CMM-SolMech 2022 conference

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APPLICATION OF LAYOUT OPTIMIZATION METHODS IN ENGINEERING ANALYSIS AND DESIGN

Matthew Gilbert[1]

[1]Civil and Structural Engineering, University of Sheffield, United Kingdom

m.gilbert@sheffield.ac.uk

To verify the safety of solid bodies and structures against collapse, engineers have traditionally had to rely either on simplistic hand type calculations, or on significantly more complex computational tools which identify the collapse state in an indirect, iterative, manner - which can be costly in terms of computer and/or operator time. Additionally, in many engineering disciplines the initial design stage is carried out in an ad-hoc manner, with engineering intuition often used to identify structurally efficient designs. Direct analysis and design methods can potentially address both these issues, and similarities between analysis and design formulations can also potentially be exploited. Here the so-called 'layout optimization' technique is described, and then applied to truss and grillage design problems and to engineering analysis problems involving identification of the critical layout of discontinuities in solid bodies at the point of collapse. In each case mathematical programming tech- niques can be used to obtain solutions and it is observed that highly accurate solutions can be obtained rapidly, permitting new insights to be drawn in a range of application areas. Future directions in the field of layout optimization will then be briefly considered.

MICROSTRUCTURE OF FERROELECTRIC CERAMICS: SIMULATION MEETS EXPERIMENT

Dennis M. Kochmann[1]

[1]Mechanics & Materials Lab, Dept. of Mechanical and Process Engineering, ETH Zürich, Switzerland

dmk@ethz.ch

Ferroelectric ceramics are the enabling factor for most actuator and sensor technologies, owing to their piezo electric effect and its nonlinear extension, the ferroelectric effect. These materials convert electrical voltages into mechanical deformation and, conversely, mechanical strains into electrical voltage - at small amplitudes the relation between those fields is relatively simple and the mechanisms are reversible. At sufficiently large applied electric fields or mechanical stresses, a complex reorganization of the atomic-scale dipole structure results in irreversible ferroelectric switching, a process that is sensitive to loading rate and temperature. Moreover, ferroelectric ceramics possess the aforementioned properties only below their Curie temperature, above which they become unpolar through a phase transformation.

Modeling the electro-thermo-mechanically-coupled behavior of ferroelectric ceramics is a challenge that extends across length and time scales: from atomic-level dipoles and thermal vibrations up to mesoscale polycrystals and, ultimately, macroscale devices. We combine information from several scales ('thermalizing' DFT-informed potentials in a phase-field setting that accounts for the influence of thermal fluctuations and uses FFT-based solvers for high resolution) with the aim to predict the effective material response and the underlying microstructural evolution. When applied to barium titanate ($BaTiO_3$) and lead zirconate titanate (PZT), the model predicts realistic microstructural domain patterns and highlights the micro-mechanical response to applied electric bias fields across a wide range of temperature. Combined with in-house experiments that probe the electro-mechanical response of ferroelectric ceramics under carefully selected loading scenarios, we gain insight into the underlying microstructural mechanisms governing the macroscale response, we discuss the importance of the kinetic assumptions that enter the phase-field model, and we outline a new phase-field formulation that may provide the much needed flexibility in realizing general kinetic relations.

SENSITIVITY ANALYSIS BASED COMPUTATIONAL MODELING

Jože Korelc[1]

[1]University of Ljubljana, Slovenia

joze.korelc@fgg.uni-lj.si

Sensitivity analysis has become an indispensable part of modern computational algorithms. Nowadays, the automation of sensitivity analysis enables efficient evaluation of sensitivities that are exact except for the round of errors. For that purpose, the use of automatic differentiation tools and techniques gained much popularity and attention in recent years. However, big differences in the numerical efficiency of the resulting simulation codes between various implementations (dual number approach, code-to-code transformation approach, forward or direct approach, backward or adjoint approach, etc.) have been revealed. The background of those differences is explained as well as the limitations of various approaches. We propose a hybrid symbolic-automatic differentiation approach with code-to-code transformation and simultaneous stochastic expression optimization implemented in AceGen (www.fgg.uni-lj.si/symech/) as one of the most efficient approaches. Yet, the true advantages of automation become apparent only if the description of the problem, the notation, and the mathematical apparatus used is changed as well. It will be shown that the unification of the classical mathematical notation of computational models and the actual computer implementation can be achieved through an extended automatic differentiation technique combined with automatic code generation and sensitivity analysis. The automatic differentiation-based form (ADB form) of a classical mathematical notation of solid and contact mechanics, multi-scale analysis, stochastic analysis, optimization, and stability analysis will be presented. While the first order sensitivity analysis is already an established tool for the improvement of numerical algorithms, (e.g., optimization) is the second order sensitivity analysis still rarely used. This is mainly due to the high numerical cost, especially in the case of time-dependent problems. The benefits and drawbacks of the second-order forward and backward sensitivity approach when applied to multi-scale modeling and stochastic analysis will be compared. The talk introduces a fully consistently linearized two-level path-following algorithm as a solution algorithm for strongly nonlinear multi-scale problems. The approach also increases the concurrency of micro problems which can significantly improve the overall speed of the execution in multi-processor and multi-core systems.

EUCLID: EFFICIENT UNSUPERVISED CONSTITUTIVE LAW IDENTIFICATION AND DISCOVERY

Laura De Lorenzis[1]

[1]Computational Mechanics Lab, ETH Zürich, Switzerland

ldelorenzis@ethz.ch

We propose a new approach for data-driven automated discovery of constitutive laws in continuum mechanics. The approach is unsupervised, i.e., it requires no stress data but only displacement and global force data, which can be realistically obtained from mechanical testing and digital image or volume correlation techniques; it can deliver either interpretable models, i.e., models that are embodied by parsimonious mathematical expressions, or black-box models encoded in artificial neural networks; it is one-shot, i.e., discovery only needs one experiment - but can use more if available. The machine learning tools enabling discovery are sparse regression from a large model space, as well as Bayesian regression, which allows for the discovery of several constitutive laws along with their probabilities. After discussing the methodology, the talk illustrates its applications to hyperelasticity, plasticity and viscoelasticity, using both artificial and experimental data.

OVERALL MICROSTRUCTURE RESPONSE FUNCTION AND ITS APPLICATION TO RECOVERY OF MICROSTRUCTURE

Dariusz Łydżba[1]

[1]Wrocław University of Science and Technology, Poland

dariusz.lydzba@pwr.edu.pl

The aim of the homogenization is up-scaling of mathematical description of the process under consideration, from the scale of heterogeneities to the scale of engineering applications. For the linear problems, the micro- and the macro- descriptions are analogous in the mathematical form, except material properties involved in both descriptions. The material properties of the micro-description are space dependent whereas that of the macro-description, called as overall ones, are constant since they characterize macroscopically homogeneous medium.

Two mathematical problems are called inverse to each other if the formulation of the first problem contains the solution of the second problem and vice versa. The evaluation of overall properties in terms of the phase properties and the microstructure morphology can therefore be interpreted as the direct problem of homogenization since it consists of projections from the known microstructure morphology. The recovery of the microstructure morphology using values of the overall material constants is therefore the inverse problem of homogenization. The inverse problem, in general, has no unique solution. In order to ensure the existence and uniqueness of the solution the problem has to be supplemented by a definite set of appropriately chosen overall material constants values as well as one has to postulate the particulate type of microstructure morphology. The set of overall material constants values may also be considered as a projection of material constants of composite components onto the space of admissible values of overall material constant; it can be also interpreted as a macroscopic manifestation of the medium microstructure and is hereinafter referred to as the overall microstructure response function.

Two type of microstructure morphology are postulated to solve the inverse problem, i.e. randomly oriented spheroidal inhomogeneities of certain distribution of the aspect ratios embedded in the matrix and a binary mixture. In this context the recovered microstructure has to be interpreted as an equivalent or replacement one since it does reproduce the overall microstructure response function but not necessary the original microstructure morphology.

For the microstructure morphology of randomly oriented spheroidal inhomogeneities, the inverse problem is formulated as a linear Fredholm equation or the system of linear Fredholm equations of the first kind, depending on the problem studied, i.e. heat conduction or elasticity problem, respectively. For a binary representation of 'replacement' microstructure, being a two-phase statistically isotropic medium, the computational micromechanics framework is used. The latter represents any microstructure morphology that can be obtained using the representation of a two-dimensional digital image composed of n x n pixels. For this case the considerations are limited to the problem of heat conduction in a two-phase medium. Simulated annealing algorithm is used to solve the inverse problem. The correctness and effectiveness of the methodology proposed is illustrated by a sequence of numerical examples.

ON-CHIP FRACTURE MECHANICS TO EXPLORE FRACTURE TOUGHNESS OF FREESTANDING ULTRA-THIN FILMS FROM BRITTLE TO DUCTILE, DOWN TO 2D MATERIALS

Thomas Pardoen[1], Sahar Jaddi[1], Malik M. Wasil[2], Bin Wang[2,3], Michael Coulombier[1], Jean-Pierre Raskin[2]

[1]Institute of Mechanics, Materials and Civil Engineering, UCLouvain, Belgium
[2]Institute of Information and Communication Technologies, Electronics and Applied Mathematics, UCLouvain, Belgium
[3]School of Physics and Electronics, Hunan University, China

thomas.pardoen@uclouvain.be

The characterization, control, and enhancement of the cracking resistance of thin films and 2D materials are major concerns for the development of fail safe flexible electronics, MEMS/NEMS devices, and structural or functional coatings. In particular, environmentally-assisted cracking phenomena affect the reliability of many thin films/2D materials-based systems. Existing approaches mostly address the cracking of films while resting on a substrate, which simplifies the testing but makes the extraction of 'intrinsic' properties more difficult often requiring advanced non-linear models. The most attractive approach is thus to work with freestanding films, but the challenges are numerous due to the small sizes.

In this context, we developed a new on-chip technique to extract the static fracture toughness and to study environmentally-assisted crack growth in freestanding thin films, 2D materials, as well as thin multilayers. The method relies on a residual-stress-based-on-chip concept taking advantage of MEMS-based fabrication principles [1]. The working principles rely on internal stress actuation and on a crack arrest measurements to avoid the problem of pre-cracking. A data reduction scheme based on finite element simulations of the test structures is used to determine the fracture toughness. The method also provides the variation of the crack growth rate as a function of the stress intensity factor under different temperature conditions and humidity levels.

Several materials were tested over the last few years varying from nominally brittle like SiN, SiO2, Al2O3 to ductile such as Cu, Ni and Al/Al2O3 multilayers, revealing several interesting effects that will be presented, e.g. [1,2]. 2D materials like graphene (Gr) and hexagonal boron nitride (h-BN) were also successfully studied providing probably the first rigorous fracture mechanics statistically representative data on these materials.

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APPLICATION OF A COUPLED DEM-CFD APPROACH TO ENGINEERING PROBLEMS

Jacek Tejchman[1]

[1]Gdańsk University of Technology, Poland

jacek.tejchman@pg.edu.pl

The paper deals with the application of a fully coupled DEM/CFD approach (discrete element method combined with computational fluid dynamics) for investigating some different combined mechanical-hydraulic-thermal problems at the meso-scale in frictional-cohesive materials (rocks, granulates and concrete). As compared with usual continuum mechanics methodologies in most existing numerical studies, discontinuous meso-scale models at the grain level (such as the discrete element method (DEM)) are more realistic since they allow for a direct simulation of meso-structure and are thus useful for studies the mechanism of the initiation, growth and formation of cracks and shear zones at the meso-level. DEM allows for a better understanding of local meso-structural phenomena that evidently affect global material behaviour [1]. We used DEM which takes advantage of the so-called soft-particle approach [1-3]. A linear contact under compression was assumed. Normal and tangential contact forces satisfied the cohesive-frictional Mohr-Coulomb condition. CFD was used to describe the laminar viscous two-phase liquid/gas flow in pores between discrete elements by employing channels.

Innovative elements of our approach with respect to other existing DEM/CFD models in the literature are the following [2,3]: 1) co-existence of two domains (a discrete and continuous one) in one physical system (the sum of domain geometries creates a complete physical system), 2) precise determination of the geometry and topology change of voids and fractures, 3) remeshing method of voids and fractures, 4) transformation schema of computation results from the old grid (before remeshing) to the new grid (after remeshing) and 5) detailed tracking of the fluid volume fraction in voids and fractures (material voids can be fully or partially filled with the fluid). Every single pore is discretized by a number of elements. Thus, the pressure field in a single pore is spatially variable while in existing DEM/CFD models, the pressure field in a single pore is constant. The flow path may be reproduced in a single pore in contrast to existing DEM/CFD models. In addition, huge pressure gradients in a single pore are captured while in existing DEM/CFD models the pressure gradient in a single pore is equal to zero. Two phases were considered in fluid flow: liquid phase and gas phase. Some engineering coupled DEM/CFD problems were discussed such as e.g. hydraulic fracturing in rocks [2-4] and capillary pressure-driven water flow in concretes [5].

References

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MODELING AND SIMULATION TOOLS FOR INDUSTRIAL AND SOCIETAL RESEARCH APPLICATIONS: DIGITAL TWINS AND GENOME-BASED MACHINE-LEARNING

Tarek Zohdi[1]

[1]University of California, Berkeley, USA

zohdi@berkeley.edu

A variety of seemingly disparate physical processes can be treated with similar modeling and simulations tools. In this talk, I discuss the modeling and rapid digital-twin simulation of. The outline of this presentation is:
Part 1: modeling of robotic machine-learning for advanced manufacturing
Part 2: modeling of laser and optical processing of materials
Part 3: modeling of multiphysical solid processing and continuum behavior
Part 4: modeling of ignition, fire propagation and ember flow
Part 5: modeling of multiple unmanned aerial vehicles for complex tasks
Part 6: modeling of industrial safety: pandemics, transmission, decontamination,
as well as aspects of genomic/evolutionary computing for system optimization, utilizing multiphysics paradigms. The tools range from discrete element methods, computational optics, voxel-based computation to agent-based modeling-all connected together via machine-learning algorithms. For more information see https://cmmrl.berkeley.edu/zohdi-publications/ and http://www.me.berkeley.edu/people/faculty/tarek-i-zohdi.