lower water mass flow rate than that required for normal operation, some of the turbine units are closed and, consequently, the remaining ones are still optimally operating. In the opposite case, when the flow exceeds its capacity, the Matrix turbine grid can be raised from its operating position like a gate. Regarding its runner, the quality of possible designs is determined by the pressure coefficient distribution over the blades, the outlet mass flow and swirl profiles and the cavitation index. The design is performed at three operating points (peak point, part load and full load) for which the aforementioned quantities are cast in the form of two objective functions to be minimized. The result of the optimization is a Pareto front of optimal solutions on a 2D space. The runner blade is parameterized using 42 design variables. Also, though the runner is designed, the stator deflection angle is allowed to vary to match the desired flow rate at the peak point. The desired mass flow rates at the other two operating points are used as constraints.

The AEA used in this paper overcomes synchronization problems due to the existence of generations and allows the highest possible degree of parallel efficiency to be achieved, since none of the available CPUs remains idle waiting to the synchronization barrier (end of generation). The AEA utilizes a structured topology of evaluation agents lying on the nodes of a 2D supporting mesh and divided into overlapping demes that interact strongly with each other. Once an evaluation terminates, the selection of the new agent to undergo evaluation on the currently idle processor is determined through a series of inter- and intra-deme processes based on two priority metrics related to the agent’s objective value and age.

DIRECT STABILITY ANALYSIS OF STEEL STRUCTURES: THEORY, SOFTWARE IMPLEMENTATION AND COMPUTATIONAL ASPECTS

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Keywords: Direct Analysis Method (DAM), Steel Framed Structures, Structural Engineering Software.

ABSTRACT

Developments in analytical software and computer hardware over the past few decades provide engineers with powerful tools for more realistically considering the behavior of steel structures. More sophisticated methods of analysis offer significant advantages in steel frame design by eliminating the need to calculate effective length factors and more directly including factors that affect system and member strength. One such approach, the Direct Analysis method (DAM), which has been established as the primary one in steel structure stability design of the 2010 ANSI/AISC Specification for Structural Steel Buildings, and indirectly proposed in other Code Provision (such as Eurocode 3), accounts for the effects of member inelasticity and frame imperfections in the assessment of both member and system strength. The latter is achieved by directly including these effects in calculating the distribution of forces in the structural system. This approach is applicable for use in the design office using commercially available software and it is applicable to a wide variety of structural problems including braced frames, moment frames and mixed systems. Just as importantly, the approach allows for a natural transition between current elastic analysis procedures and the future availability of second-order inelastic analysis programs suitable for use with an advanced analysis-design approach.

Within the above context, the present work, after a brief review of the effects that should be addressed on the overall stability analysis and design of a steel framed structure (i.e. flexural, shear and axial deformation of members, all components and connection deformation that contribute to the lateral displacement of the structure, second order P-ξ and P-Δ effects, geometric imperfections and member stiffness reduction due to residual stresses) focuses on providing specific guidance on how to implement the DAM – in the most suitable way – in analysis and design software. Discussion of the use of some common commercial software in stability design is added herein and important items design engineers must be aware of when using structural analysis software to carry out stability analysis and design are also touched upon. A simple generic computer design process flowchart is also presented to serve as a reference to design engineers.

Finally, a Direct Analysis Method case study is presented, concerning the stability of the Y-shaped 628m tall Russia Tower, developed by Halvorson and Partners in collaboration with architect Foster and partners, the construction of which – officially canceled – would lead to Europe’s largest building, whose unique form raised a number of key structural challenges to be addressed – all related to stability. The effectiveness of the DAM is demonstrated and the computational aspects of its use combined with sophisticated FE procedures is emphasized, and the crucial role of engineering judgment in achieving best performance in modeling and design is identified.
SEISMIC INELASTIC RESPONSE AND DUCTILITY ESTIMATION OF STEEL PLANAR CHEVRON-BRACED FRAMES

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Keywords: Chevron-braced steel frames, Ductility, Behavior factor.

ABSTRACT

This paper deals with an extensive study on the inelastic seismic response of steel planar chevron-braced frames. A total of 108 regular chevron-braced frames with different parametric values for the number of stories, the slenderness of braces, the columns’ stiffness and the fundamental period of vibration are subjected to 30 ordinary (i.e. without near fault effects) ground motions. The records are scaled to different intensities in order to drive the frames to 3 different damage levels. A databank of seismic inelastic response is created, including the recorded inelastic deformations and the calculated behavior and ductility factors of the frames. Based on this databank, the median and average values for the behavior and ductility factors are calculated as well as the distribution of the median maximum deformations along the height of the frames. Finally, non-linear regression analysis is adopted in order to derive simple expressions which offer a direct and reasonable estimation of the behavior factor, the drift and the ductility demands of the frames. The proposed expressions are suitable for performance-based seismic design according to the hybrid force/displacement method which combines the advantages of the force-based and displacement-based seismic design methods. A comparison of the proposed method with the procedures adopted in the current seismic codes reveals that the former estimates the seismic response in a more accurate and reasonable way.
AUTOMATED COST-OPTIMIZED PLACEMENT OF COLUMNS UNDER SEISMIC LOAD

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Keywords: Optimization, Seismic, Simulated Annealing, Numerical, Stochastic, CAD.

ABSTRACT

The placement of columns in the floor plan of a building is one of the most fundamental aspects of the seismic safety and the economics of the building. Despite its importance, this aspect is not usually given the required attention. Usually, the location of the columns is chosen by the engineer qualitatively, based on experience. And while experienced engineering judgment is indispensable for the structural safety, the structural analysis computation is rarely performed with altered location of columns, in order to quantitatively determine whether the chosen location is the most economical.

With the computing power of contemporary computers it is possible to automate the quantitative investigation of the location of the columns in order to determine the optimum. Optimum location is considered the location which yields the least weight or cost of the structure. The automated investigation can be embedded into existing structural analysis programs, as part of the overall solution process.

Determining the best location of all columns simultaneously is a strongly nonlinear problem, and it is characterized by local minima, such as for example the optimal location of a column when all the others remain constant. The analytical solution is very difficult if not impossible, and thus the simulated annealing method is employed, a stochastic numerical optimization method which is able to find the global minimum among many local, poorer, minima. The simulated annealing method generates potential random changes to an initial location of columns, which may be accepted or not. The fundamental characteristic of the method is that there is a finite probability to accept a change which increases the weight/cost of the structure, instead of decreasing it. This probability diminishes over time, until no change is accepted and the optimum location of columns is determined.

The method is independent to the structural analysis method used, which makes it ideal for incorporation into existing commercial structural analysis software, since the investment in the development of the software is not wasted.

The method was implemented in Fortran and it was integrated with an open source CAD for user friendliness. The structural analysis employed is static under seismic loads, in order to save computational time, as the method requires thousands of repetitions of the employed structural analysis. The method gives encouraging results.
FINITE ELEMENT ANALYSIS OF MASONRY BARREL VAULTS

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**Keywords:** finite elements, masonry, structural dynamics

**ABSTRACT**

In the study of historic buildings it is important to understand the way the structure behaves and to understand the origin and significance of the cracks, if they are visible. Only with a good comprehension of both aspects can the engineer or architect take decisions about the techniques of conservation which could be used. The increasing interest in historic architectural heritage and the need for conservation of historical structures has led to the continuous development of many methods for the analysis of masonry structures and special the vaults. However some type of vaults has not been thoroughly analysed, mainly because of the problem of applying simplified theories to their complicated shapes.

A cylindrical surface is a translational surface where a curve profile, moves parallel to itself, along a line. It is as if an arch extended laterally. Such a surface in masonry buildings is called barrel vault. In singly curved vault surfaces, the principle stresses along the curve will always be compressive and the inclined thrusts at the edge require enough mass of supporting system. The major simplification that is usually taken is supposed to reduce the vault to a series of adjacent arches, without transversal connection. So this model is not able to properly simulate the three dimensional effects in the vaults. Moreover the structural role of the spandrels has always been neglected, while, it is well known that they stabilise the vaults.

In order to study these effects a numerical approach based on the finite element method can be used. Vaults are modelled by means of solid elements. For each calculation, the homogenized limit analysis approach has been employed, assuming for the constituent materials experimentally determined mechanical properties. An accurate geometry of the vault is needed in order to model the existence condition, including the permanent deformations. The application of various strengthening methods on existing masonry structures leads to changes of the existing structure which could be critical in some cases of dynamic loads like seismic excitations. So the modelling of these various strengthening techniques which has been applied to the structure in parallel with the existing condition of the masonry (weak material, cracks), is important for the estimation of the structural strength and dynamic behaviour.

As case study, one of the Venetian Arsenals in Chania was selected which was a separate area for the repair of boats or build new ones. It is oblong vaulted spaces which were open to the sea for ships to come easily, but today after the construction of the wharf in the early 20th century, sea access does not exist anymore. The study was started to the elastic range, which has to be considered as a first step, but however significant for service conditions. Also the dependency of modal parameters on structural damage can be useful in the future applications of structural health monitoring.

A parametric investigation was done in order to model weak material areas, cracks, previous strengthening techniques, additional structural elements and to study their influence in static and dynamic behaviour. The static results were used for comparison to the two-dimensional thrust line results. The dynamic results consist of natural frequencies and mode shapes used for comparison to the experimental results for validation of the analytical model, while the static results are obtained by gravity loading on the validated analytical model.
RESPONSE VARIABILITY OF CYLINDRICAL SHELLS WITH STOCHASTIC SYSTEM PROPERTIES

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Keywords: Shell finite element, Translation field, Response variability, Monte Carlo simulation.

ABSTRACT

In this paper, the effect of combined uncertain material and geometric properties on the response variability of thin cylindrical shells is investigated in the framework of the stochastic finite element (SFE) method taking into account various non-Gaussian assumptions for the uncertain parameters. The TRIC shear-deformable facet shell element is used in the SFE analysis. A non-Gaussian spatial variability of the Young’s modulus and Poisson’s ratio as well as of the thickness of the shell is considered. These parameters are described by two-dimensional univariate (2D-1V) homogeneous non-Gaussian stochastic fields using translation field theory in conjunction with the spectral representation method. The stochastic stiffness matrix of the TRIC shell element is derived using the local average and weighted integral methods and depends on a minimum number of random variables representing the stochastic fields.

The numerical example focuses on the influence of the non-Gaussian assumption on the response variability of the shell structure, which is quantified in terms of exceedance probabilities by means of direct Monte Carlo simulation. The influence of the variation of each random parameter as well as of the correlation scale (length) of the stochastic fields is also investigated. It is shown that the marginal probability distribution and the correlation length of the stochastic fields used for the description of the material and thickness variability affect significantly the response statistics of the shell. Finally, as there is a significant probability of exceeding the deterministic response even for small fluctuations of the uncertain parameters, it can be concluded that the design of shells in a deterministic framework can be unsafe.
DEVELOPMENT OF NAVIER-STOKES/MOLECULAR DYNAMICS ADAPTIVE COUPLING TECHNIQUES WITHIN A MULTI-PHYSICS FRAMEWORK

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Keywords: CFD, Molecular-Dynamics, non-periodic boundary conditions, multi-physics framework

ABSTRACT

The paper describes recent developments in coupling techniques for hybrid Navier-Stokes/Molecular Dynamics simulations within the context of the multi-physics simulation framework under development with the CFD Laboratory at the University of Liverpool. This framework has been designed as a highly adaptable library of C++ template classes which form the basis of a range of different particle-based as well as mesh-based simulation methods. The Navier-Stokes equations for Newtonian flow are generally selected to form the baseline level of modeling in this framework, while locally the flow is modeled at a more detailed level of physical realism. Example of applications are the modeling of wall-slip boundary conditions for flows with partial rarefaction, as well as the modeling of detailed molecular-level phenomena taking place within shock waves at high Mach numbers.

In the present paper, the emphasis is on the coupling of a finite-volume method for the compressible-flow Navier-Stokes equations with multiple Molecular Dynamics domains in which the flow is modeled microscopic level. The main focus is on methods to impose non-periodic boundary conditions on the particle domain, originating from the non-periodicity of the flow domain as well as the particle-continuum interface conditions. A novel aspect of the present work is the development of particle forcing techniques for more general non-planar particle-domain boundary conditions than previously published in the literature. For the particle forcing in the boundary-normal direction equivalent fully-periodic simulations are used to measure the boundary contribution for the particular non-periodic boundary. The particle forcing in the direction tangential to the boundary plane is based on the equivalent shear-stress of the continuum flow, along with an empirically obtained function for the dependency of the particle forcing strength as function of distance from the boundary plane, as shown in the figure. The extension to complex non-planar boundary conditions is discussed in detail. The integration of the above particle-forcing methods into the hybrid Navier-Stokes/Molecular Dynamics simulation method forms the second part of the paper. An adaptive relaxation technique for steady-state flow problems is discussed which requires O(10) Newton-like relaxation steps, each with a number of embedded 'pseudo-steps' in which the particle forcing strengths are updated. The developed methods are discussed within the context of generic channel-flow examples, in which the Molecular Dynamics domains involve solid-wall boundary conditions as well as particle-continuum boundary conditions in rectangular/annular domains. The results show the effectiveness of the particle-forcing techniques in imposing boundary conditions. Furthermore, it is shown how the convergence of the finite-volume residuals can be used as part of the truncation criterion for the adaptive-relaxation method for the hybrid Navier-Stokes/Molecular Dynamics simulation method. Ongoing research of the developed techniques for applications to more general flow domains is also discussed.
COUPLED MD-FE MULTISCALE MODELLING AND SIMULATION OF POLYMERS

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ABSTRACT

This contribution investigates the coupling of molecular dynamics and finite element simulations of polymers. To this end, model polymer systems such as Polystyrene are going to be simulated in a multiscale approach by utilizing a bridging domain method which is essentially based on the Arlequin coupling concept. However, unlike related coupling schemes that treat crystalline matter on the particle side, polymers pose quite challenging difficulties due to their amorphous microstructure. Thus special boundary conditions in the coupling seam between molecular dynamics and finite elements have to be devised. Here we will elaborate on the recently proposed stochastic boundary conditions for the molecular simulation domain and will show how these can be incorporated into the Arlequin concept.

References

GENERALIZED VISCOELASTIC MODEL FOR POLYMER MELTS GUIDED BY PRINCIPLES OF NON-EQUILIBRIUM THERMODYNAMICS: SINGLE- AND MULTI-MODE FORMULATIONS

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Keywords: Generalized Bracket formalism, Giesekus, FENE, Non-Equilibrium Molecular Dynamics Simulations, viscoelastic model

ABSTRACT

It is well known that widely used rheological models (e.g., the Phan-Thien and Tanner or the Giesekus models [1]) for polymer melts exhibit unphysical behavior. Previous studies [2] have shown that these models are built on the basis of very simplified expressions for the chain free energy, which dramatically reduces their applicability and reliability. In an effort to improve on this, we present a generalized conformation tensor-based viscoelastic model [3] which accounts for most significant effects present in real systems, such as anisotropic drag in the form suggested by Giesekus, finite extensibility, non-affine motion, variable chain relaxation, and a bounded non equilibrium free energy, all together. The model is derived by resorting to the generalized bracket formalism of non-equilibrium thermodynamic of Beris-Edwards [4] and is thermodynamically admissible. How it reduces to well-known viscoelastic models is also analyzed in detail.

An important feature of the new constitutive model is that one can analyze its asymptotic behavior in the limits of low and high deformation rates, both in shear and elongation, and derive expressions for the material functions that can be used to fix all of its parameters except one from available rheological data (i.e., without resorting to empirical fitting). The new model (with only one fitting parameter) can describe quite accurately rheological data for short polymer melts obtained from detailed non-equilibrium molecular dynamics (NEMD) simulations both in shear and elongation [5]. By extensively comparing against the results of NEMD data for the stress tensor, we have realized that a more accurate free energy expression at the level of the conformation tensor (providing eventually the link between stress and structural or conformational properties) will be the key to further improving the predictive capability of the new constitutive model.

We have also extended the new model to multiple modes and have compared its predictions against experimental rheological data on industrially relevant polymer resins both in the linear (spectra of storage and loss moduli) and non-linear regime (shear viscosity $\eta$, first normal stress coefficient $\Psi_1$, and the transient uniaxial extensional viscosity $\eta^{(e)}_{1u}$) [6].

DIFFUSION ANISOTROPY IN TUMORS: THE EFFECT OF FIBER ORIENTATION AND IMPLICATIONS TO DRUG DELIVERY

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Keywords: Stokesian Dynamics, Random Walk, hydrodynamic interactions, drug delivery

ABSTRACT

The interstitial matrix is comprised of cross-linked collagen fibers, generally arranged in non-isotropic orientations. Spatial alignment of matrix components within the tissue can affect diffusion patterns of drugs. In this study, we developed a methodology for the calculation of diffusion coefficients of macromolecules and nanoparticles in collagenous tissues. The tissues are modeled as three-dimensional, stochastic, fiber networks with varying degrees of alignment. We employed a random walk approach to simulate diffusion and a Stokesian dynamics method to account for hydrodynamic hindrance. Hydrodynamic hindrance is determined by short-range (lubrication) and long-range hydrodynamic interactions between the diffusing particle and the fibers. For the long-range interactions, we employed the Ewald sum of the Rotne-Prager tensor accounting only for the translational velocity of the particles. To incorporate short-range forces, we calculated the interaction between the particle and each of the fibers separately using the exact two-sphere results from the literature. The incorporation of hydrodynamic forces increased the computational cost dramatically. To make the computations feasible we parallelized the algorithm, allowing the simulations to complete in approximately one hour using 28 processors. We performed our analysis for four different structures ranging from nearly isotropic to perfectly aligned. We showed that the overall diffusion coefficient is not affected by the orientation of the network. However, structural anisotropy results in diffusion anisotropy, which becomes more significant with increase in the degree of alignment, the size of the diffusing particle, and the fiber volume fraction.

To test our model predictions we performed diffusion measurements in reconstituted collagen gels and tumor xenografts. We measured fiber alignment and diffusion with second harmonic generation and multiphoton fluorescent recovery after photobleaching techniques, respectively. The results showed for the first time in tumors that the structure and orientation of collagen fibers in the extracellular space leads to diffusion anisotropy.
FINITE ELEMENT METHODS FOR 2-D FRICTIONLESS CONTACT PROBLEMS IN LINEAR ELASTICITY

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Keywords: Frictionless contact, Variational formulation, FEM, Elasticity.

ABSTRACT

A very interesting problem in computational mechanics is the two-Dimensional (2-D) frictional contact problems [1]. In this kind of problems the major interest is found in the numerical approximations considered. The Finite Element Method (FEM) [2], being a modern tool in numerical analysis, can be highly effective in the discretization and the approximation of Engineering problems. However, a variety of several boundary value problems, consisting of partial differential equations (or inequalities), can be also treated numerically using the FEM. In this paper using small deflections and linear theory, a 2-D frictional contact problem is confronted using the Finite Element Method. The paper is divided into three parts. In the first part basic assumptions are considered under which the initial non-linear problem attains its linear form. The above assumptions do not affect the mathematical formulation of the problem since the interest of the problem focuses on relatively small deflection systems. In the first part it is also formulated the system of differential equations and inequalities [1] which describe the linear contact problem (strong formulation); and then by using the strong formulation it results the weak one by introducing two linear vector spaces. The second part consists of the mathematical study of the variation inequalities [3-5], and there is also an extensive discussion about the existence and the uniqueness of solutions of this kind of inequalities. In addition, in this part of the paper it can be found thorough information about the nature as well as the discretization of the variational inequality of the first kind, which describes the mechanical problem considered. Finally, in the last section of the second part it will be developed the application of the FEM to the variational inequality of the second order. In this part of the paper there is also a brief discussion about the convergence of the method and how it can be estimated, and two conditions under which the approximation displacement field \( u_h \) converge toward the real displacement field \( u \), are given. These conditions gives the opportunity to estimate the convergence of the FEM code that simulates the above posed problem, by choosing the approximate solutions in a way that they satisfy the convergence conditions. Finally, in the last part of this study an application has been done to a contact problem, and there is also an extensive discussion about the type of elements to be used, the results and their convergence to the real solution. According to the numerical results, the numerical approximation using the Finite Element Method of the solution of the problem considered, deduces reliable results.

REFERENCES


BENEFITS FROM PARALLEL COMPUTATIONAL MECHANICS PROGRAMS IN MODERN LOW-COST SHARED MEMORY ARCHITECTURES

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Keywords: parallel computing, shared-memory, computational fluid dynamics, molecular simulation, ADREA_HF, GROMACS.

ABSTRACT

Scientific computing has started to play a significant role in many fields of scientific research due to the recent increase in the available computational power. The most promising development in computer technology has been multi-core CPUs that are now available at very low cost even for home use. Currently, such systems can contain up to 8 cores that share a common memory (shared-memory architecture), and they have already become very popular. Multi-core CPUs can be connected within a computer cluster (distributed-memory architecture) leading to even better performance, which is a common practice in scientific computing. The full exploitation of a multi-core CPU is not a straightforward task since any program that runs on such a system should be parallelized. However, the computational time saved when a parallel program runs on a multi-core CPU is not always proportional to the number of cores (proportionality is the ideal situation). A way to assess the efficiency of multi-core systems is the speed-up achieved when the number of available cores increases, i.e., the ratio of computational time of one core to the computational time of many cores.

In this work, we attempt to evaluate the benefit that can be achieved in a parallel program that tackles a computational mechanics problem. Two specific cases are examined residing in different research areas: fluid dynamics and molecular simulation. In the first case, the in-house CFD code ADREA_HF is used to simulate hydrogen release in a closed room. ADREA_HF is a powerful and versatile package that performs fluid dynamics calculations and has been successfully used to predict atmospheric dispersion of pollutants and hazardous gases. This program has recently been parallelized in order to run in either shared or distributed memory systems. For the ease of molecular simulation, the free open-source package GROMACS is used to study the properties of liquid organic compounds. Our purpose is to examine the speed-up of these programs as a function of the number of CPU cores. The effect of several parameters, such as CPU model and size of the problem, is also taken into account. The results are compared with similar results from the literature in an attempt to detect possible actions that would further improve the speed-up in each of the examined cases. Initially, we focus our study on shared-memory systems and later we try to draw some conclusions for distributed-memory systems by running both problems in a Beowulf cluster, in order to compare these two architectures.
PREDICTION OF THE CRACK KINKING IN A SANDWICH STRUCTURE BEAM SUBJECT TO THREE POINT BENDING USING THE J INTEGRAL CONCEPT

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Keywords: Sandwich Beam, Fracture Mechanics, J-Integral Criterion, Finite Element Analysis.

ABSTRACT

Sandwich structures are more and more implemented in modern industrial applications where low weight and high rigidity is very important. Since the traditional approach to structural design and material selection, tends to be replaced by the Fracture mechanics approach it is worth understanding the way it is applied. The traditional approach to structural design takes into account two variables which have to be in contrast: The applied or expected stresses and the Yield or Tensile strength. The Fracture mechanics approach [1] involves three important variables rather than two. The additional structural variable is the flaw size, and the Fracture Toughness replaces Yield or Tensile strength. This approach quantifies the critical combination of these three variables. In Fracture Mechanics there are two methods of studying a problem: The Stress Intensity criterion and the Energy criterion. In this study we get involved with the Energy criterion and specifically with the J Contour integral calculation [1].

A sandwich material consists of a core material with thin laminas on each side [2]. The laminas could be any combination of fibres and matrices, or even of a metallic material. The core is usually made of PVC, wood or a honeycomb material. The most interesting problems appeared in sandwich structures are, the failures modes in the core and the faces materials, the fracture of the core material and the interaction between the fractured core and the face materials. In sandwich structures the foam is typically the weakest part and is the first to fail under static or cyclic loading because it transfers the applied loads as shear stresses. In addition a very critical problem in sandwich structures is the debonding problem between the face and core materials [3, 4, 5]. Unstable cracking propagation and kinking in core materials represents one of the weakest failure mode in sandwich composites. The fracture behavior in sandwich composites has been directed toward the understanding of crack propagation, and at the same time toward improving the durability of composites against fracture. A crack flaw may be introduced during processing or subsequent service conditions. It may result from low velocity impact, from eccentricities in the structural load path, or from discontinuities in structures, which induce a significant out-of-plane stress.

In our study a sandwich beam under three point bending is considered. The core material of the beam contains an initially small in length crack oriented parallel to the longitudinal axis and very close to the upper skin interface. A finite element analysis code has been developed in order to predict the position and the length of the crack where kinking occurs and at the same time where the structure will finally be collapsed. The code uses the energy criterion, and the code control points of decision concerning the propagation and kinking of the crack are based on energy formulas and expressions of fracture mechanics which are taken in advance. A general flowchart of this code is presented and numerical results are given.

References:
A HYSTERETIC QUADRILATERAL PLANE STRESS ELEMENT

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Keywords: Plane Stress, Quadrilateral element, Hysteresis

ABSTRACT

In this work, a new plane stress element is proposed for the nonlinear static and dynamic analysis of plane stress / plane strain problems. The four node quadrilateral element formulation for the elastic case [1] is extended by introducing a novel hysteretic constitutive relation, based on the Bouc-Wen model of hysteresis [2]. Following the work of Casciati [3], the hysteretic model introduced is directly derived from the governing equations of classical plasticity, namely the flow rule and the hardening law. The stiffness matrix of the element is formulated using the principle of virtual displacements, where the elastic stress-strain relation is substituted by the hysteretic relation proposed. Thus, the derived stiffness matrix is conveniently decomposed into an elastic and hysteretic part that expresses the inelastic behavior of the element. The formulation proposed is further extended to account for cyclic induced phenomena such as stiffness degradation and strength deterioration [4]. Examples are presented which demonstrate the efficiency of the proposed element in the simulation of the cyclic behavior in plane structures with different materials, over existing methods.

A THREE-DIMENSIONAL HYSTERETIC TIMOSHENKO BEAM ELEMENT WITH TORSIONAL WARPING

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Keywords: Hysteresis, Timoshenko, Beam Element, Warping

ABSTRACT

In this work a three-dimensional hysteretic Timoshenko beam element formulation is presented. Torsional warping is also accounted for by introducing the rates of the twisting angles at the two ends as additional unknowns [1]. Inelasticity is treated through the definition of new degrees of freedom that account for the hysteretic part of the curvatures, shear deformations and rates of the twisting angles respectively. These additional degrees of freedom are controlled by a set of smooth hysteretic equations of the Bouc-Wen type [2]. Interaction between the stress-resultants is accounted for by modifying the interaction scheme introduced in [3] for the case of axial force – bending moment interaction in a two-dimensional Bernoulli beam element. Different types of yield surface and hardening rule can be implemented in the proposed scheme. By defining an appropriate set of shape functions the hysteretic field is interpolated at the corresponding nodal quantities. Using the principle of virtual work an elastoplastic stiffness matrix is derived that consists of a linear and a hysteretic part. Since the evolution of the hysteretic parameters is treated through the Bouc-Wen equations, the stiffness matrix remains constant throughout the analysis procedure. The governing equations of the system, namely the equations of motion and the evolution equations of the hysteretic deformations are expressed in state-space form. The derived system of first order differential equations is solved by a predictor-corrector scheme [4]. Examples are presented that demonstrate both the accuracy and the efficiency of the proposed methodology.

EXPLORING THE SOLUTION SPACE OF A MIXED FLOW CVD REACTOR WITH A COMMERCIAL COMPUTATIONAL CODE

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Keywords: Chemical Vapor Deposition (CVD), Computational Fluid Dynamics (CFD), Recursive Projection Method (RPM), FLUENT, multiplicity, stability

ABSTRACT

Chemical Vapor Deposition (CVD) is one of the most widely used processes for the production of thin solid films. CVD processes are performed in reactors [see Fig. 1(a)], equipped with wafers, where the surface reactions and the deposition of the solid film occur. The precursor, a gaseous mixture of the chemical species to be deposited, is transferred by a carrier gas from the inlet of the reactor to the wafer.

During the CVD process, multiple, competitive transport mechanisms co-exist. The mechanism that prevails is chosen indirectly via the operating conditions of the reactor (pressure, wafer’s temperature, mass inlet flow, etc.) and has a great impact on the quality of the produced film (i.e. thickness uniformity) and also on its growth rate. The quality of the deposited film becomes uncertain in cases where for the same operating conditions, represented in computations by appropriate parameters such as the dimensionless Reynolds and Nusselt numbers, different mechanisms could prevail. The latter, known as state or solution multiplicity, is owed to specific nonlinear terms [1] appearing in the partial differential equations that describe the transport phenomena in a CVD reactor. In the present study, the set of equations describing the gas flow, transport of energy and chemical species and the chemical reactions in a CVD reactor is solved numerically, under realistic boundary conditions, with the computational fluid dynamics (CFD) code Ansys/Fluent [2]. Nevertheless, even though Fluent is a powerful and general purpose code, it fails to provide all the “pieces of the puzzle” such as turning points, or solution branches comprising unstable operating states (cf. Fig. 2b). These missing pieces may hide crucial information about the limits of stability of states as well as entire solution branches which might be suggestive of advantageous operating “windows” of the process of concern. To overcome the latter, Fluent is augmented with the Recursive Projection Method (RPM) which enables it to perform certain stability analysis tasks [3], such as systematic detection and tracing of multiple solutions; in this application, there is a range of inlet flow Reynolds numbers over which three steady states exist, two stable and one unstable [see Fig. 1(b)]. The integrated computational framework RPM assisted Fluent (RPMF), is used to trace the solution multiplicity regions in the case of CVD of silicon (Si) from silane (SiH₄), at different wafer’s temperatures, mole fractions of the precursor at the inlet and carrier gases. Results for the solution branches (stable, unstable and turning points) and the corresponding growth rates along the wafer are presented.

RECONSTRUCTION OF THE KNOWN HUMAN PROTEIN-PROTEIN INTERACTION NETWORK FROM FIVE MAJOR LITERATURE-CURATED DATABASES

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Keywords: protein-protein interaction (PPI) networks, bioinformatics, biological network analysis

ABSTRACT

The protein-protein interaction (PPI) networks are essential for a wide range of biological processes, including gene regulation, signal transduction and metabolism. Their elucidation has been a major challenge of the post-genomic era. For the human, in particular, revealing the spatiotemporal protein interactome can be compared in significance with the human genome project. The challenges of the human PPI network project are even more serious, considering that the predicted proteome size is at least an order of magnitude larger than the genome, our current knowledge of the human proteome is fluid and there is a high degree of error associated with the high-throughput techniques that are currently used to identify protein interactions. Presently, there exists a plethora of databases aiming at storing the protein interactions that are supported by at least one low- or high-throughput experiment reported in the literature. Spanning usually different publications, with non-uniform curation methods and updating policies, the databases exhibit limited overlap between the PPIs that they report and the literature that has been curated by each of them. In this work, we aimed at reconstructing the network of all experimentally identified binary protein interactions, which have been recorded for the currently known human proteome by integrating the information of the five most widely used publicly-available literature-curated PPI databases, i.e. HPRD, INTACT, MINT, DIP and BioGRID. All human proteome data were retrieved from the reviewed protein entries of the UNIPROT database (www.uniprot.org), a universally accepted “comprehensive resource for protein sequence and annotation data”. Our analysis enabled the evaluation of similarities and differences among the databases and the identification of the unique PPI information that each of them contributes to the final integrated network. We were able to document the suggested limited overlap among the databases, which can be attributed to different curation practices, text mining algorithms and objectives. Our integrated PPI dataset covers a significantly larger part of the presently available human protein interactome than any of the five databases, thus providing an enhanced resource to further explore and expand the human protein interactome towards its reliable use for functional genomics, systems biology and biotechnology, and health.
A NEW KIRCHHOFF PLATE MODEL BASED ON A MODIFIED COUPLE STRESS THEORY

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Keywords: Couple stress elasticity, Kirchhoff plate, Method of fundamental solutions, Meshless methods.

ABSTRACT

The behavior of micron-scale structures has been proven experimentally to be size dependent. Therefore, the classical continuum theory is inadequate to predict their response and the utilization of strain gradient (higher order) theories containing internal material length scale parameters is inevitable. Although, the strain gradient theories encounter the physical problem in its generality, they contain additional constants – besides the Lamé constants – which are difficult to determine even in their simplified form containing only two additional constants. Thus, gradient elasticity theories of only one additional material constant are very desirable.

The work that has been done on the analysis of micro-plates is limited only to publications of linear and nonlinear plate models based on the simplified strain gradient model with one internal parameter. However, the main drawback of the above plate models is that the presence of the microstructural effect raises the order of the resulting partial differential equation from four (classical case) to six (gradient case). As well as the classical boundary conditions are supplemented by additional (non-classical) ones containing higher order traction and higher order moments. Hence, the employed analytical solutions are restricted only to simple geometric shapes.

In this paper a new Kirchhoff plate model is developed for the static analysis of isotropic micro-plates with arbitrary shape based on the simplified couple stress theory of Yang et al. [1] containing only one material length scale parameter which can capture the size effect. The proposed model is capable of handling plates with complex geometries and boundary conditions.

From a detailed variational procedure the governing equilibrium equation of the micro-plate and the most general boundary conditions are derived, in terms of the deflection, using the principle of minimum potential energy. The resulting boundary value problem is of the fourth order and it is solved using the Method of Fundamental Solutions (MFS). The MFS - like the classical Boundary Element Method (BEM) - is based on the fundamental solution of the governing equation and its solution procedure does not involve any domain discretization because it is limited only to the boundary. In the MFS the solution at any point (in the domain or on the boundary) is approximated by a series of unknown constant coefficients multiplied by fundamental solutions between the viewpoint and the source points. Since the source points are placed outside the domain, unlike the presence of singular integrals in the BEM, the MFS does not require any special treatment of singularities in the fundamental solutions since it is always regular. Hence, the MFS is considered as a boundary-type meshless method that encompasses all the advantages of the boundary methods. However, the open issue of the MFS is the location of the source points. Two schemes are referred in the bibliography for the location choice of the source points, the adaptive and the fixed one. In this work the fixed scheme is adopted due to its simple implementation, computational efficiency and convergence proof.

Several plates of various shapes, aspect and Poisson’s ratios are analyzed to illustrate the applicability of the developed micro-plate model and to reveal the differences between the current model and the classical plate model. Moreover, useful conclusions are drawn from the micron-scale response of this new Kirchhoff plate model.

REFERENCES

NONLINEAR ANALYSIS OF ELASTIC SPACE CABLE-SUPPORTED MEMBRANES

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\textbf{Keywords:} Nonlinear, large deflections, space membranes, flat membranes, cables, analog equation method, boundary elements, meshless BEM.

\textbf{ABSTRACT}

Structural membranes play an important role in the engineering field in our days. The lightness of the structure, the ability to cover very large spans and the prefabrication facility are some of their constructional advantages. They are separated into two major categories, the air-supported membranes and the prestressed membranes. The air-supported membrane derives its structural integrity from the use of internal pressurized air to inflate the structural fabric envelope, so that air is the main support of the structure. However, any prestress can be applied to the membrane of the second category by stretching it from its edges (imposed boundary displacements) or by prestressed cables which support it (cable-supported). The analysis of prestressed membranes involves three steps\textsuperscript{[1]} (i) form-finding, (ii) prestress under self-weight and (iii) in-service loading.

In this paper an iterative solution scheme to the coupled problem of elastic flat or space cable-supported membranes is presented. Starting from the minimal surface the membrane is prestressed by imposed boundary displacements on the boundary. In first instance the cables are assumed undeformed (fixed boundary) and the membrane problem is solved under self-weight and prestress. Then the external loading is applied on the deformed membrane and the membrane problem is solved again with fixed boundary taking into account the prestress forces from the previous step. The resulting reactions on the membrane boundary are applied with reversed sign on the cable as external loading and the cable problem is solved. Then the computed thus displacements of the cable are used as imposed boundary displacements for the membrane and the membrane problem is solved again under the in-service loading. The procedure is repeated until the displacement continuity conditions between cable and membrane are satisfied.

In this investigation both membrane and cable problems are solved using the Analog Equation Method (AEM). According to this method the three coupled nonlinear second order partial differential equations in terms of the displacements describing the response of the membrane are replaced with three uncoupled Poisson’s equations subjected to fictitious sources, unknown in the first instance, under the same boundary conditions. Subsequently, the fictitious sources are established using a procedure based on the BEM\textsuperscript{[1]}. A similar procedure is applied for the solution of the cable problem undergoing large displacements. The three coupled nonlinear ordinary differential equations in terms of the displacements describing the response of the cable are replaced with three linear string equations under unknown fictitious loads, which are subsequently established using the integral equation method. The final displacements due to the in-service loading as well as the stress resultants are evaluated at any point of the membrane and the cable from integral representations of the solution of the substitute problems, which are used as mathematical formulae. Example problems are presented, for both flat and space membranes, which illustrate the method and demonstrate its efficiency and accuracy.

\textbf{REFERENCES}

A MICROSTRUCTURE-DEPENDENT ORTHOTROPIC PLATE MODEL BASED ON A MODIFIED COUPLE STRESS THEORY

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Dedicated to Professor Emeritus John T. Katsikadelis on the occasion of his 72th birthday.

Keywords: Couple stress elasticity, gradient elasticity, orthotropic plate, analog equation method, meshless methods.

ABSTRACT

Since the classical continuum theory is inadequate to predict the behaviour of micron-scaled structures, which has been proven experimentally to be size dependent, the utilization of strain gradient (higher order) theories is inevitable. Although, these general theories encounter the physical problem in its generality, they contain additional constants which are difficult to determine even in their simplified form of only two constants. Thus, gradient elasticity theories involving only one additional material constant are very attractive. The couple stress theory is a special case of these higher-order theories in which the effects of the dilatation gradient and the deviatoric stretch gradient are assumed to be negligible.

The work that has been reported on the subject is restricted only to the vibration and buckling problems of orthotropic nano-plates of graphene sheet. More specifically, it has been studied the elastic buckling problem of single-layered graphene sheet by an atomistic modelling approach, the vibration problem of embedded multilayered graphene sheets and the buckling problem of single-layered graphene sheet employing the nonlocal elasticity theory of Eringen.

In this paper a new microstructure-dependent orthotropic plate model is developed for the static analysis of orthotropic micro-plates of arbitrary shape based on the simplified couple stress theory of Yang et al. [1] containing only one material length scale parameter which can capture the size effect. Yang et al. modifying the classical couple stress theory proposed a modified couple stress model in which only one material length parameter is needed to capture the size effect. This simplified couple stress theory is based on an additional equilibrium relation, which forces the couple stress tensor to be symmetric. The proposed model is capable of handling plates with complex geometries and boundary conditions.

From a variational procedure the governing equilibrium equation of the micro-plate and the most general boundary conditions are derived, in terms of the deflection, using the principle of minimum potential energy. The resulting boundary value problem is of the fourth order (instead of existing gradient theories which is of the sixth order) and it is solved using the Analog Equation Method (AEM), which is a boundary-type meshless method. Several plates of various shapes, aspect and Poisson’s ratios are analyzed to illustrate the applicability of the developed micro-plate model and to reveal the differences between the current model and the classical plate model. Moreover, useful conclusions are drawn from the micron-scale response of this new orthotropic plate model.

REFERENCES

BIOMAGNETIC FLUID FLOW IN A DRIVEN CAVITY

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\textbf{Keywords:} Biomagnetic fluid flow, magnetic fluid, BFD, FHD, MHD, driven cavity

\textbf{ABSTRACT}

\textbf{Introduction.} The influence of the magnetic field on biomagnetic fluids such as blood has numerous applications in bioengineering and medical and clinical sciences. So, it is imperative to mathematically describe the behavior of these fluids under strong magnetic fields. In this study, we numerically investigate the fundamental problem of biomagnetic fluid flow in a lid driven cavity under the influence of a steady and localized magnetic field.

\textbf{Method.} The mathematical model used for the formulation of the problem is consistent with the principles of Ferohydrodynamics (FHD) and Magnetohydrodynamics (MHD) \cite{1, 2}. The biomagnetic fluid is considered as a homogeneous isothermal Newtonian fluid and is treated as an electrically conduction magnetic fluid which also exhibits magnetization. The coupled, nonlinear system of Partial Differential Equations (PDEs) with appropriate boundary conditions is discretized using the finite volume (FV) method on a staggered and stretched computational grid. The non linear set of algebraic equations obtained form the FV discretization is numerically solved with iterative (SIMPLE method) \cite{2} or direct methods (Newton with LU decomposition or Gradient based methods) \cite{3}.

\textbf{Results.} The results show that the biomagnetic fluid is considerably influenced by the presence of the magnetic field. The velocity field is substantially changed under the influence of the magnetic field. The main, usually shown, vortex in the driven cavity is decomposed in several smaller counter-rotating vortices and investigation is made on the parameters which determine the formation of the vortices such as the form and the position of application of the applied magnetic field.

\textbf{References}


QUALITATIVE ANALYSIS OF SIMPLE MODELS CONCERNING THE TRAP-DOOR MECHANISM USING DEM SIMULATION

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In memoriam of Professor Ioannis Vardoulakis

Keywords: Subsidence, Distinct element method, stochastic, kinematic.

ABSTRACT

Compaction of a collapsible substratum, for example due to oil-production (effective stress increase) and/or water-injection (capillary action) may result in significant surface subsidence. The mathematical description of such a subsidence mechanism constitutes a complex problem due to the large number of unknowns involved in any particular setting. In situations like this, one may resort to elementary models that capture the phenomenon in a rough but satisfactory manner for engineering purposes, i.e. stochastic models. This approach allows us to condense again the response of the earth body to a minimum number of parameters, which in turn can be fitted by inverse analysis of suitably designed model experiments.

Litwiniszyn’s theory of subsidence was the first stochastic model considered by some of the authors. According to Litwiniszyn, large-scale subsidence over a yielding underground geo-structure is seen as a stochastic (Markov) process. This process may be called kinematic diffusion, since it leads to a parabolic equation which corresponds to the Fourier thermal diffusion equation where time is replaced by depth. Other stochastic-kinematic models for the granular media flow are also proposed by Mullins [1], Nedderman and Tüzün [2]. Finally, in recent works, the so called spot model for the flow of dense granular media is also proposed by Bazant et al [3], [4].

In this work, some results concerning Litwiniszyn’s theory are presented and a first effort in the evaluation and validity of the above mentioned stochastic-kinematic models is made using numerical trap-door experiments (DEM) based on data collected from small-scale model experiments [5]. In particular, using porosity measurements, displacements and velocities of grains (or of representative volumes of grains), in different phases, we can make some comparisons with the theoretical analysis, check the validity of some hypotheses of the above mentioned theories and start a discussion concerning previous published results.

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REFERENCES

FROM PORE TO NETWORK TO DeProF TO aSaPP: TOWARDS A COMPLETE DESCRIPTION OF STEADY-STATE TWO-PHASE FLOW IN POROUS MEDIA, SPANNING PORE- TO STATISTICAL THERMODYNAMICS- SCALES

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Keywords: two-phase flow, porous media, steady-state, statistical thermodynamics, process optimization

ABSTRACT
The work presents the on-going team research efforts (implementing experimental/empirical observations, true-to-mechanism hierarchical modelling and numerical simulations at multiple scales, physical interpretation of simulation predictions and experimental verification) towards the development of a complete theory for the description of steady-state concurrent two-phase flow in porous media (the DeProF theory).

First attempts are traced back in the 1980s with the analysis, description and modeling of phenomena governing two-phase flow in pore(s) scale. Appropriate simulators extending over hundreds and/or thousands of pores (network scale) were developed in the following decade (1990s); in parallel, extensive experimental research identified the three prototype flows comprising the average macroscopic flow, namely connected-oil pathway flow (CPF), ganglion dynamics (GD) and drop traffic flow (DTF), and mapped their relative contribution to the macroscopic flow in terms of the process parameters.

Efforts to provide a consistent physical rationale to explain the experimental observations, i.e. the map of flow regimes, laid the grounds for developing the DeProF -Decomposition in Prototype Flows- theory. Amongst the main results/features of the DeProF theory was the identification of the actual operational and system parameters of the process and the introduction -according to ergodicity principles- of the domain of physically admissible internal flow arrangements of the average macroscopic flow.

Use of the respective mechanistic model as a simulation tool (in the 2000s) revealed many characteristic properties of the sought process. Important is the existence of optimum operating conditions in the form of a smooth and continuous locus in the domain of the process operational parameters. The existence of the optimum operating conditions has potentially many industrial-scale applications. It remained in latency within the relative permeability curves -describing the phenomenology of the process, until recently unveiled by the DeProF theory.

Research efforts continue in the present (2010s) by elaborating appropriate physical considerations based on statistical thermodynamics and the introduction of the aSaPP -as Spontaneous as Physically Possible- concept that corroborates the correlation of the process efficiency to the multiplicity of the internal flow arrangements.
IMPLEMENTATION OF THE DEPROF THEORY FOR STEADY-STATE TWO-PHASE FLOW IN POROUS MEDIA TO IMPROVE MASS TRANSFER AROUND RECTILINEAR SINKS/SOURCES

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Keywords: two-phase flow, porous media, steady-state, statistical thermodynamics, process optimization

ABSTRACT

The work presents the on-going team research efforts (implementing experimental/empirical observations, true-to-mechanism hierarchical modelling and numerical simulations at multiple scales, physical interpretation of simulation predictions and experimental verification) towards the development of a complete theory for the description of steady-state concurrent two-phase flow in porous media (the DeProF theory).

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Research efforts continue in the present (2010s) by elaborating appropriate physical considerations based on statistical thermodynamics and the introduction of the aSaPP -as Spontaneous as Physically Possible- concept that corroborates the correlation of the process efficiency to the multiplicity of the internal flow arrangements.
J: BOUNDING-SURFACE PLASTICITY MODELS FOR STRUCTURAL BEHAVIOR OF STEEL COMPONENTS SUBJECTED TO STRONG CYCLIC LOADING

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Keywords: Bounding Surface, Cyclic Plasticity, Finite Elements, Numerical Integration

ABSTRACT

Many engineering applications in structural and mechanical engineering involve cyclic loading well beyond the elastic regime. Even in structures that are designed to perform elastically, cyclic plastic actions often occur due to discontinuities or cracks. Representative examples of plasticity affected structures are piping components, pressure vessels, off-shore structures, cranes and structural steel structures which are subjected to severe earthquake and wind loading. Under cyclic loading conditions cyclic plasticity related phenomena such as the Bauschinger effect and the accumulation of plastic strains, often referred to as ratcheting, take place affecting the total performance of a steel part or structure. This necessitates the simulation of metal cyclic behavior in the inelastic range through simple and robust cyclic plasticity models.

Significant research effort has been devoted in the formulation of phenomenological plasticity models to predict the behavior of materials subjected to cyclic loading. The earlier models developed were based on classical theory of plasticity, employing linear, nonlinear, mixed (isotropic and kinematic) and additive kinematic hardening rules and their efficiency in predicting the cyclic loading related effects has been extensively analyzed [Corona et al. (1996), Bari and Hassan (2000)]. In this class of models the hardening modulus is derived through the consistency condition, which couples the hardening modulus with the kinematic hardening rule.

An improvement to the aforementioned models is the development of a class of plasticity models which are based on the “Bounding Surface concept”. In these models, in addition to the Yield Surface, a Bounding Surface is introduced having similar properties and interacting with the Yield Surface. The main benefit of these models is that the plastic modulus is defined directly (uncoupled models) by a given expression which depends on the relative distance of the two surfaces and it is only indirectly influenced by the hardening rule adopted. Representative examples of this class of models are the Dafalias – Popov (1976) model and the Tseng – Lee (1983) model, which is the model employed in this study.

The aim of the present work is to discuss the above Bounding Surface model and its numerical implementation. The original theoretical formulation of the model is presented and some proposed modifications are discussed to account for the particularities of structural steel (plastic plateau, hardening, Bauschinger effect). Special attention is paid on the numerical integration of the incremental equations of the model and its incorporation into a finite element environment. Finally, the capabilities of the original and modified model in predicting cyclic plasticity related phenomena are examined through appropriately selected examples from industrial applications.
NUMERICAL SIMULATION OF CLAD PIPE STRUCTURAL BEHAVIOR UNDER BENDING LOADING

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Keywords: Buckling, Finite Elements, Clad Pipes, Manufacturing Process, Pipeline.

ABSTRACT

The present work concerns the numerical simulation of clad pipes and their manufacturing process as well as the structural behavior under bending and external pressure. More specifically, clad pipe is a double wall pipe, composed by two pipes that are in contact; a thick-walled “outer pipe”, and a thin-walled inner pipe, referred to as “liner” pipe. The motivation of this study stems mainly from the use of such pipes in energy pipeline applications (oil, gas, etc.) where a corrosion-resistant thin-walled liner is fitted inside a carbon steel outer pipe. Clad pipes are produced through an appropriate manufacturing process, consisting of heating the outer pipe, inserting the liner and pressurizing it until both pipes come to contact, heating the liner, and finally discharge of the internal pressure and cooling both pipes.

The lateral confinement of the liner pipe due to the deformable outer pipe constitutes the main characteristic of the clad pipe. To study the mechanical behavior of the liner, consideration of its interaction with the outer pipe is required. Therefore, to predict the response and the buckling curvature of the thin-walled liner, it is necessary to account for its contact with the confining thick-walled outer pipe. Because of this confinement, existing numerical solutions or analytical predictions for the bending buckling resistance of unconfined thin-walled pipes are inadequate to predict the buckling resistance of the bent liner.

In the present work, the problem is solved numerically, using a nonlinear finite element program ABAQUS to simulate the clad pipe and the interaction between the liner and the outer pipe. Nonlinear geometry with large strains is taken into account, and the material of both pipes is elastic-plastic. First, the manufacturing process of the clad pipe is simulated and the residual stresses in the liner pipe are measured. Then, the residual stresses are inserted to the model as initial conditions and bending curvature is applied with or without the presence of external pressure. Stresses and strains are monitored throughout the deformation stage with emphasis on possible detachment of the liner from the outer pipe and the formation of local buckling. The values of pressure and curvature at which liner buckling occurs are determined.
ACCELERATING MONTE CARLO SIMULATIONS USING GRAPHICS PROCESSING UNITS

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Keywords: molecular simulations, Monte Carlo sampling, Graphics Processing Units, polymer modelling

ABSTRACT

Computer simulation of polymers is both interesting and practically very relevant, since it can lead to faster and more economical design of tailor-made materials and processes for specific applications. The challenge faced by polymer modelers, especially those interested in connecting macroscopic material behaviour to the chemical structure and architecture of constituent macromolecules, is that polymer structure and dynamics are characterised by extremely broad spectra of length and time scales. Our ability to equilibrate atomistic models of synthetic polymers and biopolymers has been significantly enhanced through the development of Monte Carlo (MC) schemes employing moves which modify the connectivity of monomers along the chains. MC schemes based on such moves may induce equilibration many orders of magnitude more efficiently than Molecular Dynamics (MD) simulations, for the same model of molecular geometry and energetics. In the past, methodologies for accelerating MC simulations by use of parallel and vector machines have been developed. These were system specific and very hard to maintain and port across different computer architectures and environments.

Nowadays, by exploiting the power offered by an heterogeneous computing architecture, we reduce by an order of magnitude the time needed to perform a MC move. Graphics Processing Units (GPUs) now provide unprecedented computational power for scientific applications. The most time consuming part of a MC algorithm, which is the calculation of the non-bonded interactions, is suitably adjusted in order to be executed by a GPU. The exploitation of a device with thousands of parallel threads makes the calculation of the non-bonded energy one order of magnitude faster than can be accomplished by a serial algorithm. At an instant of time the parallel threads can compute the pairwise interactions of a specific monomer with its environment. The efficiency of the developed GPU algorithm is mainly restricted by its memory access operations. Special consideration has been taken in order to optimize the use of memory access operations by exploiting the different levels of device memory hierarchy. Moreover, logical operations, especially comparisons, were strictly avoided inside the device code and replaced by purely arithmetic ones.

The proposed implementation of a MC algorithm on GPU scales fairly well. For small systems (less than $10^4$ monomers) the serial application is as fast as the GPU enhanced application. For larger system, the GPU enhanced version has the clear advantage of very weak scaling versus the size of the system (while the serial version scales almost quadratically). The non-bonded energy calculation, which is the limiting rate step of a computer simulation algorithm, has a smoother increase as systems grow. In the case of a device offering more threads than system monomers, the time per MC step would be even independent of the size of the system.

Even by using an inexpensive GPU embedded chip of a laptop, the time needed for the GPU enhanced application approaches one eighth of that needed for the serial application. The achieved acceleration lies in the same order of magnitude as that of already ported to GPUs MD applications (LAMMPS, NAMD).

To the best of our knowledge, no molecular simulation MC technique has harnessed the power provided by GPU computing architecture up to now. The true equilibration of large systems of long polymeric chains can only be achieved by means of MC simulation. Porting the intensive calculations to a massively parallel GPU can enable efficient treatment of large systems. The transparency and facility of the proposed approach can find several applications to other frameworks of MC sampling formalism. Equilibrated configurations obtained by GPU enhanced connectivity-altering MC methods can serve as starting points for atomistic studies of dynamics in the Rouse and reptation regimes and for topology-preserving reductions to entanglement networks useful in the mesoscopic analysis of melt flow and large-scale deformation of solid amorphous polymers. Thus, the exploitation of GPU environments will significantly boost MC methods, which already play a strategically important role in the prediction of polymer properties through hierarchical and multiscale modelling.
INFLUENCE OF A CIRCULAR EXIT WALL BOUNDARY ON THE AXISYMMETRIC JET FLOW

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Keywords: Engineering Education, Axisymmetric Jet, Computational Fluid Dynamics.

ABSTRACT

In the frame of “engineering education” activities, the Laboratory of Fluid Mechanics and Turbomachinery (FMTULAB/ASPETE) is continuously targeting to create links between education and basic research activities in fluid mechanics/dynamics. This task is expected to attract and motivate young engineers and scientists to join the fluid dynamics sector, which significantly contributes to the improvement of efficiency of applications relating clean energy sources and air pollution control. For this purpose computational and experimental studies are combined mainly in fundamental topics, while innovative results are produced to improve the knowledge of additional effects rising from the adoption of alternative flow configurations.

Axsisymmetric jet flow constitutes a subject of research from the origins of fluid dynamics; however it remains a subject of interest due to the new findings regarding the influence of flow and geometry conditions utilized in configurations that diverge from the theoretical “free-jet” case. Parameters under consideration include the type of the exit nozzle that can be smoothed contraction or long pipe, the dimensions of the room or channel used for jet’s evolution, and the range of the Reynolds number at which the jet emanates from nozzle exit. The influence of a flat plate placed on nozzle’s exit also, appears to be capable of altering typical jet’s features.

In the present study, the effect of a wall boundary produced by a circular disk of twice the jet diameter placed on the exit of the jet is investigated numerically. Mean and turbulent velocity statistics are compared to typical “free” jet profiles. Computational simulations are performed to predict the flow characteristics by incorporating several turbulence models, while supportive pressure measurements are used to evaluate the predictions within the initial region of jet’s development.
USE OF VIRTUAL INSTRUMENTATION AND COMPUTATIONAL FLUID DYNAMICS IN AN UNDERGRADUATE RESEARCH PROJECT

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Keywords: CFD, Virtual Instrumentation, Venturi Tube, Engineering Education.

ABSTRACT

The current paper demonstrates how to introduce a combination of CFD (Computational Fluid Dynamics) and virtual instrumentation to undergraduates in a research setting in the framework of a fluid mechanics course. A laboratory research project has been developed to enable students to compare and analyze pressure and velocity measurements obtained experimentally in a “Venturi tube” setup to those generated using a commercial CFD software package. An old but proven laboratory setup has been retrofitted with computer data acquisition system and custom written software has been developed to suit the experimental module. Pressure measurements received along the tube for five Reynolds numbers are directly compared with corresponding predictions using CFD code and all are contrasted with the 1-d inviscid flow solution. It is shown that, although undergraduate students may have limited knowledge in the underlying theories and equations used by CFD codes to solve flow problems, they are capable of using the code in solving classical and more complex problems with supervision by a faculty member. The developed project provides a cost-effective means for laboratory improvement in addition to educational benefits derived by the students since they have the opportunity to explore first-hand the various capabilities of CFD as an analysis tool and additionally to familiarize using modern measurements techniques such as pressure and temperature transmitters, experimental data acquisition and processing.
OPTIMAL SEISMIC DESIGN OF STRUCTURES USING APPROXIMATE METHODS

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\textbf{Keywords:} Performance-based design, genetic algorithm, mean annual frequency, incremental dynamic analysis, static pushover.

\textbf{ABSTRACT}

This study presents an alternative seismic design approach for steel frames that is nested within a structural optimization algorithm. The capacity assessment of the structure can be carried out using approximate performance estimation methods such as the SPO2IDA tool (Static Pushover to Incremental Dynamic Analysis)\cite{Vamvatsikos2005} thus expediting the capacity assessment process compared to using the resource-consuming nonlinear response history analysis approach. SPO2IDA is employed to quickly provide an estimate of the median demand and its dispersion at various performance levels. The mean annual frequencies of the limit-states considered are compared to preset values in order to decide whether each candidate design is acceptable\cite{Fragiadakis2011}. A Genetic Algorithm is used to handle the resulting seismic design problem by locating the most efficient design in terms of the minimum weight of the structure. A three and a nine storey steel moment-resisting frames (SMRF) are used to demonstrate the efficiency of the proposed seismic design approach. The proposed methodology leads to efficient building designs within reasonable computing time and therefore is suitable for practical design applications.

\textbf{REFERENCES}


Abstracts of the

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THE NATURAL NEIGHBOUR RADIAL POINT INTERPOLATION METHOD - SOLID MECHANICS AND MECHANOBIOLOGY APPLICATIONS

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Keywords: Meshless Methods, Non-Linear Analysis, Elastoplasticity, Large Deformations, Biomechanics, Bone remodelling analysis.

ABSTRACT

This work presents and develops the Natural Neighbour Radial Point Interpolation Method (NNRPIM) [1], a new truly meshless method. The NNRPIM is extended to several engineering fields, such as solid mechanics static and dynamic linear analysis and structural nonlinear analysis, and bone remodelling biomechanical analysis. Within the NNRPIM the nodal connectivity is enforced using the Natural Neighbour concept. After the Voronoi diagram construction from the unstructured nodal mesh, which discretizes the problem domain, small cells are created, the “influence-cells”. These cells are in fact influence-domains entirely nodal dependent. The Delaunay triangles are used to create a node-depending background mesh used in the numerical integration of the NNRPIM interpolation functions. The NNRPIM interpolation functions, used in the Galerkin weak form, are constructed with the Radial Point Interpolators. In the construction of the NNRPIM interpolation functions no polynomial base is required, which is an innovation and the used Radial Basis Function (RBF) is the Multiquadric RBF. The NNRPIM interpolation functions possess the delta Kronecker property, which simplify the imposition of the natural and essential boundary conditions.

In the nonlinear analysis, large deformations [2] and elastoplastic material behaviour [3] are considered. The solution of the nonlinear equation system is obtained resorting to incremental/iterative methods, such as the Newton-Raphson method or the orthogonal actualized Ramm’s method, this last permitting the analysis of structures that in some point evidence instability phenomena such as the “snap-through” and the “snap-back”. The material nonlinear behaviour is dealt considering for the elastoplastic model the Von Mises yield function and the efficient “forward-Euler” procedure is used in order to return the stress to the yield surface.

In the biomechanical analysis, a new mathematical model to obtain the bone material properties is proposed. This material law is based in experimental data, which support the idea that the law governing the mechanical behaviour of the bone tissue is the same for cortical bone and trabecular bone. A bone remodelling algorithm is proposed, adapted from Carter’s remodelling algorithm. It is based on the assumption that the adaptation of bony tissue responds mainly to mechanical stimulus. A simple forward Euler scheme is implemented, resulting in an iterative remodelling process.

After the respective exposition, several benchmark solid mechanics static and dynamic linear examples are solved, and well-known demanding nonlinear reference examples are analysed. In biomechanics applications, bone remodelling validation tests are made and then two important bone structures in the human body are studied. The obtained results indicate that NNRPIM is an accurate, flexible and reliable meshless method that can be used in several fields of solid mechanics and biomechanical analysis [4,5].

REFERENCES

QUALITATIVE METHODS FOR INVERSE SCATTERING IN SOLID MECHANICS

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Keywords: Inverse Scattering, Elastodynamics, Topological Sensitivity, Linear Sampling Method.

ABSTRACT

Nowadays, inverse scattering problems in solid mechanics bear relevance to a wide range of applications such as seismic tomography and imaging, non-destructive material testing, and medical diagnosis. To help advance the state of the art on the subject, this research deals with detecting and identifying unknown scatterers i.e. obstacles (e.g. material defects, cracks, or lesions in soft tissues) in an elastic background solid through the use of acoustic or elastic illuminating waves. To circumvent the limitations underpinning the conventional imaging algorithms based on e.g. weak scatterer approximations or non-linear optimization techniques, a variety of the so-called sampling methods have been proposed over the past decade or so. Jointly, these methods constitute a paradigm shift in the approach of inverse scattering in that they seek only a qualitative information on the scatterer geometry and material characteristics within a computationally efficient and robust framework based on full-waveform (or partial) measurements of the scattered field.

The recent emergence of these non-iterative probing methods allows to consider the study of two or three-dimensional elastic waves propagation inverse problems in a new light. Earlier works have shown in particular, within the framework of the hypothesis adopted in this subject, the interest of methods such as i) the Topological Sensitivity Method that relies on a heuristic interpretation of the asymptotic perturbation of a featured cost functional generated by introducing an infinitesimal flaw at a prescribed location (the so-called sampling point), and ii) the Linear Sampling Method based on the resolution of a linear integral equation of the first featuring a fundamental singular solution to the wave equation.

The present study comes within the scope of the development of the two methods mentioned with application within the framework of the mechanics of deformable solids, i.e. inverse scattering problems in acoustic and elastic media. The proposed developments aim to i) provide key results underpinning the validity of these two techniques, ii) demonstrate their usefulness as implemented in conventional computational platforms for approximate but fast defect/lesion detection, and iii) extend their range of application in terms of the geometry and nature of hidden scatterers.

Figure: 3D time-domain identification of a helicoidal crack (in blue) in a thin pipe using the Topological Sensitivity approach. (left) Map of the indicator function; (right) Reconstruction of the local crack orientation.
CONTRIBUTION TO THE STRENGTH DESIGN OF MECHANICAL STRUCTURES MADE OF ADVANCED LAMINATED MATERIALS

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Keywords: GLARE, Fiber-metal laminate, Impact, Indentation.

ABSTRACT

Recently, advanced laminated materials have been constructed which cannot be classified in any category of classic composite materials. These are hybrid materials composed of alternating metal layers and prepreg layers. The layers are bonded together and form the hybrid laminate. The new materials are called fiber-metal laminates and are primarily used in aerospace industry. GLARE (GLAss REinforced) is a successful example of fiber-metal laminates that consists of alternating aluminum layers and glass fiber-reinforced polymer layers.

Since 1991, when GLARE manufacturing for commercial use started, there has been intensive research, from many organizations, concerning the strength of GLARE when subjected to various loading conditions. In this regard, the research of this thesis focuses in the strength design of GLARE under impact loading, which plays an important role as far as the integrity of aircraft structures is concerned since impact damages are often caused due to impacts of foreign objects to the structures.

The first chapter of this thesis includes details about the structural arrangement, the available grades, the basic properties and the main applications of GLARE in mechanical engineering. Furthermore, details concerning the experimental equipment used by researchers in order to study the response of GLARE to impact loading are also included.

In the second and third chapter of this thesis the problem of the response of circular GLARE plates under lateral indentation is solved analytically using the Ritz method [1] and numerically using the finite element method respectively [2]. Based on the current international literature, it is the first time that an analytical solution for this problem is given and it is also the first time that it is solved numerically using the finite element method.

In the fourth chapter, an innovative procedure is proposed in order to minimize the weight of circular GLARE plates which are subjected to lateral indentation using linear programming techniques.

In the fifth chapter, the problem of unloading response of circular GLARE plates which have been previously subjected to lateral indentation is treated analytically, in association with the results obtained in the second chapter, and numerically using the finite element method. Both analytical and numerical solutions of this problem have not been published elsewhere in the current international literature.

In the sixth and seventh chapter, the post-impact permanent deformation of circular GLARE plates due to low velocity impact is calculated numerically using the finite element method and analytically, in association with the results obtained in the second and fifth chapter, respectively. Also, no other solution of this problem has been published in the current international literature.

Finally, in the eighth chapter a numerical solution is given to the problem of the dynamic response of circular GLARE plates due to low velocity impact, after the formulation of the differential equations of motion which represent the examined impact phenomenon using the results obtained in the second and fifth chapter [3]. This problem has not been treated theoretically elsewhere in the current international literature.

REFERENCES

NUMERICAL MODELLING AND CREDIBILITY ANALYSIS OF FREE SURFACE FLOWS IN SELECTED INDUSTRIAL PROCESSES

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Keywords: free surface flow, curing, moulding process, electrical transformers.

ABSTRACT

Main objective of this work is to design and carry out the hierarchical validation and verification (V&V) procedure of the numerical model of the free surface flow in casting applications [1]. Casting processes encompass many techniques that may significantly differ from each other. However, for the purpose of this study one specific process, namely gravitational epoxy casting of an electrical transformer was chosen. Nevertheless, the proposed V&V procedure have rather universal character.

Gravitational casting technique is commonly used in production process of many electrical devices such as bushings, switchgears or instrument transformers. From modelling point of view it is characterized with a very complex shape of the free surface and coupling between physical properties of the epoxy composition, velocity, temperature and polymerization reaction, making its modelling very demanding task.

The Volume of Fluid (VOF) method was used as a framework for development of the mathematical model of the transformer casting process [2]. The polymerization reaction of the epoxy composition was modelled by introduction of the curing degree transport equation and the reaction kinetics determined experimentally. The strong coupling between rheological properties of the epoxy composition, kinetics of the polymerization reaction and temperature was considered in the model as well. The surface tension and wall adhesion effects were modelled with the Continuum Surface Force (CSF) model. The dynamics of the surface wetting was also considered. Computations were performed with all purposes Computational Fluid Dynamics code ANSYS Fluent. It was customized with the User Defined Functions (UDFs) to incorporate all listed phenomena.

The hierarchical verification and validation procedure consisted of three experiments with different levels of complexity. The first experiment was a simple benchmark problem in which only the free surface flow was considered. The second and the third experiment were appropriately isothermal and non-isothermal transformer casting processes. In the former an analog of the epoxy resin was utilized, while in the later the original epoxy resin was used.

Selected Quantitative Imaging (QI) techniques were used in the experimental part of this work. The Particle Image Velocimetry was applied to measure velocity at the free surface of flowing liquid. Characteristic features of the free surface flow were captured and quantified with application of the machine vision techniques. In case of the non-isothermal experiment, temperature field was measured at a few points inside the casting mould.

FINITE ELEMENT ANALYSIS OF CAROTID ARTERY STENTING

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Keywords: cardiovascular, finite element analysis, patient-specific simulation.

ABSTRACT

Cardiovascular diseases (CVDs) are nowadays the leading cause of death in the Western countries, corresponding to high social and economical costs. CDVs are often related to atherosclerosis, a degeneration of the vessel wall causing a number of events, ranging from arterial hardening to lumen narrowing (stenosis), potentially resulting in heart attack or stroke. In particular atherosclerotic stenosis of the carotid artery (CA), narrowing the bifurcation neck, causes 20\% of all ischemic strokes and transient ischemic attacks. Several treatment options are nowadays available for managing CA stenosis but, thanks also to the encouraging outcomes achieved for coronary stenosis treatment, the application of percutaneous minimally invasive techniques, such as stenting, for CA revascularization is rapidly arising. Accordingly, carotid artery stenting (CAS) is a procedure which restores the vessel patency by enlarging the narrowed lumen by the expansion of a metallic mesh, which is driven to the target lesion through a catheter, running inside an endoluminal path accessed by groin incision. A low profile angioplasty balloon can be used for pre-dilation and an embolic protection device can be used to minimize the risk of ischemic attacks due to migration of clots, released during the procedure.

Design, development and performance assessment of the devices used in this procedure are the natural application field of (computational) biomechanics, which applies the principle of mechanics to investigate biological systems and their interaction with artificial implants. The present study is collocated within this scenario since it aims at investigating several aspects of carotid artery stenting (CAS) by means of numerical simulations and supporting the clinical practice through a quantitative assessment of the relation between the complex mechanical features of a given stent design and a given patient-specific anatomy.

In particular, the study investigates: i) the role of filter design on its capability to adapt to the vessel wall; ii) the impact of different stent designs on the revascularization of a single vessel anatomy in order to quantitatively assess the relation between a given carotid stent design and a given patient-specific CA anatomy; iii) the impact of carotid stent apposition on CA wall stress distribution and in particular the influence of constitutive vessel wall modeling on the predicted tensional state over the CA wall; iv) the influence of stent cell type (open versus closed) on vessel scaffolding in a realistic, experimentally-validated case.

Bearing in mind the multidisciplinary nature of the proposed investigation, this study can be considered as a contribution to integration process between the computational tools and clinical practice, in order to support the procedure standardization.
A LAGRANGIAN FINITE ELEMENT METHOD FOR THE INTERACTION BETWEEN FLEXIBLE STRUCTURES AND FREE SURFACES FLUID FLOWS

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Keywords: Fluid-structure interaction, Lagrangian approach, non-Newtonian fluids.

ABSTRACT
The numerical treatment of fluid-structure interaction phenomena, increasingly important in many fields of engineering, is always critical. One of the main problems is the identification of the free surfaces and of the interfaces between solid and fluid. Different techniques have been developed to recover the position of these surfaces (e.g. the Arbitrary Lagrangian Eulerian method (ALE), the level set algorithm or the meshless approaches). A possibility to overcome the difficulties concerning the tracking of the interfaces is to adopt a Lagrangian approach for both fluid and structure. In the present work a fluid-structure interaction algorithm is presented based on a staggered approach in which the fluid is treated in a Lagrangian framework using a new implementation of the so called Particle Finite Element Method (PFEM) [1], and the structure using a classical finite element method.

An advantage of the Lagrangian approach for the fluid flow is that the convective terms in the momentum conservation disappear. The difficulty is however transferred to the necessity to frequently regenerate the mesh. In fact, if a fixed finite element mesh is used and the position of element nodes is updated as a consequence of the fluid flow, very soon the element distortion becomes excessive. A remedy which allows to avoid these distortions consists of systematically remeshing the volume of the problem. To this purpose, an efficient Delaunay triangulation has been adopted. Moreover to define the integration domain and to correctly impose the boundary conditions a method to identify the external boundary is necessary. This has been achieved using a criterion based on the mesh distortion called alpha shape method.

The proposed Lagrangian PFEM is particularly suited for the solution of fluid-structure interaction problems in the presence of free-surfaces, in conjunction with a classical finite element method for the solid part. A critical issue of fluid-structure interaction schemes is the identification of the contact interfaces between the solid and fluid domains. The evolution of the interaction surfaces is tracked using a novel algorithm which exploits the features of the Lagrangian approach based on the continuous remeshing introduced for the fluid solution. The proposed algorithm is based on the superposition of a set of fictitious fluid particles to the nodes of the solid domain, which can come in contact with the fluid domain. When the Delaunay triangulation is performed, the alpha-shape criterion selects those parts of the interface where the fluid particles can possibly come into contact with the structure. Once the fluid-structure domain is determined, a coupled analysis is performed with a Dirichlet-Neumann iterative approach.

The proposed scheme has been applied to both Newtonian and non-Newtonian fluids. Comparisons with numerical benchmarks and with experimental results are presented to show its potentialities and to find possible defects. The non-Newtonian solver has been also used to simulate typical tests on fresh concrete, mortar and cement pastes showing a good agreement between numerical and experimental results.

REFERENCES
STRONG DISCONTINUITIES IN THE SCOPE OF THE DISCRETE CRACK APPROACH

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Keywords: Strong discontinuities, discrete crack approach, non-homogeneous jumps, embedded discontinuities, generalized/extended FEM.

ABSTRACT

The use of the discrete crack approach and Nonlinear Fracture Mechanics opened the possibility of accurately modelling fracture behaviour of quasi-brittle materials, such as concrete, mortar and masonry. In this approach, it is assumed that microcracking localises into a surface of discontinuity, designated fictitious crack. Traditionally, the discontinuities are modelled by interface elements within the scope of the finite element method. In this case, some numerical problems exist related to the fact that the discontinuities must evolve along the finite element boundaries, although the crack path is not usually known in advance.

More recently, the possibility of embedding strong discontinuities in finite elements overcame these difficulties. In general, in these formulations constant strain triangles are used and constant jumps are adopted in each parent element. Furthermore, the additional degrees of freedom are local and, as a consequence, both the discontinuity jumps and the tractions are discontinuous across element boundaries.

In this work, two variationally consistent innovative strong embedded discontinuity formulations are introduced: i) the Discrete Strong Discontinuity Approach (DSDA); and ii) the Generalised Strong Discontinuity Approach (GSDA). Their main characteristics are: i) non-homogeneous jumps are introduced in each parent element using the shape functions of an interface element in the parent element; ii) additional edge nodes are global nodes and, since they are shared by two elements at a common boundary, iii) continuous jumps and tractions across interelement boundaries are automatically obtained; and iv) no stress locking is found. In the DSDA the discontinuity jumps are transmitted by means of a rigid body motion, whereas in the GSDA stretching is also included.

In order to assess the capabilities of the presented formulations, a comparison is established with: i) the Discrete Interface Approach (DIA); and ii) the Generalised Finite Element Method (GFEM). It is found that both the DSDA and the GSDA often present similar results in structural problems with soft discontinuities, in particular under mode-I fracture. Nevertheless, in some cases in which either mixed-mode or mode-II fracture is predominant, the DSDA may lead to a more rigid behaviour when compared to the GSDA, the DIA and the GFEM.

Furthermore, several benchmark tests concerning mode-I, mixed mode and mode-II fracture are computed and the numerical results are compared to the corresponding experimental results. It is emphasised that all numerical results are similar to the available experimental data, even with coarse meshes (see for e.g. Fig. 1).

As a final result of this work, an efficient and robust numerical tool has been introduced for modelling fracture behaviour of quasi-brittle materials, which is already being applied so several ongoing projects.

![Figure 1. Four-point shear test - load vs. CMSD curves superposed with experimental results; $\sigma_f$ map obtained with the GSDA when CMSD=0.15 mm (displacements amplified 100 times)](image)
GALERKIN PROJECTION VIA SUPERMESH CONSTRUCTION

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Keywords: Galerkin projection; supermeshing; finite elements; interpolation; coupling.

ABSTRACT

At the heart of the finite element method is the concept of a discrete function space. Searching for solutions to a partial differential equation inside an infinite-dimensional function space is very difficult; the search space is simply too big. The finite element method restricts the search space to a smaller function space of manageable size, and computes an approximate solution within the discrete function space. If the approximate solution is not accurate enough, then the discrete function space may be enlarged and a better approximation sought.

As discrete function spaces are fundamental to the finite element method, the question of transferring data between these function spaces commonly arises in the course of the analysis. For example, the mesh may be adapted in the hope of improving the quality of the solution; this necessitates transferring the computed solutions from the previous mesh to the adapted mesh; or perhaps two simulations have been conducted on different meshes, and the analyst wishes to compute a diagnostic that is a function of both. This problem of transferring data between function spaces is referred to as the interpolation of discrete fields, and is the primary focus of this thesis.

The key contribution of this thesis is the novel implementation and analysis of Galerkin projection between discrete function spaces, an interpolation technique with three principal advantages over its alternatives. Firstly, it is optimally accurate in the L2 norm; no other interpolation technique can improve on its accuracy. Secondly, it is naturally conservative, which is a crucial and non-negotiable requirement for many application areas. Thirdly, it is well-defined in the case of spaces of discontinuous functions; it works for cases where standard approaches of nodal evaluation are not well-defined. While the highly desirable properties of this projection have been known for some time, the implementation of Galerkin projection is very challenging; this thesis reports the first successful general implementation.

The fundamental difficulty of implementing Galerkin projection is that it requires the computation of the inner products of the basis functions associated with the target and donor function spaces. These inner products cannot be exactly computed on either the target or donor meshes. This thesis describes the efficient computation of these inner products by introducing the geometric concept of the supermesh of the two meshes; the supermesh is simply the mesh of the intersections of the elements of the input meshes. Given the supermesh of the target and donor meshes, the construction of the Galerkin projection is simple; therefore, the focus of the thesis turns to the construction of the supermesh of two meshes. The major practical contribution of this work is an efficient algorithm for the construction of the supermesh.

With efficient algorithms for its construction in hand, a wide range of applications become possible. The discussion will focus on the computation of diagnostics of unstructured-mesh or adaptive-mesh simulations, and the applications of supermeshing to coupling different models.
NUMERICAL APPROXIMATION OF THE LINEAR CANONICAL TRANSFORM
AND APPLICATIONS

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Keywords: Linear canonical transforms, Fourier optics, optical signal processing, sampling, digital holography.

ABSTRACT

The linear canonical transforms (LCTs) are a three-parameter group of linear integral transforms. They were first discovered in the field of quantum mechanics, where they constitute the dynamical group of the N-dimensional harmonic oscillator. Later, they were linked to the ABCD matrix, which characterizes certain optical systems including lens systems and optical fibres with certain refractive index profiles. Also linked to these matrices was the Wigner distribution function, a bilinear time-frequency pseudo-distribution with many applications in optics. Together, these mathematical tools provide a number of consistent approaches to solving many problems related to optical systems.

The Fourier transform is an LCT, one which is ubiquitous in signal processing, communications, Fourier optics and many other technical areas. Where the Fourier transform describes a signal in the frequency domain, the LCTs in general transform signals into mixed time-frequency domains. By comparison with the FFT, it is evident that fast and accurate numerical approximation of the LCTs is of great importance for applications involving LCT-based analysis. In particular, we mention the numerical reconstruction of an image in digital holography, an example of the modern trend towards combined opto-numeric imaging systems.

Consequently, numerical approximation of the LCT is an active area of research, of interest for system design and analysis, holography, signal processing and other areas. We examined the discretizations of the transforms available in the literature, selected the most suitable one, and showed a number of practical considerations regarding setting resolution and window size. Sampling requirements for the wave fields at the input and output of such calculations were established for the first time; previous sampling theory in the area was shown to be insufficient to guarantee reconstruction of the signal. Lohmann’s phase space diagrams (PSDs) were modified for use with discrete fields, illustrating clearly the failings of previous sampling theories by making use of the LCTs simple co-ordinate transforming effect on such diagrams. In doing so, we were obliged to ignore the implications of the cross-terms present in the Wigner distribution function for the accuracy of the simulations and for the selection of sampling schemes. However, we later revisited this question and showed that neglecting such cross-terms is a reasonable approximation. A number of algorithms were previously proposed for performing the LCTs in \( O(N \log N) \) time. We compared these, determining the relative merits of algorithms which decompose the optical system into special cases for which fast algorithms are better developed and algorithms which decompose the calculations into smaller ones iteratively. We used the PSD-based sampling analyses to show how to perform the former type of calculation with fewer samples (and hence faster), and proposed a new algorithm of the latter type which is more flexible than previous algorithms in terms of the numbers of samples it can support.

More recent work on the LCT has focused on a number of topics. An algorithm has been proposed for numerically approximating non-separable 2-dimensional LCTs. We have extended our PSD sampling analysis to apply to this case. Algorithms have also been proposed for the generalization to complex parameters, and in the case of our algorithm even a complex output domain. Though this has no physical significance in optics, it does suggest some applications. We have shown that our discrete LCTs are Hadamard matrices if certain restrictions are placed on the parameters. Hadamard matrices are used in quantum computing. Turning to more traditional territory – digital holography - we have quantified the 2.5D imaging performance of digital holographic systems using an LCT-based methodology, and proposed the space-bandwidth ratio as a means of choosing between Fresnel and other linear canonical transform algorithms for the reconstruction of holograms.
MESHLESS NUMERICAL FORMULATION FOR ANALYSIS OF SHELL-LIKE STRUCTURES

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Keywords: Meshless methods, Meshless Local Petrov-Galerkin method, Moving Least Squares approximation, plates, shells, Poisson’s thickness locking, transversal shear locking

ABSTRACT

Meshless computational methods for the analysis of plate and shell structures are proposed in this contribution. The developed algorithms are based on the local Petrov-Galerkin approach. A shell is considered as a three dimensional (3-D) solid continuum, and the solid-shell concept, which allows the implementation of complete 3-D material models, is adopted. It is assumed that the material fibres that are initially normal to the shell middle surface remain straight, but not necessarily normal to the mid-surface. However, the stretching of the fibre in the thickness direction is allowed, which enables the more realistic description of shell deformation response. The geometry of the shell is described by employing a parametric mapping technique, whereby the middle surface of the shell is defined mathematically exactly. Discretization is carried out by the couples of nodes located on the upper and lower surfaces of the structure. The nodes forming a couple lay on the same fibre in the direction of the normal vector to the shell middle surface.

The governing equations are obtained by constructing the local weak forms (LWF) of the 3-D equilibrium equations, which are written over the local sub-domains surrounding the node couples. The approximation of all unknown field variables is carried out by using the Moving Least Squares (MLS) approximation scheme in the directions that are tangential to the structure middle surface, while simple polynomials are applied in the thickness direction. For simplicity, the test functions are assumed to be linear across the thickness, and the Heaviside step function is applied in the tangential directions. The causes of Poisson’s locking and transversal shear locking are identified and explained from the theoretical point of view for the classical displacement-based approach. Both the purely displacement-based (primal) and mixed formulations are proposed and special attention is given to the elimination of locking effects.

Two different primal formulations are presented where only the displacement field is approximated. The Poisson’s thickness locking effect is circumvented by adopting the hierarchical quadratic interpolation over the thickness for the transversal displacement component. The transversal shear locking phenomenon is alleviated by applying a sufficiently high order of the MLS functions in the tangential directions. The proposed strategy performs well in the analysis of thick structures, but it is sensitive to the shear locking effects. The application of high-order approximation functions leads to prohibitively high computational costs.

The mixed approaches, based on the mixed MLPG paradigm, are developed. Therein, the appropriate strain and stress components are approximated separately from the displacement field. A closed system of equations includes the LWF of the 3-D equilibrium equations, and suitable collocation relations enforcing the compatibility between approximated strains/stresses and approximated displacements at the nodes. The nodal strain and stress values are eliminated from the equations by the algebraic manipulation of the discretized equations, which is performed locally, and a global system of equations containing only the unknown nodal displacement variables is obtained. In the formulation for plates, Poisson’s thickness locking is eliminated by modifying the nodal values of the normal transversal strain component. In the curved shell structures, the transversal normal stress is approximated directly instead of the transversal normal strain, leading to a simpler and computationally less costly efficient algorithm. Transversal shear locking in the thin structural limit is efficiently suppressed by means of the separate strains approximation. It is theoretically proved that the developed mixed approach is numerically more efficient than the comparable primal meshless formulations. The numerical efficiency of the derived algorithms is demonstrated by numerical examples.
MULTISURFACE ELASTOPLASTIC YIELD CRITERIA.
NUMERICAL IMPLEMENTATION IN PRINCIPAL STRESS SPACE AND
APPLICATION IN GEOTECHNICAL ENGINEERING PROBLEMS

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Keywords: Plasticity, multisurface yield criteria, nonsmooth, spectral decomposition, return-mapping algorithm.

ABSTRACT

Plasticity models possessing multiple yield surfaces are used in many engineering applications, especially in
gеotechnical engineering. The multiple yield surfaces may or may not intersect in a smooth manner, with the
latter case being a superset of the former and typically encountered more often in engineering problems. While
the importance of these models is widely acknowledged, difficulties arising from the singularities induced by the
non-smooth intersections of the yield surfaces, introduce severe algorithmic and numerical complexities.

Three main problems can be identified, namely, (a) the elastic domain is subdifferential with respect to the
stress vector at the intersections of the yield surfaces, (b) the application of the normality hypothesis concerning
the flow rule suffers from severe numerical errors in near singular areas and (c) the set of the yield surfaces
assumed to be ultimately active is not known a priori.

To overcome these problems a number of different approaches can be found in the literature, which focus
either on (a) the modification/smoothening of the yield surfaces in the vicinity of non-smooth intersections,
leading however to inevitable gradient jumps and reduced accuracy, (b) the replacement of all the yield surfaces
with a smooth one, raising as a consequence modeling issues, or (c) the proper treatment of the plastic corrector
near corner regions following specific, non general, surface dependent implementations.

In this work a new algorithmic treatment of the non-smooth multisurface plasticity problem is proposed,
based on:

- The utilization of the complete set of yield surfaces used to describe the model, employing the
  fundamental work of Koiter.
- The use of convex programming to define the active yield surfaces. Only the Karush-Kuhn-Tucker
  complementarity conditions are used to provide the characterization of plastic loading/unloading and
  thus characterize the constraints induced by the yield surfaces.
- And more importantly, the reformulation of the return-mapping algorithm into the principal stress
  space. If isotropy in the elastic response is assumed, then the strain spectral directions coincide with the
  stress spectral directions and therefore the return mapping algorithm may be conveniently formulated in
  the principal stress space, a concept which is exploited for the case of multisurface plasticity.

The proposed algorithm is applied into four typical multisurface plasticity models, namely the Tresca, the
Mohr-Coulomb, the Hoek-Brown and the Drucker-Prager (supplemented with a tension cut-off surface) yield
criteria. It is proven that all the singularities induced by the non-smooth intersections of the yield surfaces are
removed and an extremely efficient algorithm is provided, characterized by generality, simplicity and robustness.
Especially in the case where linear surfaces in the principal stress space are considered (as in the Mohr-Coulomb
and Tresca yield criteria), it is shown that the return mapping scheme reduces to a one step closest point
projection, leading to a closed form solution.

For the validation of the theoretical work, a fully featured, flexible and extendable finite element program is
developed, where the proposed algorithm is implemented. State of the art programming techniques are used,
including the object oriented programming paradigm, parallel programming and scripting capabilities. The
resulting software, which is freely available at www.nemesys-project.org, is capable of dealing with static/transient/eigenvalue problems accounting for material and/or geometrical nonlinearities, employing a
variety of solution algorithms, material implementations and element formulations.

The algorithm's behavior is thoroughly examined, verified and validated in a wide range of geotechnical
problems with excellent results.
FAST NUMERICAL METHODS FOR MIXED-INTEGER NONLINEAR MODEL PREDICTIVE CONTROL

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Keywords: optimal control, direct and simultaneous methods, mixed-integer nonlinear programming

ABSTRACT

We present new developments towards the solution of nonlinear mixed-integer optimal control and model-predictive control problems under real-time constraints [1].

In this contribution, we present a new numerical framework for the efficient solution of mixed-integer nonlinear optimal control problems. Such problems frequently arise from challenging industrial processes and have seen significant research efforts in the past. This probably is due to the enormous potential for optimization. The hybrid and nonlinear nature of these problems however still is challenging to cope with from a numerical and algorithmic point of view. The developed methods for this combinatorial and nonconvex dynamic problem are based on direct and simultaneous approaches such as Bock's direct multiple shooting method. Using a new partial outer convexification and reformulation of dynamics and constraints affected by integer or binary controls, we show how to efficiently compute approximate solutions with feasibility and optimality certificates, and how to do so without experiencing exponential runtime in practice. The idea of real-time iterations allows to transfer this framework also to nonlinear model-predictive control problems. Here, it effectively allows to rapidly compute mixed-integer feedback for real-time predictive control of hybrid nonlinear dynamic processes. The computational performance of this scheme is determined by the computational effort required to solve a nonconvex feedback QP in each real-time iteration. We show how this effort can be reduced further by using a tailored block structured active set method in each real-time iteration. The described methods achieve real-time capable mixed-integer control feedback and their applicability is demonstrated on several real-world problems from research and industry.

REFERENCES

NUMERICAL MODELLING OF HEAT, MASS AND MOMENTUM TRANSFER IN NATURAL DRAFT WET-COOLING TOWER

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Keywords: Natural Draft Wet-cooling Towers, CFD, Heat and Mass Transfer, POD-RBF networks

ABSTRACT

This thesis presents investigations on numerical modelling of Natural Draft Wet-cooling Towers (NDWCT) using computational fluid dynamics tools. The aim of a cooling tower is to reject waste heat into the atmosphere. From the viewpoint of heat and mass transfer intensity the most important regions of the tower are the fill, rain zone and spray zone. In all three zones the heat and mass is transferred from the cooling water to the air in a counter-current flow. The NDWCTs are the most frequently used cooling systems in conventional power plants and are often used in other industrial applications. The efficiencies of the power plants strongly depend on the cooled water temperature, therefore the cooling effectiveness translates into fuel consumption, flue gas emissions and earnings. The cooling towers are large structures whose heights often exceed 100 m and sometimes even attain 200 m. They are expensive in retrofitting and difficult to operate and adjust. The so called global models (e.g. Merkel, e-NTU and Poppe methods together with aerodynamic calculations), most frequently used in the design and performance test computations, lack generality in the sense that they operate on average flow parameters. This in turn does not allow to investigate the flow parameters distributions inside and outside the tower, the changes in some design parameters and reduces the possibilities to predict e.g. the effect of wind, non-uniform water load and fill depth, introduction of flue gases into the tower, etc. The aim of the thesis was to develop a numerical model of a NDWCT that comprises a complete computational tool for cooling tower simulations and that overcomes the aforementioned difficulties. A natural choice was to use a CFD code and supplement it with submodels suited for transport phenomena occurring in NDWCTs. The major difficulty occurring when developing the CFD model was the large difference in geometrical scales in the tower and its surroundings. The dimensions of the channels of the labyrinth like fill present inside the cooling tower are of the order of centimeters, while the dimensions of the surrounding air domain in the model are of the order of a kilometer. This scale difference makes the task of generating a good quality mesh of reasonable number of degrees of freedom almost impossible. In order to obtain the results within an acceptable time submodels of each of the transfer zones have been created. The submodels allow coupling of the small and large scale phenomena and preserve details of the flow down to the scale of interest maintaining the accuracy of the computations. The approaches used in modelling of the fill deserve most attention. Firstly the fill zone has been treated as a porous medium. The gain was that the detailed geometry need not be reproduced. The complex transport phenomena in this zone are modelled by including appropriately defined distributions of heat and mass sources. The spatial distribution of the flow parameters in the fill have been accounted for by dividing this region into a set of vertical conduits. The heat and mass sources are obtained by solving mass and heat transfer problems in each conduit. A new approach to the solution of this problem has been developed. Secondly the heat and mass transfer in the fill has been approximated by a Proper Orthogonal Decomposition Radial Basis Function (POD-RBF) network. This approach allowed reduction of the computational time in each conduit by two orders of magnitude preserving high accuracy of the calculations. The flow of water droplets in the rain zone has been represented using the Euler-Euler multiphase model. The heat and mass transfer in the spray zone has been included in the analysis of the fill. The developed computational procedures have been then used in the simulation a real cooling tower. Comparison of the experimental results on this tower and the computations was used to successfully validate the CFD model. The created CFD model of the NDWCT comprises a complete computational tool that can be used for both design computations, typical what-if analyses as well as cooling tower performance tests.
APPLICATION OF HOMOGENIZATION METHODS AND CRYSTAL PLASTICITY TO THE MODELING OF HETEROGENEOUS MATERIALS OF TECHNOLOGICAL INTEREST

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Keywords: Homogenization, Crystal Plasticity, Heterogeneous Materials, Image Processing.

ABSTRACT

The relation between microstructure, material properties and mechanical response is a basic issue of research in material science and material mechanics. E.g., the prediction of the macroscopic stress-strain response of composite materials is related to the description of their complex microstructural behavior. In this contribution different aspects of the modeling of heterogeneous materials of technological interest while taking the microstructure into account are addressed. In a first step homogenization methods in the context of linear elasticity are considered. Three strategies to determine the effective macroscopic material behavior for composites consisting of irregular shaped inclusions are discussed: (i) Homogenization methods using an analytical description for the Eshelby tensor, (ii) Computation of the contribution of one isolated inclusion into an infinite matrix material and its influence on the effective behavior, and (iii) Direct computation of the effective elastic properties for a given microstructure by discretizing the domain and using FEM. Different inclusion shapes are investigated and the results are compared. In this context an exemplary study will be reported about the characterization and parameter identification of single constituents in thermally arc-sprayed coatings as well as whole coatings. Based on results in nanoindentation tests the mechanical properties are identified for each constituent in the coating. A general procedure is presented to predict the effective mechanical properties based on the microstructure, porosity, chemical composition and properties of the coating after thermal spraying.

Thermally arc-sprayed coatings show a heterogeneous microstructure, however, the microstructure is composed of a layered structure which is determined by the nature of the manufacturing process. This was the motivation to develop a homogenization method for the material behavior of two-phase composites characterized by a thin-layer-type microstructure. The basic idea of this approach is to idealize the thin-layered microstructure as a first-order laminate. Comparison of the method with existing homogenization schemes demonstrates the advantage of the current approach for such microstructures. Further a first extension to a variable interface orientation is presented.

Finally an experimental and theoretical investigation of a large-grained Fe-3%Si sheet metal oligocrystal undergoing incremental tensile loading at room temperature is performed. To this end an explicit finite-element-, crystal-plasticity-based model is developed for each grain, the grain morphology, and the thin sheet specimen as a whole. In particular, the crystal plasticity model is rate-dependent and accounts for (local) dissipative hardening effects. In order to compare model predictions with experiment, the material parameters have been identified with the help of single-crystal data from the literature. Identified model predictions are compared with the experimental results for the deformation behavior of thin sheets of Fe-3%Si loaded incrementally in tension at room temperature. To this end, attention is restricted to the two slip families \{110\} and \{112\} expected to be active at room temperature. Comparison of model predictions for grain morphological evolution with the corresponding experimental results up to 19.5% deformation imply good agreement. In addition, model predictions for the development of the strain field, the grain reorientation field, the orientation gradient and geometrically necessary dislocations are discussed and evaluated.

REFERENCES

DEVELOPMENT OF A LATERALLY PRESSED QUADRILATERAL SHELL ELEMENT

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Keywords: Drilling degree of freedom, Quadrilateral shell element, Stress in thickness direction

ABSTRACT

The numerical simulation of shell like structures presents a major challenge in the field of computational mechanics. Thereby, the derivation of accurate and robust shell elements for geometrically and physically nonlinear analysis is somehow the supreme discipline. Within this two-parted thesis two main issues in that field are discussed and resolved:

Within the first part of the present thesis a highly efficient quadrilateral shell element is derived, especially for use within an explicit time integration scheme. Special emphasis is put on the incorporation of in-plane rotational degrees of freedom (drilling degrees of freedom). Thereby, the micro polar theory of elasticity (Cosserat's theory of elasticity) is found to be a suitable starting point, since the corresponding field problem consists of rotational degrees of freedom. Requiring the absence of couple stresses and enforcing the symmetry of the stress tensor in a weak form enables the derivation of a functional which can be used to propose low order finite element formulations. It is worth noting that the derived functional does not require any mathematical regularizations resulting in a physically based, straightforward approach. The computational efficiency and the predictive quality of the finite elements can be increased using a Hu-Washizu variational principle in connection with suitable strain interpolations. Avoiding any internal degrees of freedom which would have to be condensed at element level, the proposed formulation shows excellent in-plane and out-of-plane bending characteristics, while fulfilling all relevant patch test conditions. Furthermore, the evaluation of element stiffness matrices can be carried out analytically avoiding any Gaussian quadrature and resulting in a computationally efficient formulation. The generalization of the theory to geometrical and physical nonlinearities is carried out in a straightforward manner according to an Updated Lagrangian scheme and the predictive quality of the formulation is equal or even better compared to results within standard benchmark problems. The incorporation of drilling degrees of freedom enhances the performance of the shell element at beam to shell connections significantly.

The second part of the thesis tackles the frequently used assumption of vanishing normal stress components in thickness direction. It is observed within the simulation of sheet metal forming operations that the corresponding stress values are of the order of the material's yield stress and cannot be neglected. It is proved analytically and numerically that this lateral stress component has a major impact on damage and on mechanical properties like force and deformation histories. In contrast to recently proposed seven-parameter shell formulations the suggested algorithm avoids any additional degrees of freedom to cover this three dimensional stress state. It is stated that a linear lateral stress distribution can be extracted from applied boundary conditions, i.e. tractions from externally applied pressures or normal contact stresses acting on the top and/or the bottom surface of the shell bound the stress distribution in thickness direction. According to the proposed “constrained plasticity” algorithm the constitutive update is able to account for these stresses and, consequently, the membrane and bending behavior of the shell becomes more realistic. Furthermore, a novel contact algorithm is developed suitable for the description of element impact at rigid contact surfaces. Based on a scalar coefficient of restitution which influences the transmission of energy from the impacting shell to the rigid contact surface and analytical considerations of stress waves between impacting bodies a physically based contact stress extraction procedure is derived. The performance of these derivations is tested extensively within several specific benchmark problems of sheet metal forming. The numerical results are in close agreement with three dimensional continuum formulations, where conventional plane stress shell elements yield erroneous solutions. Consequently, the proposed derivations, algorithms and modifications enable computationally efficient numerical simulations of real world manufacturing processes with a substantial increase of predictive quality.
EXPLORING THE PHYSICS OF FRAGMENTATION THROUGH PARALLEL SIMULATIONS

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Keywords: dynamic fragmentation, heterogeneous brittle materials, parallel computing, fragment size distribution, energy conversion, stress release waves

ABSTRACT

The physical mechanisms underlying the dynamic fragmentation of heterogeneous brittle materials are explored through numerical simulations. The use of computational facilities, rather than experimental or fundamental sciences, ensures the accurate tracking of rapidly evolving fields (such as stress field, energies and damage). The numerical framework is based on Galerkin approximations coupled to the Cohesive Zone model, which addresses the failure response. Depending on the number of degrees of freedom, serial or parallel simulations are performed. The finite element method with dynamic insertion of cohesive elements constitutes the basis of the serial calculations. However, it is replaced by the scalable discontinuous Galerkin formulation for parallel computing. Both frameworks recover accurately the physical mechanisms behind dynamic fragmentation.

The thesis is organized to handle gradually increasing complexity. First, the fragmentation of a quasi one-dimensional expanding ring, constituted of a heterogeneous material, is simulated. It involves two major mechanisms: crack initiation and crack interaction. Fragment sizes are highly dependent upon strain rate, material properties, and microstructural heterogeneity. Scaling laws of the average fragment size, as well as of the distribution of fragment masses, are proposed and lead to predictable laws.

Then, crack propagation mechanisms are investigated through parallel simulations of the quasi three-dimensional breakage of a thin plate. By analyzing the energetic response, two regimes are defined: the strength controlled and the toughness controlled. At low strain rates, defects play a key role and govern energy levels. They correspond to the strength controlled regime and induce disordered responses. At high strain rates, fragmentation is more organized, fragment masses follow Weibull distributions, and crack interactions become secondary. This is the toughness controlled regime, governed by energetic arguments. The transition between the two regimes is derived as a function of material parameters.

Finally, the transition between two- and three-dimensional fragmentation is analyzed. Massively parallel simulations of the fragmentation of a hollow sphere with variable thickness are conducted. The effect of dimensionality upon fragment shape and fragment mass distributions is analyzed.

Interestingly, although these three tests involve distinct mechanisms due to the specimen geometry, they share common behaviors. Quasi-static loadings lead to highly dynamic fragmentation processes, involving extensive stress wave interactions. Defect distributions play a key role. By contrast, dynamic loadings are associated to smoother and more deterministic responses. They are primarily controlled by energy arguments. This results in a predictable dependence of the average fragment size and strain rate, characterized by a power law.

Therefore, the interpretation of these numerical results sheds light on the complexity of the physics underlying fragmentation. The dynamics of stress waves, energetic arguments, the loading conditions, the dimensionality of the geometry, and the material itself (bulk and defects) must be all evoked to draw a global picture of the phenomenon. Reproducing such processes requires a high level of accuracy that novel parallel numerical frameworks are able to provide.
OPTIMIZATION OF RAILWAY VEHICLES FOR CRASHWORTHINESS

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Keywords: Crashworthiness, Railway, Multibody, Optimization, Sensitivities, Automatic Differentiation.

ABSTRACT

Although the railway industry uses structural passive safety principles in the design of railway vehicles their design is mostly based in the experience of the designer rather than in any systematic approach. The need for design methodologies that systematize the process ensuring that the best results are obtained has been recognized by leading railway manufacturers. The use of optimization methods applied to a large number of highly nonlinear problems in different areas of mechanics is accepted in most of the industries including in the design of road vehicle passive safety systems, but rarely used in railway crashworthiness. This work presents an optimization based approach to the design of crashworthy railway components that fulfill existing regulation.

A multibody formulation is developed for the dynamic analysis of trains under collision. Specific railway force elements are developed to describe the suspension system of the train cars, the interaction between wheels and rail, and the contact between train cars. Of particular importance to characterize the crashworthiness of trains, a force-deformation element is developed to describe the energy absorption due to the deformation of crashworthy components of the train car based on a generic spring force element with nonlinear force-deformation characteristics that considers loading and unloading conditions in both linear and plastic domain. The developed multibody dynamics methodology is demonstrated in a study case for the assessment of effects concerning overriding of train cars and design specifications for anti-climbers components. A validation of a multibody model for railway crashworthiness is developed in the context of a train crash experimental test, revealing similar dynamic responses which enable to demonstrate the validity of the model.

A methodology for the sensitivity analysis of multibody systems is developed. Automatic differentiation is introduced as a valid tool to obtain complex derivatives to overcome the drawback of using the finite difference method to obtain an approximation of the sensitivities whenever the analytical solution of the sensitivities is impracticable to establish. Automatic differentiation is implemented using the computer tool ADIFOR. Particular focus is given on the evaluation of sensitivities related to the force-displacement curves that characterize the behavior of train car components that deforms during train collisions. A set of case studies is defined to describe particular characteristics of the sensitivities evaluation process and the suitability of using the automatic differentiation ADIFOR tool.

Optimization in the context of railway crashworthiness is introduced, based on the regulations for the structural integrity of the passenger train cars. Considering the dynamics of train collisions characterized by the absorption of maximum kinetic energy as a result of structural deformation of train car components in designated areas, optimization studies are carried out in order to determine the crashworthiness design parameters representing major characteristics of crush behavior for those components. Case studies highlight the suitability and advantages of using automatic differentiation to obtain the optimization gradients, instead of using finite differences that imply a large number of dynamic analyses necessary to compute each design sensitivity with prohibitive computational costs.

It can be concluded that the proposed optimization methodology is computationally efficient for the design of crashworthy structures and that the methodology efficiently integrate the main requirements associated to the dynamic analysis of trains in crash scenarios. In particular, the design methodology that systematize the process of optimization of energy absorbing components, based on design parameters associated with the force-displacement curves that characterize the crush behavior of such components, constitute advances in the area of railway crashworthiness.
STABILIZED 3D X-FEM CRACK SIMULATION WITH INTERFACE FRICTIONAL CONTACT: APPLICATION TO FRETTING FATIGUE

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Keywords: X-FEM, crack propagation, frictional contact, LBB condition, fretting fatigue.

ABSTRACT

Numerous local nonlinear phenomena impact directly the propagation rate and path of cracks. Contact with friction between crack faces notably occurs in contact-fatigue problems, at the interface between contacting mechanical parts for instance. In this case, the possible time-dependent, multi-axial, non-proportional loadings may induce a very complex distribution of open, sliding and adherent areas between the crack faces. Moreover, the spatial scale of these local phenomena is usually much smaller than the scale of the global structure problem.

In this context, a stabilized global-local quasi-static contact algorithm for 3D non-planar frictional crack is presented in the X-FEM / Level-Set framework. A three-field weak formulation is considered and allows a refined discretization of the crack interface according to the possible complex local contact state independently from the mesh in the bulk [1]. Furthermore, an efficient stabilized non-linear LATIN solver dedicated to contact and friction is proposed [2]. It allows solving in a unified framework frictionless and frictional contact at the crack interface with a symmetric formulation, no iterations on the local stage (unilateral contact law with/without friction), no calculation of any global tangent operator, and improved convergence rate.

2D / 3D patch tests are presented to illustrate the relevance of the proposed model. Then, an actual 3D frictional crack problem under cyclic fretting loading is modelled [3,4]. A multi-model strategy based on experimental analysis and numerical X-FEM simulation is proposed to simulate fretting crack propagation. 3D cyclic contact loadings and experimental 3D non-trivial crack geometries (cf. figure 1) are extracted. Crack initiation prediction and 3D X-FEM crack propagation simulations are performed using multi-axial non proportional path criteria and a dedicated crack growth law [5].

REFERENCES

VISCOPLASTIC DAMAGE ANALYSIS OF PLATE-SHELL STRUCTURES SUBJECTED TO IMPACT LOADING

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Keywords: Plate, impact loading, explosion, damage, failure modelling, numerical simulation.

ABSTRACT

The work presents the investigation in the response of plate-shell structures subjected to impact loadings – gas mixture explosions. This rather complex phenomenon is studied in the context of its mechanical aspects, mainly the ductile failure prediction (failure mechanics). A primary problem of this domain is associated with formulation of sufficiently simple and accurate criterion of crack initiation and propagation for multiaxial stress concentrations in structural elements. The area of design against failure potential applications is very wide. The examples are: aeronautical industry (assessment of safety against a threat posed by on-board commercial aircrafts explosions), industrial transport or storage (assuring a reliability against metallic pressurised vessels accidents or ductile tearing of pipelines), metal-forming processes (localisation of potential damage during stamping and extrusion of aluminium or steel plates), army applications (ballistic penetrations) and other general problems of life prediction.

The work starts with the literature review and the description of theories, which are nowadays in common use in damage and failure modelling. Four main groups are distinguished and described: fracture mechanics, continuum damage mechanics, porous solids plasticity models and abrupt failure criteria. Among them, for the further applications, two groups are chosen. The first is continuum damage mechanics (the Lemaitre model [1]), which is the example of the approach fully coupled with a constitutive law (affects weakening of a material stiffness). The second is the group of abrupt failure criteria (based on the critical value of the equivalent plastic strain at fracture [2], based on the total strain energy density constancy assumption [3] and based on the triaxiality stress ratio dependency [4]), which is the example of the uncoupled approach. As a constitutive law, in both groups, the viscoplastic model proposed by Chaboche [5] is used.

After selecting the theoretical models and the numerical tools (MSC.Marc software) for the analyses, the detailed report of all realised experiments (tests on plates subjected to explosions, quasi-static tests on plates and uniaxial tests on bar samples) and their results is presented. Then, for the assumed constitutive and damage laws, the identification of elastic-viscoplastic material parameters and fracture criteria parameters is described.

Finally, the realisation and the results of numerical simulations are illustrated. The main analysis is preceded by the determination of model’s fixing boundary conditions. The description of final simulations is divided into the analyses realised using axisymmetrical and 2-D shell elements. All presented results are verified by the results of corresponding experiments. The work finishes with the summary and conclusions, where the best approaches (from those, which have been tested) are pointed, all assumptions or limitations used in the study are discussed and the objectives for the further research are indicated.

REFERENCES

NUMERICAL ANALYSIS OF THE NONLINEAR DYNAMICS OF A DRILL-STRING WITH UNCERTAINTY MODELING

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Keywords: nonlinear dynamics, uncertainty modeling, stochastic analysis, drill-string dynamics.

ABSTRACT

This work analyzes the nonlinear dynamics of a drill-string including uncertainty modeling. A drill-string is a slender flexible structure that rotates and digs into the rock in search of oil. A mathematical-mechanical model is developed for this structure including fluid-structure interaction, impact, geometrical nonlinearities and bit-rock interaction. After the derivation of the equations of motion, the system is discretized by means of the Finite Element Method and a computer code is developed for the numerical computations using the software MATLAB. The normal modes of the dynamical system in the prestressed configuration are used to construct a reduced-order model of the system. To take into account uncertainties, the nonparametric probabilistic approach, which is able to take into account both system-parameter and model uncertainties, is used. The probability density functions related to the random variables are constructed using the Maximum Entropy Principle and the stochastic response of the system is calculated using the Monte Carlo Method. A novel approach to take into account model uncertainties in a nonlinear constitutive equation (bit-rock interaction model) is developed using the nonparametric probabilistic approach. To identify the probabilistic model of the bit-rock interaction model, the Maximum Likelihood Method together with a statistical reduction in the frequency domain (using the Principal Component Analysis) is applied. Finally, a robust optimization problem is performed to find the operational parameters of the system that maximize its performance, respecting the integrity limits of the system, such as fatigue and torsional instability. Four papers have been published from this PhD thesis [1-4].

It should be remarked the author, now Associate professor at Universidade Federal Fluminense (Brazil), has published till now a total of 10 Journal papers and 25 conference papers. In addition, this PhD thesis has won the CSMA prize (http://csma.fr, France) and the ABCM-EMBRAER prize (http://www.abcm.org.br/premios/7-4.shtml, Brazil).

REFERENCES

GEOMETRIC MULTIGRID METHODS ON SEMI-STRUCTURED TRIANGULAR GRIDS

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Keywords: Multigrid Methods, Local Fourier Analysis, Finite Element Methods, Triangular grids, Semi-Structured Grids, Computational Mechanics.

ABSTRACT

Finite element methods are one of the most popular techniques for solving numerically elliptic partial differential equations (PDEs), because of their flexibility to handle unstructured meshes. However, the large sparse algebraic linear systems arising from the discretization of PDEs by this kind of methods require an efficient resolution. By other hand, geometric multigrid algorithms are among the most efficient methods for solving large algebraic systems of such type, with optimal computational complexity, taking advantage of the regularity of structured meshes. Thus, our interest lies in the combination of these techniques by using semi-structured grids which offer a suitable framework for the application of both. This type of meshes combine the flexibility of a totally unstructured input grid to capture the geometry of the domain, with the advantages obtained from the structured patches arising from the regular refinement of the initial triangular elements, where the stencil-wise implementation of a geometric multigrid method can be done very efficiently. Besides, in this framework, it is exploited the regularity of the grids in such a way that it is not necessary to assemble the global discretization matrix for problems with constant coefficients, and therefore the multigrid method can be implemented by using stencil-based operations, drastically reducing the memory required.

Moreover, since the good performance of the method depends on the particular choice of the components of the algorithm for an individual problem, the local Fourier analysis (LFA) is often used to predict the convergence rates of the multigrid method, and thus to design suitable components. In particular, LFA on triangular grids, see [1], is used in the framework of semi-structured grids, being applied to each triangular block of the initial unstructured grid to choose suitable local components giving rise to a block-wise multigrid algorithm which becomes a very efficient solver, see [2,3]. This strategy is here developed for problems of practical relevance in the context of computational solid mechanics, as for example the elasticity problem and the Biot’s consolidation model.

REFERENCES


NONLINEAR MULTIRESOLUTION ALGORITHMS AND VARIATIONAL PROBLEMS FOR IMAGE DENOISING

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Keywords: Multiresolution algorithms, nonlinear schemes, filtered methods, denoising, cell-average discretization.

ABSTRACT

The design of fast multiresolution algorithms for image denoising problems is deeply connected with three important aspects. The first one is the specific multiresolution chosen, the second one is the filter, that must be appropriate and the third one is the choice of the thresholding parameter. We will start our work from the classical solution, i.e., linear wavelet algorithms plus Donoho and Johnstone’s Soft-thresholding with the universal shrinkage parameter, and we will try to improve the classical results in the three mentioned aspects. To do so, a new nonlinear approach will be proposed and analyzed. This analysis will be based on the fact that the linear approach proposed by Donoho and Johnstone is based upon a well known variational problem. Starting from this point we will propose a different but related variational problem for the new approach, that will be more adapted to the denoising problem. It is important to mention that the theoretical analysis of a nonlinear setting is usually much more difficult than its linear counterpart. In order to test the performance of the new algorithm proposed, comparisons with other state of the art approaches will be done.
LAGRANGIAN FE METHODS FOR COUPLED PROBLEMS IN FLUID MECHANICS

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Keywords: fluid-structure interaction, PFEM, mesh-free methods, CFD, monolithic FSI, coupled problems

ABSTRACT

Lagrangian finite element methods emerged in fluid dynamics when the deficiencies of the Eulerian methods in treating free surface flows were faced. Their advantage relies upon natural tracking of boundaries and interfaces, a feature particularly important for interaction problems. Additionally, the absence of the convective term in the fluid momentum equations written in the Lagrangian framework leads to a symmetric discrete system matrix, an important feature in case iterative solvers are utilized.

This work aims at developing formulations and algorithms where maximum advantage of using Lagrangian finite element fluid formulations can be taken. We concentrate our attention at fluid-structure interaction and thermally coupled applications, most of which originate from practical "real-life" problems. Two fundamental options are investigated - coupling two Lagrangian formulations (e.g. Lagrangian fluid and Lagrangian structure) and coupling the Lagrangian and Eulerian fluid formulations. This work is restricted to the Lagrangian finite element methods based on classical FE shape functions and adopts the Particle Finite Element Method (PFEM) philosophy.

In the first part of this work the basic concepts of the PFEM Lagrangian fluids concept are presented. These include nodal variable storage, mesh re-construction using Delaunay triangulation/tetrahedralization and alpha shape-based method for identification of the computational domain boundaries. This serves as a general basis for all the further developments of this work.

Next we show how an incompressible Lagrangian fluid can be used in a partitioned fluid-structure interaction context. We present a strategy for coupling the incompressible Lagrangian fluid with a rigid body.

In the following, an extension of the method is proposed to allow dealing with fluid-structure problems involving general flexible structures. The method developed takes advantage of the symmetry of the discrete system matrix and by introducing a slight fluid compressibility allows to treat the fluid-structure interaction problem efficiently in a monolithic way. Thus, maximal benefit from using a similar description for both the fluid (updated Lagrangian) and the solid (total Lagrangian) is taken. We show next that the developed monolithic approach is particularly useful for modeling the interaction with light-weight structures.

The second part of this work aims at coupling Lagrangian and Eulerian fluid formulations. The application area is the modeling of polymers under fire conditions. This kind of problem consists of modeling the two subsystems (namely the polymer and the surrounding air) and their thermo-mechanical interaction. A compressible fluid formulation based on the Eulerian description is used for modeling the air, whereas a Lagrangian description is used for the polymer. For the surrounding air we develop a model based upon the compressible Navier-Stokes equations. Such choice is dictated by the presence of high temperature gradients in the problem of interest, which precludes the utilization of the Boussinesq approximation. The mechanical interaction of the subsystems is modeled by means of a one-way coupling, where the polymer velocities are imposed on the interface elements of the Eulerian mesh in a weak way. Thermal interaction is treated by means of the energy equation solved on the Eulerian mesh, containing thermal properties of both the subsystems, namely air and polymer.

Each part of the work concludes with an example section that includes both the validation tests and/or applications to the real-life problems. The future lines of research that naturally evolve from the results of this work are also highlighted.
REDUCED INTEGRATION FINITE ELEMENT TECHNOLOGIES WITH APPLICATON TO SHEET METAL FORMING

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Keywords: solid-shell, reduced integration, large deformations, sheet metal forming

ABSTRACT

In the last decades finite element simulations of sheet metal forming processes often have been carried out by means of shell elements including the assumption of a plane stress state. Such formulations reach its limit if fully three-dimensional material models are required to take the structural behavior precisely into account. In this context so-called solid-shell finite elements represent a competitive alternative. These elements are usually based on classical continuum finite elements, but they include kinematic concepts which allow the use of only one element over the sheet thickness. Due to their three-dimensional nature the implementation of arbitrary three-dimensional material models can be easily accomplished.

The present contribution deals with the derivation and application of a new eight-node solid-shell finite element based on reduced integration with hourglass stabilization. In order to overcome artificial stiffening effects (called locking), the derivation of the element requires the implementation of techniques of the finite element technology. The present solid-shell element is based on the enhanced assumed strain (EAS) method and the assumed natural strain (ANS) method. The implementation of the latter represents a new aspect in the development of reduced integration solid-shell finite elements. It has been achieved by means of a consequent application of a concept of Taylor series.

The proposed element is studied in many tests of finite element technology. Starting in [1] with verifications in geometrically linear applications the element fulfills both the membrane and the bending patch test exactly. To the author’s knowledge the exact fulfillment of the bending patch test is not yet documented in literature for a reduced integration eight-node solid-shell element. The element’s large deformation counterpart obtains very good agreements with reference solutions in a range of very thin to very thick shell problems. It shows high robustness against mesh distortions and obtains also in problems under strong plastification results of high quality.

The application of the new solid-shell formulation in sheet metal forming processes is a main objective of the present work. Numerical results are validated using experimental measurements. The well-known s-rail problem is a typical benchmark problem for deep drawing simulations. The computed punch forces and final geometries of the workpieces are in excellent agreement with experiments. Furthermore the solid-shell element has been successfully applied in springback simulations. In draw-bending tests the springback after unloading has been predicted with high precision. Moreover in [2] it is shown that the proposed solid-shell finite element has the potential to analyze the earing deformation pattern of anisotropic sheet metals.

REFERENCES

ASSESSMENT OF THE DISPERSION ERROR AND GOAL-ORIENTED ADAPTIVITY FOR WAVE PROBLEMS

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Keywords: Wave Problems, Helmholtz Equation, Error Estimation of Wave Number, Dispersion/Pollution Error, Goal-oriented Adaptivity, Local Indicators, Finite Element Method, Stabilized Method

ABSTRACT

This work presents an a posteriori estimator for the error in the wave number in the context of finite element approximations of the Helmholtz equation, both for standard and stabilized formulations. We also introduce a new goal-oriented adaptive strategy using post-processing techniques.

The simple strategy assessing the error in the wave number is based on the determination of the numerical wave number that better accommodates the numerical solution. Compared to other goal-oriented error estimation strategies, the approach proposed in this work is innovative because it adopts a new paradigm.

A distinctive feature of this method is that the error estimation procedure is devoted to obtain the numerical wave number, corresponding to the approximate solution, instead of the exact one, which is known as part of the data of the problem. Thus, the error in the wave number is consistently defined as the outcome of a global minimization problem. This problem is computationally unaffordable and, for practical error estimation purposes, is approximated. An enhanced approximation is obtained from the finite element solution using a simple local least-squares technique. Once the enhanced solution is obtained, the associated numerical wave number is readily recovered using a simple closed expression. An alternative improved recovery technique is developed to take advantage of the nature of the solutions of wave problems. The standard polynomial least-squares technique is replaced by a new exponential fitting, yielding much sharper results in most cases.

The proposed new goal-oriented adaptive strategy is based on post-processed solutions and is valid both for linear and non-linear quantities of interest. In the non-linear case the linear contribution to the quantity of interest is assumed to be the leading term. Two different representations to recover the error in the quantity of interest are studied, both providing similar results in the adaptive procedures. It has been shown that the accuracy of these representations, which involve the post-processing of either the primal or adjoint finite element approximations, is related to the dispersion error of its corresponding problems. Moreover, the adaptive procedure leads to a faster reduction of the error when compared with a uniform refinement. The proposed error estimate properly identifies the areas most contributing to the error in the quantity of interest and consequently the adaptive procedure yields adapted meshes that provide accurate results.
COMPUTATIONAL MODELING OF FAILURE IN COMPOSITE LAMINATES

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Keywords: Composite laminates, progressive failure, X-FEM, continuum damage, cohesive zone.

ABSTRACT

Composite laminates are increasingly popular as engineering materials because of their favorable stiffness-to-weight and strength-to-weight ratios. However, predictive simulation of failure in laminates is a challenging task, because different processes may play a role, such as matrix cracking, delamination and fiber failure. For reliable simulations, all relevant processes and their interaction must be represented realistically in a single framework. In this thesis, an effort has been made to build such a framework.

It is shown that a continuum approach, even if it distinguishes between matrix failure and fiber failure, is inadequate for the simulation of some failure mechanisms, particularly those where interaction between matrix cracking and delamination is important. In this observation the motivation is found to model matrix cracks as real discontinuities in the displacement field with the eXtended Finite Element Methods (X-FEM). The fiber direction is used to determine the direction of crack propagation. This gives rise to mixed mode failure, for which two new cohesive laws are developed.

The model for matrix failure is combined with interface elements for delamination, a continuum damage model for fiber failure and a damage/plasticity model for shear nonlinearity. All components give results that are objective with respect to element size. Analyses are performed in an implicit quasi-static solution scheme. Together with the interaction between the different nonlinear processes that are occurring, the brittle nature of laminates renders it difficult to find convergence and follow the equilibrium path. Therefore, much attention is paid to the robustness of the solution algorithm with an appropriate arc-length method and adaptive time-stepping. Furthermore, efficiency of the algorithm with respect to growth of numerous cracks is highlighted.

The framework is validated against different experiments. Measured size effects, which are understood to be related to the specific interaction between the different failure processes, are reproduced well.

Figure 1. Failure in a notched laminate with matrix cracking and delamination. Discrete matrix cracks follow the $45^\circ$ fiber direction and cause stress concentrations that trigger interface failure.
TREFFTZ-BASED MID-FREQUENCY ANALYSIS OF GEOMETRICALLY COMPLEX VIBRO-ACOUSTIC SYSTEMS - HYBRID METHODOLOGIES AND MULTI-LEVEL MODELLING

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Keywords: mid-frequency vibro-acoustic analysis, Wave Based Method, hybrid coupling, multiple scattering.

ABSTRACT

Numerical modelling techniques have become an indispensable part of many product design processes. In the context of optimising the design of mechanical systems, the acoustical and vibrational comfort of a product has taken up a predominant place among more traditional design criteria such as strength, durability and maintainability. Unfortunately, none of the virtual prototypes constructed using the most commonly applied vibro-acoustic simulation techniques are capable of adequately capturing this behaviour in the mid-frequency range. At these frequencies, the deterministic element-based approaches lead to unrealistically dense problem discretisations and unfeasibly long calculation times, while the basic assumptions required for adopting a statistical energy-based description are not yet fully met.

This dissertation fits in the development of an alternative Trefftz-based deterministic modelling approach which specifically aims at accurately capturing the low- and mid-frequency vibro-acoustic behaviour of complex mechanical systems at an affordable computational cost. Through the use of a set of wave-like basis functions for the approximation of the dynamic response variables, this so-called Wave Based Method provides a flexible way of analysing problems at higher frequencies. Unfortunately, as a direct result of the use of these functions, the efficiency of this approach can only be fully exploited for problems of moderate geometrical complexity. This dissertation presents two extensions to the Wave Based Method which allow this methodology to cope with two of the most limiting types of commonly encountered geometrical features. The limitations imposed by the presence of superficial geometrical details are overcome by extending the existing family of hybrid Finite Element-Wave Based approaches to fully coupled vibro-acoustic problems and by further improving this method's efficiency through the use of Finite Element model reduction techniques [1-2]. In a parallel research line, the introduction of an innovative Multi-Level modelling framework allows the Wave Based Method to successfully and flexibly model multiple scattering and inclusion problems [3-4].

REFERENCES

A MODEL FOR 3D FRACTURE USING A MESHLESS METHOD AND LEVEL SETS AND ITS APPLICATION IN GEOMECHANICS

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Keywords: 3D fracture modelling, level sets, meshless methods, partition of unity, rock slope stability.

ABSTRACT

The spatial distribution and evolution of fractures in a rock stratum control the heat flow, fluid flow and the overall stability. From an engineering perspective, understanding the 3D mechanical behavior of a fracture network is of prime importance for rock slope stability in hydropower station construction, deep oil exploration, waste reservoirs and exploitation of geothermal power. In these areas, accurate analysis of the fracture network is of vital importance yet methods for effective 3D calculations are currently unsatisfactory. A numerical framework is described here for 3D fracture modelling where a meshless method is used for stress analysis, and level sets are used to describe and capture the crack evolution. In this paper the level set method is coupled with the element-free Galerkin method (EFGM). The developed method is now being applied to slope stability analysis, especially for rock slope stability governed by a number of dominating discontinuities where joints are modeled as embedded elliptic or penny shaped cracks. Level set functions are utilized to refine the nodal arrangement, perform partition of unity based integration and reduce the computational cost of including the displacement jump across a crack. Results are presented showing the performance of the proposed method. Remaining issues to be addressed in further studies are discussed, namely, the use of level sets for intersecting joints in 3D and the construction of meshless approximations for cohesive zones ahead of a joint front.

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