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Computational Science

"Understanding and Solving Multiphysics Problems for Industry and Society with Large Scale Simulation"

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Computational Mechanics and Multi-Physics of Materials and Structures

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In 2004, the name of the former Institute for Strength of Materials of Vienna University of Technology was changed to Mechanics of Materials and Structures, accounting for the change of paradigms in this traditional engineering discipline. This change involves enhanced consideration of problems which require coupling of mechanics with other branches of physics and beyond, referred to as "multi-physics problems", and of macroscopic material laws based on information from smaller scales, i.e. on so-called "multi-scale formulations".

After a brief description of the historical development of the Institute for Mechanics of Materials and Structures, pertinent research activities will be reported. The following topics will be touched:

- Nano-to-macro mechanics of biological materials (bone, wood, skin)
- Nano-to-macro chemomechanics of early-age concrete / shotcrete / jet-grouted soil
- Concrete subjected to high temperatures
- Performance-based optimization of asphalt
- Soil mechanics
- Frictional behavior of rubber tread patterns
- Numerical prognosis of extrusion process of rubber
- Computational investigation of structural stability
- Biomechanics of human skins

Multi-scale mechanics of biological materials exhibits common principles of micromechanical design. Despite the complex hierarchical organization and the astonishing variety of these materials, elementary components can be identified for each class. Macroscopic material properties are determined by mechanical properties of elementary components, their dosages, and their mechanical interactions.

Chemomechanics of early-age concrete is an example for a multi-physics approach, accounting for thermo-chemo-mechanical couplings. Multi-scale modelling of this material is based on continuum micromechanics. The experiments include macroscopic and low-scale characterizations.

The theory of concrete subjected to high temperatures involves consideration of coupled transport processes in heated concrete and nano-to-macro up-scaling of transport properties of different temperatures.

An Evolutionary Robust Design Method for the Wing Drag Reduction with Variable Operating Flight Condition Parameters.

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Abstract :
In Aerospace engineering there are many applications where some values of the design parameters cannot be provided accurately. These values are related either to the geometry (wingspan, length, angles) or to operational flight conditions that vary due to the presence of fluctuations (Mach, angle of attack, air density and temperature, etc....). In this case an alternative strategy is to estimate the variability of input parameters by the mean and variancevalues of the objective function associated to the design optimisation procedure.

In this frequent aerodynamic situation the use of the well known Taguchi methods aims to look for design solution with better performance and stability simultaneously within a certain interval where input parameters can randomly vary.

In this lecture, a Taguchi robust optimisation concept is implemented with Hierarchical Asynchronous Parallel Evolutionary Algorithms (HAPEA) to solve numerically wing drag reduction problems with uncertainties and compared to a traditional single point optimization approach .

It is shown how the approach can provide robust solutions using game theory in the sense that they are less sensitive to little changes of input parameters. Starting from a statistical definition of stability, the method captures, simultaneously Pareto non-dominated solutions with respect to performance and stability criteria, offering alternative choices to the designer.

It is concluded from the preliminary obtained results that a general design framework integrating evolutionary algorithm procedures coupled to a robust optimisation technique can be used advantageously when some of the design parameters, such as operating conditions fluctuate within specified design intervals and that uncertainties in the design have a non-linear effect on the objective functions.

CHALLENGES AND SOLUTIONS FOR SIMULATION-ASSISTED ENGINEERING

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Abstract

Modelling and simulation has been a promising engineering aid for decades, gaining gradually popularity in industry. However, there are still some major problems to overcome before simulation break through can really happen. Such challenges include:
- Seamless support for simulation in different levels of details i.e. conceptual level simulation at the beginning of the product life cycle, more detailed simulation in later phases and seamless moving between these levels.
- There should exist a way for software component based simulation i.e. model algorithms can be developed, added, removed and changed run time as part of the larger scale model.
- Support for multi-domain and multi-physics simulation.
- Model configuration has to be neutral i.e. it should not be simulation tool specific.
- Need for distributed simulation model configuration and usage including version and access control.
- Simulation data visualization using suitable modern methods of computer graphics (2-D, 3-D, augmented reality) should be common for different models and different levels of details. This way results from these models can be visualized in a common and intuitive way.
- There should be better links from simulators to different engineering applications. Only this way simulation can find its way to the everyday engineering.
- Support for validation and verification of simulation models should be a built-in feature in a modelling and simulation framework.
- There should be general, unified model composing and modification tools for different background tools.
- There should exist high level component modelling, meshing, model topology editing, simulation management and runtime adaptive tools.
- The simulation system should provide seamless exchange of model and simulation results data between different modules in the simulation process.

In the expected presentation we will describe how many of these challenges have been and are addressed at VTT. Examples include
- Ontology-based semantic modelling to implement better interconnectivity
- Simulation and digital product processes
- Simulation-assisted testing, verification, and validation of automation applications in process plants
- Multi-disciplinary simulation and middleware-technologies

Direct and inverse modelling in environmental sciences

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The evolution of natural systems, in the short, mid, or long term, has extremely important consequences for both the global earth system and humanity. Forecasting this evolution is thus a major challenge from the scientific, economic, and human standpoints.

Mathematical and numerical tools are omnipresent and play a fundamental role in these fields of research. As a matter of fact, designing a forecasting system in geophysics require several complex ingredients :
- Models : they allow a global view of the dynamics, consistent in time and space on a wide spectrum of scales. They are based on complex equations, are often strongly nonlinear, deal with the irregular shape of domains, and include a number of specific parameterizations. Moreover, it is often necessary to couple different models.
- Observations : since models are characterised by an imperfect physics and some poorly known parameters (e.g. initial and boundary conditions), it is important to also have observations of natural systems. Such observations are now increasingly numerous due, in particular, to satellite techniques. However, they provide only a partial view of reality, localised in time and space, and their accuracy is not always satisfactory.
- Data assimilation techniques : Since models and observations taken separately do not allow for a deterministic reconstruction of real geophysical flows, it is necessary to use these heterogeneous but complementary sources of information simultaneously, by using data assimilation methods. These tools for inverse modelling are based on the mathematical theories of optimal control and stochastic filtering. Their aim is to identify system parameters which are poorly known in order to correct, in an optimal manner, the model trajectory, bringing it as close as possible to the available observations.

Moreover, given the size of the applications, challenging scientific computing issues have to be addressed.

Several examples linked to the design of such forecasting systems for geophysical phenomena will be given in this talk, with an emphasis on some generic mathematical and computational tools.

Solving multiphysical problems with Elmer finite element software

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Multiphysical problems arise when two or more different physical phenomena are coupled with one another. The solution of multiphysical problems is not necessarily particularly difficult -- in many fields it has been done long before the concept even existed. The difficulty depends very much on the nature of coupling. In this paper we go through some different solution strategies for multiphysical problems. We also show number of examples computed with the Elmer finite element software [1]. Elmer is on Open Source finite element software package particularly targeted for coupled problems.

When the coupling is weak at least in one direction the solution may easily be found by a iterative procedure where the relevant equations are solved one after the other until convergence is reached. This iteration approach is also the one that we usually use in the Elmer software
For strongly coupled problems the iteration method may not converge or does it very slowly. For such cases the ideal solution strategy may be to treat the system as one large problem. In terms of finite element method this means that all degrees of freedom are solved from the same matrix equation. Unfortunately this monolithic approach is often very laborious to code and difficult to verify. Also the matrix structure may become such that efficient linear algebra solvers may be difficult to find. However, when the coupling is inherently strong the monolithic has sometimes been the method of choice [2].

Sometimes there is also a third alternative that combines the good convergence properties of the monolithic method with the easy implementation of the iteration method. Often this involves the modification of the original set of equation in a consistent manner. We have, for example, applied this approach to the simulation of fluid-structure interaction in human arteries [3], and to the simulation of the electro-mechanical pull-in phenomenon [4]. If such a hybrid method exists it often provides the best alternative for solving the coupled problems.

References

[1] http://www.csc.fi/elmer, Elmer finite element software homepage
[2] Mika Malinen, Mikko Lyly, Peter Råback, Asta Kärkkäinen and Leo Kärkkäinen, A finite element method for the modeling of thermo-visoucs effects in acoustics. ECCOMAS 2004, Jyväskylä, Finland, 24-28 June 2004.
[3] Peter Råback and Antti Pursula, Finite element simulation of the electro-mechanical pull-in phenomenon. ECCOMAS 2004, Jyväskylä, Finland, 24-28 June 2004.
[4] Peter Råback, Juha Ruokolainen, Mikko Lyly, Esko Järvinen. Fluid-structure interaction boundary conditions by artificial compressibility. ECCOMAS CFD 2001, Swansea 4-7 September.

Realistic numerical modeling of electromagnetic wave propagation in head tissues using discontinuous Galerkin methods designed on unstructured tetrahedral meshes

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The ever-rising diffusion of mobile phones has determined an increased concern for possible consequences of electromagnetic (EM) radiation on human health.
As a matter of fact, when a cellular phone is in use, the transmitting antenna is placed very close to the user's head where a substantial part of the radiated power is absorbed. In the last decade, several research projects have been conducted in order to evaluate the possible biological effects resulting from human exposure to such an electromagnetic radiation.
In this context, it is widely accepted that a distinction must be made between thermal and non-thermal biological effects.
Thermal biological effects of microwave radiation have been investigated both from the experimental and numerical viewpoints. Concerning numerical modeling, the power absorption in a user head is generally computed using discretized models built from Magnetic Resonance images. The vast majority of such numerical studies have been conducted using the widely known Finite Difference Time Domain (FDTD) method due to Yee[Yee:1966] for solving the time domain Maxwell equations. In this method, the computational domain is discretized using a structured cartesian grid, which can be directly derived from the structure of MR images. Due to the possible straightforward implementation of the algorithm and the availability of computational power, the FDTD method is currently the leading method for numerical assessment of human exposure to electromagnetic waves [Bernardi-etal:2001][Gandhi-etal:2001].
However, limitations are still seen, due to the rather difficult departure from the commonly used rectilinear grid and cell size limitations regarding very detailed structures of head tissues as well as of a handset which might be essential for reliable compliance testing. So far, little attention has been pt to the application of numerical methods able to deal with nstructured rids, i.e. Finite Element, Finite Volume or Discontinuous Galerkin Time omain (respectively FETD, FVTD, DGTD) methods. This situation is essentially ue to the lack of reliable automated tools for the Unstructured iscretization of human heads.
Such tools have been recently developed at INRIA Sophia Antipolis n the ontext of a multi-disciplinary project involving specialists of medical mage rocessing and geometrical modeling. Starting from MR data, the head issues ave to be segmented. Each voxel of the cartesian representation of he MR mage is recognized as made (mainly) of a single material. After hving ecided the relevant number of different materials for the dosimetry analysis
(each material having its own electromagnetic characteristics), the different issues are segmented and the interfaces between tissues are meshed, sing riangle facets [Boissonnat-Oudot:2005]. Starting from the triangular urfacic eshes of the interfaces between different materials, tetrahedral
Volumic eshes of the tissues are generated using a tetrahedral mesh eneration tool George-etal:1991].

In this talk, we will discuss of our recent efforts aiming at the development f discontinuous Galerkin methods for the numerical simulation of lectromagnetic wave propagation in head tissues using nstructured etrahedral mesh based geometrical models. Discontinuous Galerkin methods [DG:2000] enjoy a renewed favor nowadays and are now used in a wide ariety of pplications as eople (re)discover the abilities of these methods to andle omplicated geometries, media and meshes, to achieve a high order of ccuracy y simply choosing suitable basis functions, and, last but not least, to emain highly parallelizable at the end. Our contributions are concerned with oth Discontinuous Galerkin Time Domain (DGTD) methods Fezoui-etal:2005]-[Bernacki-etal:2006] and Discontinuous Galerkin Time armonic (DGTH) methods [Dolean-etal:06].

[Bernacki-etal:2006]
M. Bernacki, L. Fezoui, S. Lanteri and S. Piperno.
Parallel Discontinuous Galerkin unstructured mesh solvers for the
calculation of three-dimensional wave propagation problems.
Appl. Math. Model., Vol. 30, No. 8, pp. 744-763, 2006.
[Bernardi-etal:2001]
P. Bernardi, M. Cavagnaro, S. Pisa and E. Piuzzi.
Power absorption and temperature elevations induced in the human head by
a dual-band monopole-helix antenna phone.
IEEE Trans Microwave Theory Tech, Vol. 49, No. 12, pp. 2539-2546
(2001).
[Boissonnat-Oudot:2005]
J.-D. Boissonnat and S. Oudot.
Provably good sampling and meshing of surfaces.
Graphical Models, Vol. 67, No. 5, pp. 405-451 (2005).
[DG:2000]
Discontinuous Galerkin methods. Theory, computation and applications.
Lecture Notes in Computational Science and Engineering, Vol. 11,
B. Cockburn and G.E. Karniadakis and C.W. Shu Eds., Springer-Verlag (2000).
[Dolean-etal:06]
V. Dolean and H. Fol and S. Lanteri and R. Perrussel.
Resolution of the time-harmonic Maxwell equations using discontinuous
Galerkin methods and domain decomposition algorithms.
20th International Congress on Computational and Applied Mathematics
(ICCAM06), Leuven, Belgium, July 10-14 (2006).
http://hal.archives-ouvertes.fr/hal-00106201
[Fezoui-etal:2005]
L. Fezoui, S. Lanteri, S. Lohrengel and S. Piperno.
Convergence and stability of a Discontinuous Galerkin time-domain method
for the 3D heterogeneous Maxwell equations on unstructured meshes.
ESAIM: Math. Model. and Numer. Anal., Vol. 39 No. 6, pp. 1149-1176 (2005).
[Gandhi-etal:2001]
O.M.P. Gandhi, Q.X. Li and G. Kang.
Temperature rise for the human head for
cellular telephones and for peak SARs prescribed in safety guidelines.
IEEE Trans Microwave Theory Tech, Vol. 49, No. 9, pp. 1607-1613 (2001).
[George-etal:1991].
P.-L. George, F. Hecht and E. Saltel.
Automatic mesh generator with specified boundary.
Comput. Methods Appl. Mech. Engrg., Vol. 92, pp. 269-288 (1991).
[Yee:1966]
K.S. Yee.
Numerical solution of initial boundary value problems
involving Maxwell's equations in isotropic media.
IEEE Trans. Ant. and Prop., AP-16, pp.302-307 (1966).

Experience in Parallel Computational Mechanics on MareNostrum

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We present in this paper our experience in solving very large problems of computational mechanics. The authors of the paper are researchers of the Barcelona Supercomputing Center-Centro Nacional de Supercomputación (BSC-CNS), a brand new research center in Spain, which hosts the fastest supercomputer in Europe and the fifth in the world: MareNostrum.

A brief presentation of MareNostrum is given in the first section. In the next section, we describe the physical problems we are faced with, followed by the section on the associated numerical strategies.

The following section presents the parallelization strategy employed; emphasis will be put on those ``new" problems that appear when running huge problems on a large number of processors.

Finally, in the last section we describe some applications together with performance results.

Simplifying numerical solution of constrained PDE systems through involutive completion

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When analysing general systems of PDEs, it is important first to find the involutive form of the initial system.
This is because the properties of the system cannot in general be determined if the system is not involutive.
We show that the notion of involutivity is also interesting from the numerical point of view.
The use of the involutive form of the system allows one to consider quite general situations in a unified way.
We illustrate our approach on the numerical solution of several flow equations with the aim of showing the
impact of the involutive form of the systems in simplifying numerical schemes.
For instance, one shows that for the Stokes system, the discrete involutive form does not need the classical LBB stability condition.

Tommi Karkkainen

The theme of the presentation is a two-fold evaluation of clustering algorithms. On the real world application side, we are concerned with the feasibility of clustering in Business Intelligence, in providing meaningful information from vast amounts of data on company operations. We evaluate the algorithms in this application context.

The clustering objective function considered is the multisource Weber problem or K-spatial medians, with Euclidean metric extended for missing data. That is, we want to minimise the sum of the distances from each prescribed data point to the closest cluster centre. The conventional method to locally approximately solve this problem is the K-means type algorithm: successively assign each data point to the closest cluster centre, and update the centre to be the spatial median of this cluster. The spatial median can be approximated with an extension of the Weiszfeld algorithm (to support missing data).

We evaluate this conventional algorithm against a recent extension of the Weiszfeld algorithm to include concave perturbations. By suitable choice of of the perturbation, and lifting of the data points, the multisource Weber problem can be modelled in this form. The perturbed Weiszfeld algorithm then actually becomes in some sense a ``dual'' to the K-means type algorithm: the vertices are assigned to clusters between K parallel iterations of the Weiszfeld algorithm.

Both of these algorithms are parallelisable, so we implement them on a parallel computing architecture. We then test and compare the scalability of the algorithms in such implementation.

Model reduction in Bayesian inverse problems

Jari Kaipio

Inverse problems can be characterized as problems that tolerate poorly measurement and modelling errors. While the classical measurement error issues, such as electronic noise, have been studied widely, there are only sparse results and even fewer methods to deal with modelling errors.While this problem is difficult to deal with in the classical deterministic framework for inverse problems, the Bayesian counterpart provides a possibility to deal with modelling errors. We discuss a recently proposed approach for approximation and modelling errors. We consider especially the problem of model reduction in which problem the implemented forward solvers (simulation models) have to be poor. This is a relevant topic in process industry in which the inverse problems might have to be solved in a few milliseconds.

Challenges in fruitful management of data generated by simulation of complex flowfields

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When some one covers present and anticipated large numerical simulations, the weaker link of the chain delivering useful data for Industry and Society appears to be the quality evaluation of these data. Of course the points to be first improved in multi-physics computations can only be identified after evaluations of the uncertainties coming from knowledge in quality of validation of physics, of mathematical modelling and of algorithms, of numerical solvers in relation with mesh and boundary conditions.

But the indicators of such quality are actually too poor for good evaluation of uncertainties; indicators decent for simple and not too complex simulations survey only some characteristic local and global parameters. Among such parameters are the ones to be selected for optimisation in Industry and research. However the quality is to be evaluated in all critical parts of the flowfield from the smaller sizes defined by the smaller mesh spacing and the larger scales where emerge the properties of the complete system to be simulated. For rapid survey of large number of data we need to extract images allowing survey of the field from different points of view not only geometric but also quality-oriented and physically right.

Starting from two examples of visualization of very large data generated by super computations we will analyse the components of future multi-scale evaluation of quality extracted from specific image processing : one is search for abnormal cells after RMN exploration of human body, the other try to recover uncertainty to be associated with a figure of global aerodynamic drag of a transcontinental business aircraft in transonic regime.

A major contribution to such evaluation of the uncertainties will be the small scale analysis of discrete critical events and there large scale effects cumulated randomly.

All that new effort requires new dynamic view as can be given by images in movies of specific "objects in the fluid"; such new images needs supercomputing to test the better parametric objects and a methodology to put their contribution on a proposed tree of derivation by computations of trajectory in a space of physical parameters for consolidation of the overall quality

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SCOMA (scientific computing and optimization with multidicipline applications) activities with industrial partners

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Super-Computing in France, Finland and Europe

Author: Olivier PIronneau

Finland is exceptionnally well equipped for super-computing; France exceptionnally badly.
Fortunately the situation will change very soon thanks to an exceptional program launched by the French ministry of Research.
The program will be presented and adequation to the needs will be discussed. Comparison with the rest of Europe and the world will also be sketched.