Modelling 2014

Blaheta, Radim
2014

Institute of Geonics AS CR, Ostrava

VŠB - Technical University of Ostrava

IMACS: International Association for Mathematics and Computers in Simulation

Modelling 2014

Scientific program

Abstracts

List of participants

June 2 – 6, 2014

Rožnov pod Radhoštěm, Czech Republic

The project SPOMECH *Creating a multidisciplinary R&D team for reliable solution of problems in mechanics*, reg. no. CZ.1.07/2.3.00/20.0070, is supported by Operational Program Education for competitiveness funded by Structural Funds of the European Union and state budget of the Czech Republic. It is a joint activity of the VŠB-Technical University of Ostrava and the Institute of Geonics AS CR. More about SPOMECH activities can be found on the official project website: `http://spomech.vsb.cz`

The final conference of the SPOMECH project is a part of this event.

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Edited by Radim Blaheta, Jiří Starý, Dagmar Sysalová
ISBN 978-80-86407-47-0

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Plenary invited speakers

J. Karátson	ELTE University, Budapest, Hungary
B. Khoromskij	Max-Planck Institute MIS, Leipzig, Germany
J. Kraus	University of Duisburg-Essen, Germany & RICAM, Austria
U. Langer	RICAM and JKU Linz, Austria
F. Magoulès	Ecole Centrale, Paris, France
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D. Szyld	Temple University, Philadelphia, USA

Preface

MODELLING 2014 is a conference on Mathematical Modelling and Computational Methods in Applied Sciences and Engineering, which is held in Rožnov pod Radhoštěm, Czech Republic, in June 2 - 6, 2014. The conference is organized by the IT4Innovations Centre of Excellence, Institute of Geonics AS CR, VŠB - Technical University of Ostrava and International Association for Mathematics and Computers in Simulations (IMACS).

MODELLING 2014 aims to be a forum for an exchange of ideas, insights and experience in different areas of mathematical modelling – from numerical methods and computer aspects to applications of mathematical modelling methods. This international conference belongs to a series of conferences held in Rožnov 2009, Pilsen 2005, Pilsen 2001, Prague 1998 which started 20 years ago in Prague 1994.

Main topics of the conference include computational modelling in engineering and science: multiscale modelling, multiphysics modelling, progress in discretization methods, efficient solvers, nonlinear problems, reliable computations, challenging applications of mathematical modelling methods, exploiting massively parallel computing facilities.

The conference is organized in honour of Professor Owe Axelsson on the occasion of his 80th birthday to give a tribute to his inspiring scientific work as well as long term collaboration with the Czech numerical analysis community, see also the following Laudatio.

The organization of the conference is supported by the project *Creating a Multidisciplinary R&D Team for Reliable Solution of Mechanical Problems* (SPOMECH, CZ.1.07/2.3.00/20.0070), which is described in more details on a separate page. The final conference of the SPOMECH project becomes a part of this event.

The conference is held as one of the conferences co-sponsored by the IMACS society. The aim of this society is to promote the exchange of scientific information, see `https://imacs-online.eu`. Due to this support, selected reviewed papers will be published in a special issue of the IMACS journal Mathematics and Computers in Simulation (IMACS, Elsevier). The deadline for paper submission is September 15, 2014.

This booklet contains the scientific programme and abstracts of invited and contributed talks.

On behalf of organizers, I would like to thank all participants for their interest and coming and wish them a nice experience of the scientific programme, friendly atmosphere and good feeling of Rožnov pod Radhoštěm with its famous Open Air Museum and surrounding Beskydy mountains.

Radim Blaheta

Laudatio to Professor Owe Axelsson

Owe Axelsson, born on February 16, 1934 in Gothenburg (Göteborg, Sweden), celebrated his jubilee birthday this year. On this occasion, I would like to outline some facts from his very rich and fruitful scientific life.

Owe's professional carrier has begun in Gothenburg. He studied there and later he became a chairman of the Department of Computer Science, including Numerical Analysis, at the Chalmers University of Technology and the University of Gothenburg. There, he was appointed Full Professor in 1973.

For the twenty-five years, from 1979 till 2004, Owe held the position of Professor of Numerical Analysis at the University of Nijmegen. Beside Gothenburg and Nijmegen, Owe also spent a lot of time as a visiting professor at many famous institutions, such as CERN, Geneva; Ecole Polytechnique Federale, Lausanne; University of Texas at Austin; Rice University, Houston, Texas; University of Lund, Sweden; Bulgarian Academy of Sciences, Sofia; Florida State University, Tallahassee; Lawrence Livermore National Laboratory, Livermore, California.

In 2004, Owe Axelsson accepted an invitation from the Academy of Sciences of the Czech Republic to join the Applied Mathematics Centre at the Institute of Geonics, Ostrava. Further, we shall provide more details about his activities there in the last decade.

The overall work of Owe Axelsson is very broad and therefore difficult to describe. I just try to mention some of his great scientific achievements, but the list will be far to complete.

We can start with the highest appreciation of Owe Axelsson's merits in the development of the concept of preconditioning. His fundamental work started by publishing the paper [1] and has successfully continued up to the present days. In the first period, this work concerned mainly incomplete factorization methods with diagonal balancing, further he engaged in the development of block methods, efficient and robust variants, application of incomplete factorization preconditioning to different type of problems. See references [1-7].

Next research achievements were gained in combination of factorization and multilevel ideas and led to optimal solvers. The first work on two level method [10] appeared in 1982, in a refined form published in 1984, see [11]. A sophisticated multilevel variant – Algebraic Multi Level Iterative (AMLI) methods appeared in the end of eighties in joint papers with Panayot Vassilevski [12-14]. The method was further enhanced with respect to robustness to coefficient jumps and anisotropy, efficient parallelization etc., see e.g. [15,16, 22].

Owe's work included much more e.g. parallel algorithms, investigation of the convergence of the conjugate gradient and generalized conjugate gradient methods [8,9], multilevel Newton-like methods [17], approximate methods for initial-boundary value problems. The richness of his work is also visible from his work in the last decade [22-40].

In total, Owe published two books and a big amount of highly appreciated research papers. The quality of these publications is confirmed by their broad influence on the numerical community as well as e.g. re-edition of the book by Axelsson and Barker in SIAM series Classics in Applied Mathematics in 2001. Moreover, Owe's work was appreciated by being selected to the list of Highly Cited Research (The people behind the most influential research, `http://highlycited.com`) of Web of Science Database by Thomson Reuters.

Last but not least, I would like to mention Owe's relation to the numerical analysis community in Ostrava, which now last about three decades. The first decade can be characterized by Owe's influence and first contacts. It started after 1984, when the book by Axelsson and Barker appeared in Ostrava as a real miracle in those times. Of course, the work of Owe was already known, especially due to his earlier contacts with Ivo Marek and other mathematicians in Prague. The EQUADIFF conference in Brno 1988 was for me a first opportunity to meet Owe. I remember his interest and friendly encouragement for submitting a paper. After 1989 I got the first possibility to visit Owe at University of Nijmegen. It happened in 1992, in the period when Owe prepared his second book Iterative Solution Methods.

These contacts consequently led to an invitation of a group from the Institute of Geonics in Ostrava to EU project HIPERGEOS (High Performance Computing in Geosciences), which was led by Owe Axelsson. This project enabled fruitful joint work with Owe and many others including M. Neytcheva, B. Polman, A. Padiy and others from the University of Nijmegen, R. Beauwens, Y. Notay and others from ULB Brussels, S. Margenov, P. Vassilevski and a group from BAS Sofia and another Czech group from the Institute of Computer Science AS CR led by J. Nedoma. Due to successful first period, this project was prolonged and both periods of HIPERGEOS created a framework for this second decade of collaboration. Note that beside the research in numerical methods, this project enabled also our first experiments in parallel computing.

The third decade started in 2004, at the conference IMET 2004 (Iterative methods) in Prague. At this conference Owe obtained Bolzano medal of Academy of Sciences of CR for Merits in Mathematical Sciences. The medal was awarded by the president of the Academy, Prof. H. Illnerova, and in a discussion with her, an idea was born to invite Owe to the Academy. This idea was consequently realized – Owe joined the Applied Mathematics Department at the Institute of Geonics AS CR. We are very glad that from that time, we have a very close collaboration with Owe, even much strengthened after Owe bought a flat in Ostrava and coming to Ostrava became really like going home.

The recent decade was also decade of very fruitful work, as confirmed by many publications, see selected papers [22-40]. And moreover, these publications again show Owe's broad interests as they concern many topics: macroelementwise and block type of preconditioners, preconditioning saddle point systems appearing in mixed FEM and poroelasticity, investigation higher order time discretization schemes and suitable preconditioners for them, modelling two-phase flow problems, homogenization, operator preconditioning

and PCG in general setting, etc. He even found time for writing some review papers, as e.g. [24] and [26].

Owe Axelsson has reached many excellent scientific results, but remains all the time a kind, generous man inviting people for collaboration. He serves the numerical community by managing the high quality journal Numerical Linear Algebra with Applications and organizing several very successful events. He influenced lot of students and researchers worldwide. In personal contact, Owe succeeded in transferring to people his unceasing energy and enthusiasm for the research work.

On behalf of the conference participants, his friends and the whole scientific community working in numerical analysis, I would like to wish Owe many happy returns of the days, further successful research and good health.

Radim Blaheta

For more details about Owe Axelsson, see also:

- R. Blaheta, I. Marek: *Laudatio to Owe Axelsson*, Applications of Mathematics, 50 (3), 2005, pp. 179-182, `http://dml.cz/dmlcz/134601`.

Books:

- O. Axelsson, V. A. Barker: *Finite Element Solution of Boundary Value Problems: Theory and Computation.* Academic Press, Orlando 1984, SIAM series Classics in Applied Mathematics, 2001.
- O. Axelsson: *Iterative Solution Methods.* Cambridge University Press, 1994.

Scientific papers:

[1] O. Axelsson: *A generalized SSOR method.* BIT 12, 1972.

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SPOMECH

Creating a Multidisciplinary R&D Team for Reliable Solution of Mechanical Problems

Short title: SPOMECH Reg. No.: CZ.1.07/2.3.00/20.0070

Applicant:	VŠB - Technical University of Ostrava	From - To:	July 1, 2011 - June 30, 2014
Partner:	Institute of Geonics AS CR, Ostrava	Budget:	CZK 29 925 962.00

The SPOMECH project was approved by the Ministry of Education, Youth and Sports under the Operational Programme Education for Competitiveness, area of intervention Human Resources in Research and Development.

The aim of the project is to create an excellent research team working in the important field of reliable modelling of problems in non-linear mechanics and geomechanics, involve this team in international cooperation, and present the results of its research to academic and research workers and students who are the project's target groups.

The researchers who make up the core of the research team include Prof. Marek Kwasniewski, a renowned expert in laboratory material research, and doc. Jan Valdman, an expert in reliable numerical solutions of non-linear problems in mechanics.

The key project activities are as follows:

- Enhancing and developing the existing research team in the field of reliable solution of non-linear problems in mechanics and geomechanics
- Organizing thematic international workshops and conferences
- Organizing thematic seminars
- Organizing series of specialised courses for students, the announcing and supervising of their thesis

The project's target groups are academic and research workers and university students of technical subjects.

The main project output is to improve the research team, increase its members' competences, provide a large amount of expert results, and create and maintain a project website. Other project outputs include events organised as part of the key activities mentioned above for individual target groups.

Activities of the SPOMECH project are documented at: `http://spomech.vsb.cz`

The project is implemented under the IT4Innovations National Supercomputing Centre: `http://www.it4innovations.cz`, `http://www.facebok.com/it4innovations`

esf european social fund in the czech republic | EUROPEAN UNION | MINISTRY OF EDUCATION, YOUTH AND SPORTS | OP Education for Competitiveness

INVESTMENTS IN EDUCATION DEVELOPMENT

IT4Innovations
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Centre of Excellence IT4Innovations

Reg. No.: CZ.1.05/1.1.00/02.0070

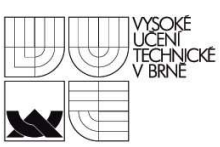
The IT4Innovations project aims at creation a unique structure with both national and international significance that represents an exceptional synergy of scientific, research and development capacities in computer science and computational mathematics with the goal of stimulating the development of a wide range of modern and progressive technologies. Integral part of the project is installation of a high-performance supercomputer enabling solution of computing intensive tasks.

The project IT4Innovations started in 2011 and is still under development. So far it provides computing at a Terraflop High Performance Cluster ANSELM, a further computing facility with Petaflop performance will be installed in 2015 .

The Anselm cluster consists of 209 compute nodes, providing 3344 compute cores with 15 TB RAM and giving over 94 Tflop/s theoretical peak performance. Each node is a powerful x86-64 computer, equipped with 16 cores, at least 64 GB RAM, and 500 GB harddrive. Nodes are interconnected by fully non-blocking fat-tree Infiniband network and equipped with Intel Sandy Bridge processors. A few nodes are also equipped with NVIDIA Kepler GPU or Intel Xeon Phi MIC accelerators. The cluster runs bullx Linux operating system, which is compatible with the RedHat Linux family. A wide range of software packages targeted at different scientific domains are provided to users.

More details about the IT4Innovations project: `http://www.it4i.cz`

The project is funded by Operational Programme R&D for Innovations. Partners of the project are VŠB - Technical University of Ostrava, University of Ostrava, Brno University of Technology, Silesian University in Opava, and Institute of Geonics AS CR.



Part A
Scientific program

June 2 – Monday — Hotel Relax

10:00 - 13:30 Registration 1 (Hotel Relax)

12:00 - 13:30 Lunch

June 2 – Monday — Hotel Eroplán, "The cone"

13:00 - 14:00 Registration 2 (Hotel Eroplán)

14:00 - 14:45 Opening the conference
Modelling and IT4Innovations
SPOMECH project
IMACS society
Laudatio to Owe Axelsson

Plenary talks — Chairman: Z. Dostál

14:45 - 15:30 O. Axelsson: Easy Way to Analyze Some Preconditioners for Saddle Point Problems

15:30 - 16:15 Y. Saad: Multilevel Low-rank Approximation Preconditioners

16:15 - 16:45 Coffee break

Plenary talks — Chairman: T. Kozubek

16:45 - 17:30 U. Langer: Discontinuous Galerkin Multipatch Isogeometric Analysis of Diffusion Problems on Surfaces and in Volumetric Domains

17:30 - 18:15 J. Karátson: Equivalent Operator Preconditioning

18:30 Welcome dinner

June 3 – Tuesday — Hotel Relax

Plenary talks — Chairman: Y. Saad

09:00 - 09:45 B. Khoromskij: Recent Advances in Grid-based Tensor Numerical Methods with Applications to Multidimensional PDEs

09:45 - 10:30 J. Kraus: Robust Preconditioning of Weighted $H(div)$-norm and Applications

10:30 - 11:00 Coffee break

Plenary talks — Chairman: J. Valdman

11:00 - 11:45 S. Repin: Guaranteed and Fully Computable Bounds of Approximation and Modeling Errors for Problems with Divergence Free Condition

11:45 - 12:30 F. Magoulès: Chaotic Iterations of Domain Decomposition Methods

12:30 - 14:00 Lunch

Parallel session A: **Nonlinear mechanics 1** — Chairman: T. Roubíček

14:00 - 14:20 J. Málek: Termodynamics of Rate-type Fluid Models and Their Applications to Deformations of Apshalt Binders

14:20 - 14:40 M. Kružík, J. Valdman: Modeling of Ferro/paramagnetic Transition

14:40 - 15:00 S. Sysala: On Control of the Loading Process in Hencky's Perfect Plasticity

15:00 - 15:20 K. Goyal, M. Mehra: Diffusion Wavelet Based Space-time Adaptive Numerical Method

15:20 - 15:40 P. Salač: The Two Steps Optimization of Plunger Cooling in the Glass Forming Process

Parallel session B: **High-performance computing** — Chairman: F. Magoulès

14:00 - 14:20 T. Kozubek: Acceleration of Direct and Iterative Solvers Used in Domain Decomposition Based Algorithms by Novel Techniques and Novel Many-cores Accelerators

14:20 - 14:40 P. Pařík, J. Plešek: Efficient In-core Sparse Direct Solution of Large Finite Element Problems

14:40 - 15:00 A. Markopoulos, F.-X. Roux: Domain Decomposition Method, Plasticity, Krylov Subspace Method with Multiple Search Directions

15:00 - 15:20 A. Polovinkin, K. Barkalov, I. Meyerov et al: SVM Regression Parameters Optimization Using Parallel Global Search Algorithm on Intel Xeon Phi

15:20 - 15:40 V. Hapla: FLLOP: A Massively Parallel QP Solver Compatible with the TFETI Substructuring Scheme

June 3 – Tuesday — Hotel Relax

15:40 - 16:10 Coffee break

Parallel session A: **Nonlinear mechanics 2** Chairman: D. Lukáš

16:10 - 16:30 J. Haslinger, V. Janovský, R. Kučera: On Parameter Dependent Static Contact Problems

16:30 - 16:50 P. Beremlijski, A. Markopoulos: Shape Optimization in 3D Contact Problems with Coulomb Friction

16:50 - 17:10 I. Bock: Mindlin-Timoshenko Beam in a Dynamic Contact with a Rigid Obstacle

17:10 - 17:30 D. Gabriel, J. Kopačka, J. Plešek: Searching for Local Contact Constraints in the Finite Element Procedures for Contact Problems

17:30 - 17:50 J. Kopačka, D. Gabriel, R. Kolman, J. Plešek: Influence of Mass Lumping Techniques on Contact Pressure Oscillations in Explicit Finite Element Contact-impact Algorithm Based on Isogeometric Analysis with NURBS

17:50 - 18:10 J.- J. Shu: Heat Transfer of an Impinging Jet on a Plane Surface

Parallel session B: **Homogenization and multiscale** Chairman: J. Kruis

16:10 - 16:30 E. Rohan: Waves in Large Contrast Fluid-saturated Porous Deformable Media

16:30 - 16:50 F. Kolařík, J. Zeman, B. Patzák: On Homogenization-based Models for Fresh Concrete Flow through Reinforcing Bars

16:50 - 17:10 J. Vondřejc, J. Zeman, I. Marek: Accurate Guaranteed Bounds on Homogenized Matrix by FFT-based Methods

17:10 - 17:30 N. Mishra, J. Vondřejc, J. Zeman: A Comparative Study on Iterative Solvers for FFT-based Homogenization of Periodic Media

17:30 - 17:50 R. Cimrman, M. Novák, R. Kolman, M. Tůma, J. Vackář: Isogeometric Analysis in Electronic Structure Calculations

17:50 - 18:10 M. Theuer, D. Lukáš, J. Bouchala: BEM for Homogenization in 2D

18:30 Dinner at the hotel

June 4 – Wednesday — Hotel Relax

Plenary talks — Chairman: M. Kružík

09:00 - 09:45 H. Petryk: The Energy Approach to Material Instability and Microstructure Evolution in Rate-independent Dissipative Solids

09:45 - 10:30 T. Roubíček: Various Solution Concepts in Rate-independent Evolution Systems

10:30 - 11:00 Coffee break

Plenary talks — Chairman: J. Málek

11:00 - 11:45 K. Rajagopal: On Implicit Constitutive Relations

11:45 - 12:30 D. Szyld: Old and New Iterative Methods for the Solution of Generalized Lyapunov Equations

12:30 - 14:00 Lunch

Excursions

14:00
- A. Visiting *the Wallachian open air museum*
- B. Hiking to *Radhošť*
- C. Trip to *Hukvaldy*

18:00 - 20:00 Dinner at the hotel

Poster session

20:00
1. R. Blaheta, O. Jakl, J. Starý: Parallel Processing of High Resolution FEM Systems in Micromechanics
2. D. Horák, V. Hapla, L. Říha, A. Markopoulos: Solution of Contact Problems Using FLLOP Library
3. R. Kohut: Parallel Solution of Elasticity Problems using Aggregations
4. P. Maršálek: Passenger Safety in Railway Traffic
5. P. Rálek, M. Hokr: Application of the 3D Numerical Model in the Control and Predictions during the Underground Rock Heating Experiment
6. J. Říha, J. Šembera: Model of the Water Balance of a Lake Created by Hydrological Recultivation of an Open Pit Coal Mine
7. O. Vlach: Thermomechanical Contact Problems in MatSol
8. J. Zapletal, M. Merta: BEM4I - Parallel BEM Library and its Applications

June 5 – Thursday — Hotel Relax

Plenary talks — Chairman: M. Tůma

09:00 - 09:45 J. Mandel, J. Beezley, M. Jenkins et al: A Coupled Weather and Wildland Fire Forecasting System with Assimilation of Satellite Remote Sensing Data

09:45 - 10:30 J. Nordbotten: Finite Volume Methods for Elasticity and Poro-elasticity

10:30 - 11:00 Coffee break

Parallel session A: **Porous media flow** — Chairman: J. Zeman

11:00 - 11:20 J. Kruis, T. Koudelka: Moisture Transport in Partially Damaged Materials

11:20 - 11:40 J. Vala: Identification of Moisture Distribution in Porous Building Materials from Microwave Measurements

11:40 - 12:00 J. Březina, J. Stebel: Flow123d - Modeling Tool for Processes in Fractured Media

12:00 - 12:20 J. Březina, J. Stebel: Robust Discontinuous Galerkin Method for Transport Processes in Fractured Porous Media

Parallel session B: **Flow problems** — Chairman: M. Brandner

11:00 - 11:20 J. Šístek: Parallel Performance of Iterative Solvers for Pressure-correction Methods for Incompressible Flows

11:20 - 11:40 P. Burda, M. Hanek, J. Šístek: Analytical Solution for Singularities of Rotationally Symmetric Stokes Flow and Applications to Finite Element Solution

11:40 - 12:00 B. Bastl, M. Brandner, E. Turnerová et al: Isogeometric Analysis for Navier-Stokes Equations

12:00 - 12:20 O. Bublík, J. Vimmr, A. Jonášová: On Modelling of Non-Newtonian Free Surface Flows Using the Lattice Boltzmann Method

12:30 - 14:00 Lunch

June 5 – Thursday — Hotel Relax

Parallel session A: **Environmental problems** — Chairman: V. Vondrák

14:00 - 14:20 K. Georgiev, Z. Zlatev: Comparison Results of Running of an Eulerian Computer Model for Long Range Air Pollution on Different High-performance Computers

14:20 - 14:40 D. Fedorčák, M. Theuer, R. Vavřík et al: Calibration Methods for Rainfall-runoff Simulations inside FLOREON+ System

14:40 - 15:00 J. Mandel, I. Kasanický, M. Vejmelka: Spectral Diagonal Covariance in EnKF

15:00 - 15:20 J. Resler, P. Juruš, K. Eben et al: Fine Resolution Modelling of Meteorological Conditions and Air Quality in Urbanized Areas

15:20 - 15:40 U. Schaarschmidt, S. Subbey, T. Steihaug: A Stock-recruitment Relationship Derived from a Slow-fast Population Dynamic Model

Parallel session B: **Numerical linear algebra** — Chairman: D. Szyld

14:00 - 14:20 M. Tůma: On Incomplete Symmetric Decompositions

14:20 - 14:40 V. Khoromskaia: Black-box Eigenvalue Solver for the 3D Integro-differential Hartree-Fock Equation by Tensor Numerical Methods

14:40 - 15:00 J. Kraus, M. Lymbery: Incomplete Factorization by Local Exact Factorization (ILUE)

15:00 - 15:20 J. Alvarez, A. Duran: Numerical Treatment of Algebraic Equations with Symmetries

15:20 - 15:40 A. Y. Wang, F.-X. Roux: A Coupling Method for the Parallel Solution of Vibro-acoustic Problems

15:40 - 16:10 Coffee break

June 5 – Thursday — Hotel Relax

Parallel session A: **Flow and environmental problems** — Chairman: P. Burda

16:10 - 16:30 M. Lanzendörfer: Thin Film Flows of Piezoviscous Fluids in Lubrication Problems

16:30 - 16:50 V. Aggarwal, B. Srinivasan: An Adaptive Mesh Strategy for Convection Diffusion Problems

16:50 - 17:10 R. Blaheta, M. Hasal, Z. Michalec: Hydro-mechanical Modelling of SEALEX Experiments

17:10 - 17:30 I. Bruský, J. Šembera: Coupled Model of Flow-through Experiment in Novaculite Fracture

17:30 - 17:50 J. Šembera, V. Žabka: Geochemical Model of Calcite Dissolution in Column Experiments

17:50 - 18:10 L. Zedek, J. Šembera: ODE's for Description of Reactive Transport Including Equilibrium Reactions

18:10 - 18:30 I. Oguoma, T. Acho: Mathematical Modelling of the Spread and Control of Onchocerciasis in Nigeria

Parallel session B: **Numerical methods** — Chairman: P. Råback

16:10 - 16:30 R. Kolman, S.-S. Cho, K. Park: On an Accurate Explicit Time Integration Algorithm for Wave Propagation Problems in Solids

16:30 - 16:50 M. Neumüller: A Parallel Space-time Multigrid Solver for the Stokes Equations

16:50 - 17:10 U. Langer, H. Yang: Partitioned and Monolithic Approaches for Fluid-structure Interaction Simulation

17:10 - 17:30 M. Čermák, V. Hapla, D. Horák: Solving Elastoplastic Problems with the FLLOP Solver

17:30 - 17:50 Z. Dostál, L. Pospíšil: The Projected Barzilai-Borwein Method for Solving Quadratic Programming Problems with Separable Elliptic Constraints

17:50 - 18:10 M. Jarošová, Z. Dostál: The Monotonic Algorithm for the Solution of the Variational Equations with Bound Constrains Exploiting Weakly Feasible Steps

18:10 - 18:30 S. Basterrech, V. Snášel: A Study of the Impact of the Pseudospectra on the Stability of the Recurrent Neural Networks

19:00 Conference dinner at the hotel

June 6 – Friday — Hotel Relax

Parallel session A: **Boundary elements** — Chairman: J. Malík

09:00 - 09:20 D. Lukáš, P. Kovář, T. Kovářová et al: Parallel Fast BEM

09:20 - 09:40 J. Bouchala, D. Lukáš, L. Malý et al: BEM-based Domain Decomposition for Polygonal Subdomains

09:40 - 10:00 M. Merta, J. Zapletal: BEM4I - parallel BEM Library with Applications

Parallel session B: **Meshes and images** — Chairman: O. Jakl

09:00 - 09:20 M. Jaroš: Rendering and Post-processing of OpenFOAM CFD Simulations

09:20 - 09:40 A. Kolcun: Goldberg-like Decompositions and Voxel Representation of 3D Space

09:40 - 10:00 A. Ronovský, A. Vašatová: Elastic Image Registration with Mesh Adaptation

10:00 - 10:20 Coffee break

Plenary talk — Chairman: R. Blaheta

10:20 - 11:05 P. Råback: Building Blocks for Multiphysical Simulation Software

11:05 Closing the conference

11:20 - 12:20 Lunch

Part B
Abstracts of plenary talks

Easy Way to Analyze Some Preconditioners for Saddle Point Problems

O. Axelsson

A survey is given of some block triangular and block diagonal preconditioning methods for saddle point problems such as appear in porous media flow. Various forms of regularization of the problem and a short way to prove diagonalizability of the preconditioned matrix are presented.

The methods uses inner iterations for the arising block diagonal matrices and a nonlinear (variable preconditioner, flexible) version of a Krylov subspace based acceleration method for the outer iterations. The eigenvalue spectrum depends on the regularization parameter. For comparison, some more robust methods, but with, in general, less efficient spectrum are also presented.

Equivalent Operator Preconditioning

J. Karátson

A class of efficient preconditioners for discretized elliptic problems can be obtained via equivalent operator preconditioning. This means that the preconditioner is chosen as the discretization of a suitable auxiliary operator that is equivalent to the original one. Under proper conditions one can thus achieve mesh independent convergence rates. If the discretized auxiliary problems possess efficient optimal order solvers (e.g. of multigrid type) regarding the number of arithmetic operations, then the overall iteration also yields an optimal order solution.

The talk is based on the joint work of the speaker with Prof. Owe Axelsson. First some earlier results are summarized, then some recent applications are shown such as parallel preconditioning for transport type systems and streamline diffusion preconditioning for convection-diffusion problems.

Recent Advances in Grid-based Tensor Numerical Methods with Applications to Multidimensional PDEs

B.N. Khoromskij

Grid-based tensor methods provide the efficient tools for numerical approximation of d–dimensional PDEs (discretized on large $n^{\otimes d}$–grids) with linear complexity scaling in the dimension, $O(dn)$. Traditional methods of separable approximation combine the canonical, Tucker, as well as the matrix product state type (MPS) formats and, in particular, TT/HT representations.

The quantized-TT (QTT) approximation [2] is proven to provide the logarithmic data-compression on a wide class of functions and operators. In combinations with the

Tacker/TT formats, it makes possible to efficiently solve multi-dimensional steady-state and dynamical problems by their reformulation in quantized tensor spaces, reducing the complexity to logarithmic scale in the size full data on the grid, $O(d \log n)$.

In this talk, we are going to discuss how the grid-based tensor approximation applies to hard problems arising in electronic structure calculations, such as computation of many-electron integrals, solution of the nonlinear eigenvalue problem for the Hartree-Fock equation, including the case of huge lattice- structured/periodic compounds, arising in numerical modeling of metals, crystals and polymers [1, 4, 6]. We will also discuss applications to the solution of multi-parametric PDEs [3], and to the efficient simultaneous times-space tensor approximation to the dynamical chemical master equations arising in stochastic modeling of multi-particle reaction processes [5].

Numerical tests indicate the efficiency of tensor numerical methods on realistic examples in electronic and molecular structure simulation and for stochastic PDEs.

[1] B.N. Khoromskij, V. Khoromskaia, and H.-J. Flad. *Numerical solution of the Hartree-Fock equation in multilevel tensor-structured format.* SIAM J. Sci. Comp., **33**(1), 2011, 45-65.

[2] B.N. Khoromskij. $O(d \log N)$-*Quantics Approximation of N-d Tensors in High-Dimensional Numerical Modeling.* J. Constr. Approx. v. 34(2), 257-289 (2011).

[3] B.N. Khoromskij, and Ch. Schwab, *Tensor-Structured Galerkin Approximation of Parametric and Stochastic Elliptic PDEs.* SIAM J. Sci. Comp., **33**(1), 2011, 1-25.

[4] V. Khoromskaia, B.N. Khoromskij, and R. Schneider. *Tensor-structured calculation of two-electron integrals in a general basis.* SIAM J. Sci. Comput., **35**(2), 2013, A987-A1010.

[5] S. Dolgov, and B.N. Khoromskij. *Simultaneous state-time approximation of the chemical master equation using tensor product formats.* arXiv:1311.3143, 2013; http://arxiv.org/abs/1311.3143, (NLAA, 2014 to appear).

[6] V. Khoromskaia and B.N. Khoromskij. *Grid-based Ewald-type lattice summation of electrostatic potentials by low-rank tensor approximation.* Preprint 116/2013, MPI MiS, Leipzig 2013 (CPC, 2014 to appear).

Robust Preconditioning of Weighted $H(div)$-norm and Applications

J. Kraus

A robust multigrid method is presented for the systems arising in leastsquares or mixed finite element methods when modelling flow processes in highly heterogeneous media. The main focus of the talk is on the design and analysis of a preconditioner for the weighted $H(\mathrm{div})$-norm.

A combination of ideas from domain decomposition and fictitious space preconditioning based on additive Schur complement approximation (see [2, 3]) provides a general framework for building *auxiliary space multigrid methods*. Justified by theory and numerical tests, this approach allows to construct iterative methods that are robust with respect to the contrast of the media, defined as the ratio between the maximum and minimum values of the coeffcient (related to the permeability/conductivity). The uniformity of a block-diagonal symmetric and positive definite preconditioner for the saddle-point problem arising from the mixed formulation is established via a discrete inf-sup condition, which links our work to the classical theory in [1].

[1] D. Arnold, R. Falk, R. Winther, Preconditioning in H(div) and applications, *Math. Comp.*, 66, (1997), pp. 957–984.

[2] J. Kraus, Additive Schur complement approximation and application to multilevel preconditioning, *SIAM J. Sci. Comput.* 34 (2012), pp. A2872-A2895.

[3] J. Kraus, M. Lymbery, S. Margenov, Auxiliary space multigrid method based on additive Schur complememt approximation, *Numer. Linear Algebra Appl.*, (submitted).

Discontinuous Galerkin Multipatch Isogeometric Analysis of Diffusion Problems on Surfaces and in Volumetric Domains

U. Langer

Isogeometric analysis (IGA) uses the same class of basis functions for both, representing the geometry of the computational domain and approximating the solution. In practical applications, geometrical patches are used in order to get flexibility in the geometrical representation. This multi-patch representation corresponds to a decomposition of the computational domain into non-overlapping subdomains also called patches in the geometrical framework.

We will present Discontinuous Galerkin (DG) Methods that admit discontinuities along the subdomain (patch) boundaries. The required smoothness is obtained by the DG terms associated with the boundary of the subdomains. The construction and the corresponding discretization error analysis of such DG multi-patch IGA schemes will be given for heterogeneous diffusion model problems on open and closed surfaces as well as in volumetric computational domains, but can be generalized to other elliptic boundary value problems as well. The construction of isogeometric segmentation algorithms that automatically deliver a decomposition of a volumetric computational domain into patches with a patch-wise volumetric NURBS parametrizations is a challenging geometrical task.

The result of such segmentation algorithms frequently induce non-conforming meshes along the patch interfaces or even non-matching patches. Therefore, the DG technology is very helpful to handle such cases successfully. Finally, we present the implementation in **G+SMO**, and some numerical results confirming our theoretical estimates.

Acknowledgement:This talk is based on joint work with B. Jüttler, A. Mantzaflaris, S. Moore and I. Toulopoulos within the National Research Network S117 on "Geometry + Simulation", see `http://www.gs.jku.at` for more information about this research network. The research work presented in this talk has been supported by the Austrian Science Fund under the grant NFN S117-03.

Chaotic Iterations of Domain Decomposition Methods

F. Magoulès

Existing numerical algorithms often face their limits when running on a large number of cores. For instance, parallel iterative methods meet some scalability limitation due to the synchronization procedure occurring between the processors at the end of each iteration.

Iterative domain decomposition methods are a particular type of methods, well suited for parallel computations. This talk shows how the domain decomposition methods have efficiently evolved over the years by using specially designed boundary conditions on the interface between the subdomains. In order to use such methods on massive parallel computers, the iterative scheme should be modified, and chaotic iterations are here proposed for the solution strategy of the interface problem, leading to some convergence difficulties. After the presentation of the method, numerical experiments are performed on large scale engineering problems to illustrate the robustness and efficiency of the proposed method.

[1] F. Magoulès, F.-X. Roux, and S. Salmon. Optimal discrete transmission conditions for a non-overlapping domain decomposition method for the Helmholtz equation. SIAM Journal on Scientific Computing, 25(5):1497-1515, 2004.

[2] M.J. Gander, F. Magoulès, and F. Nataf. Optimized Schwarz methods without overlap for the Helmholtz equation. SIAM Journal on Scientific Computing, 24(1):38-60, 2002.

[3] D.P. Bertsekas and J.N. Tsitsiklis. Parallel and Distributed Computation: Numerical Methods. Prentice-Hall, 1989.

A Coupled Weather and Wildland Fire Forecasting System with Assimilation of Satellite Remote Sensing Data

J. Mandel, J. D. Beezley, M. A. Jenkins, A. K. Kochanski, V. Y. Kondratenko, L. Lu, S. Shranz, M. Vejmelka

We describe a system in development, which will provide a wildland fire forecasting capability integrated with weather forecasting systems. The system is based on on the WRF-SFIRE software, which couples atmospheric modeling by the Weather Research Forecasting (WRF) model with a fire spread (SFIRE) model and a dynamic fuel moisture model. Fuel moisture data from from automated weather stations are assimilated

into the simulation. Smoke dispersion and advection and chemical weather forecast for pollution forecasting are also available by coupling with WRF-Chem. Static Geographic Information System (GIS) data (topography and fuel maps) are obtained from US government databases. Fire simulation can be started from an ignition point or a developed fire perimeter, provided in near real time. This type of data can be also assimilated dynamically to change the course of a running simulation. Dynamical data from NASA and NOAA orbital platforms are assimilated into the simulations, including MODIS and VIIRS and fire detection, and vegetation indices for fuel moisture estimation. The system is accessed through NOAA FX-Net system as well as a website. It provides on-screen output and KML file download for visualization in Google Earth.

Finite Volume Methods for Elasticity and Poro-elasticity

J. Nordbotten

We introduce a new class of cell-centered finite volume methods for elasticity and poro-elasticity. This class of discretization methods has the advantage that the mechanical discretization is fully compatible (in terms of grid and variables) to the standard cell-centered finite volume discretizations that are prevailing for commercial simulation of multi-phase flows in porous media.

For a specific variant of the proposed discretization, we give an overview of a convergence proof in the setting of isotropic elasticity, and address from a theoretical perspective the issues of a discrete Korn's inequality and robustness with respect to locking. Furthermore, we give numerical results for both structured and unstructured grids for both elasticity and poro-elasticity. The talk concludes with an application to simulation of fractured and fracturing porous media.

The Energy Approach to Material Instability and Microstructure Evolution in Rate-independent Dissipative Solids

H. Petryk

Material instability is typically linked to spontaneous emergence of non-uniform deformation patterns and to the formation and evolution of microstructures. For the modelling purposes, regularization methods with rate-dependence or strain-gradient effects are commonly used. However, they can eliminate the instability phenomena observed in real materials unless suitable initial imperfections are adjusted.

An alternative method emerges from the energy criterion of material instability. The essence of the energy approach lies in the incremental minimization of the rate-independent work that is not quasiconvex. However, for dissipative solids this is not

automatically a valid approach, as sometimes claimed, since the path dependence of energy dissipation can destroy a potential structure of the incremental problem. It is shown that if multiple mechanisms of inelastic deformation operate simultaneously and interact, as in plasticity of metal crystals deformed by multislip, then the interaction matrix for active mechanisms must be symmetrized in advance.

The energy approach describes in a natural way the formation and evolution of material microstructures, with no need for initial imperfections. An intrinsic length-scale is required to predict characteristic dimensions of the microstructures. For this purpose, sharp interfaces of a specified surface energy can be used. Then, the microstructure dimensions are determined by the energy minimization without assuming any artificial length-scale parameter. That approach is also applicable to multi-scale modelling.

A number of 3D examples have been calculated which demonstrate computational effectiveness of the incremental energy approach. The examples include multi-scale modeling of the formation and evolution of martensitic microstructures in shape memory alloys, emergence of shear bands in polycrystalline metals, and deformation banding in ductile single crystals.

Building Blocks for Multiphysical Simulation Software

P. Råback

Multiphysical simulation software requires a large selection of numerical methods combined with an implementation that enables the flexibility required by arbitrary couplings. In this presentation the essential building blocks related to Elmer finite element software are reviewed. Examples are given on the combination of these in some challenging real-world examples.

The required numerical methods include space and time discreatization techniques, stabilization methods, meshing techniques, linear solvers and preconditioners, projectors, constraints, and solution methods for nonlinear and coupled systems etc. These are library functionalists for individual physical solvers that may be coupled with one another without an *a priori* defined way. Also all material parameters may depend on the field values in any way. To be able to study large problems the implementation should always target for parallel computation.

Different combinations of numerical techniques are needed in different application fields. For example, the 3D simulation of continental ice-sheets uses novel meshing techniques, robust stabilization methods and block preconditioners to enable large scale computations. Simulation of electrical machines on the other hand uses combination of edge elements, mortar projectors, constraints from electrical circuits, and tailored partitioning routines.

In solving complex problems there are often two competing design paradigms: The reuse of code and ease of individual problems favors *divide and conquer* approach where

the problem is split to simpler subproblems. On the other hand, strong physical couplings sometimes require a monolithic approach which may be more complicated to implement and don't allow for efficient solution techniques – but provides the solution. Finding a good balance here with numerical methods that fit together is often a challenge in multiphysical problems.

[1] http://www.csc.fi/elmer

[2] M. Malinen and P. Råback, Elmer finite element software for multiphysical and multiscale problems in http://books.google.fi/books?id=PeF8QGJEKKIC.

On Implicit Constitutive Relations

K.R. Rajagopal

In this talk, I will present implicit new classes of constitutive relations to describe the response of both solids and fluids and discuss how such models can describe phenomena that have not been described adequately by existing constitutive relations.

Guaranteed and Fully Computable Bounds of Approximation and Modeling Errors for Problems with Divergence Free Condition

S. Repin

Mathematical models of incompressible media arise in the theory of fluids, some models of solids, electromagnetic problems. We present an overview of key results related to quantitative analysis (stability, reliability, and adaptivity) of these problems and discuss recent results in the field. The main subject is fully guaranteed a posteriori estimates for approximate solutions of models with divergence free condition and closely related questions on computable bounds of the constants in functional inequalities, which enter these a posteriori estimates.

[1] S. Repin. A posteriori estimates for partial differential equations, Walter de Gruyter, Berlin, 2008.

[2] S. Repin. Estimates of deviations from exact solutions of the generalized Oseen problem, Zap. Nauchn. Semin. POMI, 410(2013), 110–130.

Various Solution Concepts in Rate-independent Evolution Systems

T. Roubíček

Evolution of mechanical systems is often governed by nonconvex stored energies together with dissipation potentials. If the outer loading is much slower than the time-scale

of internal disipative processes, these systems can approximately be considered as rate independent and the dissipated energy potential as positively homogenoues of degree -1. Typical examples are damage, plasticity, phase transformations, or fracture in the bulk, or delamination or friction in adhesive contacts. The usual global-minimum concept for incremental problems preserves energy in the limit but may be computationally difficult and often less physical than some force-driven locally-minimal solutions. The various concepts of solutions and various time-discretisations will be discussed, together with the role of the maximum-dissipation principle. Abstract considerations will be illustrated on a delamination problem (=an adhesive contact problem), together with some of its variants as a brittle contact or a mixity-mode sensitive delamination (illustrated by numerical experiments performed by C. G. Panagiotopoulos and R. Vodicka), or a combination with a rate-dependent healing.

Multilevel Low-rank Approximation Preconditioners

Y. Saad

This presentation will discuss preconditioning methods for solving linear systems of equations that are based on exploiting low-rank approximations to certain matrices. These methods have a number of appealing features. Because they are essentially approximate inverse techniques, they handle indefiniteness quite well. At the same time they are amenable to SIMD computations such those inherent to GPUs. We will first describe the methods for Symmetric Positive Definite model problems arising from Finite Difference discretizations of PDEs. We will then show how to extend them to general situations, by exploiting the domain decomposition framework.

Old and New Iterative Methods for the Solution of Generalized Lyapunov Equations

D. B. Szyld

There has been a flurry of activity in recent years in the area of solution of matrix equations. In particular, a good understanding has been reached on how to approach the solution of large scale Lyapunov equations; see, e.g., [1]–[3]. An effective way to solve Lyapunov equations of the form $A^T X + XA + C^T C = 0$, where A and X are $n \times n$, is to use Galerkin projection with appropriate extended or rational Krylov subspaces. These methods work in part because the solution is known to be symmetric positive definite with rapidly decreasing singular values, and therefore it can be approximated by a low rank matrix $X_k = Z_k Z_k^T$. Thus the computations are performed usually with storage which is lower rank, i.e., much lower than order of n^2.

Generalized Lyapunov equations have additional terms. In our work, we concentrate on equations of the following form

$$A^T X + XA + \sum_{j=1}^{m} N_j X N_j^T + C^T C = 0,$$

Such equations arise for example in stochastic control [4]. It has been proposed, e.g., in [5], to use approximations to conjugate gradients or to BiCGStab, appropriately preconditioned, where the basis vectors (matrices) and iterates are "truncated" throughout the algorithm to keep all these elements represented by low-rank matrices.

In the present work, we propose a return to classical iterative methods, and consider instead stationary iterations, where the iterate $X_{k+1} = Z_{k+1} Z_{k+1}^T$ is the solution of

$$P(X) := A^T X + XA = Q(X_k), \quad k = 0, 1, \ldots \tag{1}$$

where $Q(X) = -\sum_{j=1}^{m} N_j X N_j^T - C^T C$; cf. [6]. The classical theory of splittings applies here, while imposing certain conditions on $P(X)$ and $Q(X)$.

One of the advantages of this classical approach is that only the data and the low-rank factors of the old and new iterates X_k and X_{k+1} need to be kept in storage. Furthermore, the solutions of the Lyapunov equations (1) can be performed with the Galerkin projection methods mentioned above, where the growth of rank can usually be well contained.

Furthermore, in this instance, the solution of (1) for each column of $Q(X_k)$ gives us further reduction of the memory usage (and CPU times), as compared to a simultaneous (block) solution for all columns. This is because the singular values of the matrix solution for a right hand side of low rank decay much fatser than those of a right hand side of larger rank.

Numerical experiments show the competitiveness of the proposed approach.

This is joint work with Stephen D. Shank and Valeria Simoncini.

[1] P. Benner, J.-R. Li, and T. Penzl. Numerical solution of large-scale Lyapunov equations, Riccati equations, and linear-quadratric optimal control problems. *Numerical Linear Algebra with Applications*, 15:755–777, 2008.

[2] V. Druskin, and V. Simoncini. Adaptive rational Krylov subspaces for large-scale dynamical systems. *Systems and Control Letters*, 60:546–560, 2011.

[3] V. Simoncini. A new iterative method for solving large-scale Lyapunov matrix equations. *SIAM Journal on Scientific Computing*, 29:1268–1288, 2007.

[4] T. Damm. *Rational Matrix Equations in Stochastic Control*. Lecture Notes in Control and Information Sciences, vol. 297, Springer, Berlin and Heidelberg, 2004.

[5] P. Benner and T. Breiten. Low rank methods for a class of generalized Lyapunov equations and related issues. *Numerische Mathematik*, 124:441–470, 2013.

[6] Ch.-H. Guo and A.J. Laub. On the iterative solution of a class of nonsymmetric algebraic Riccati equations. *SIAM Journal on Matrix Analysis and Applications*, 22:376–391, 2000.

Part C
Abstracts of contributions

An Adaptive Mesh Strategy for Convection Diffusion Problems

V. Aggarwal, B. Srinivasan

It is well known that whenever central finite difference schemes (second order or higher order central schemes) are applied to solve convection diffusion singularly perturbed problems (SPP) numerically on uniform meshes, non physical oscillations observed in the numerical solution and their magnitude increases in the layers (boundary and interior) regions. The presence of these large non physical oscillations in the approximated solution shows that central finite difference operators on the uniform meshes are unstable. To eliminate these oscillations while retaining the order of accuracy, one needs either a fine mesh at the layer. This maybe done either via uniformly fine meshing or via an adaptive mesh strategy. The former strategy increases significantly in computational cost as the small parameter decreases.

In this paper, a new adaptive mesh strategy has been developed for solving SPP with higher order central compact schemes. Our strategy uses a novel, entropy-like variable as the adaptation parameter for convection diffusion SPP. Further, unlike the popular Bakhvalov and Shishkin type meshes, no pre-knowledge of the location and width of the layers (boundary as well as interior) is needed. The method is completely free of arbitrary parameters and results in oscillation free solutions to a range of convection-diffusion SPP. Numerical results for various test problems are presented and comparison have been shown with the existing non uniform meshes. This method is expected to aid in robust computations of convection dominated SPP.

Numerical Treatment of Algebraic Equations with Symmetries

J. Alvarez, A. Duran

The resolution of systems of algebraic equations with symmetry groups appears in the mathematical treatment of many models, [2, 3]. These groups consist of transformations that map solutions of the algebraic system into other solutions. Some consequences of the existence of such symmetry groups, from an analytical point of view, have been described in e. g. [3]. The main goal of this talk is discussing the influence of the symmetries in the numerical procedures to approximate the solutions of the system. This question that is more or less implicitly observed but, to our knowledge, not formally discussed, except in particular cases, [1]. The study is focused on fixed-point iteration algorithms.

[1] J. Alvarez, A. Duran, The Petviashvili method and its applications: I. Analysis of convergence, J. Comput. Appl. Math. 266 (2014) 39-51.

[2] J.E. Marsden, T.S. Ratiu: Introduction to Mechanics and Symmetry, Springer, New York (1994).

[3] P.J. Olver: Applications of Lie Groups to Differential Equations, Springer, New York (1986).

A Study of the Impact of the Pseudospectra on the Stability of the Recurrent Neural Networks

S. Basterrech, V. Snášel

Recurrent Neural Networks (RNNs) have been used for information processing in biological neural systems and to solve machine learning problems. The recurrent topology ensures that the non-linear transformation of the input history can be stored in internal states. As a consequence, they are a powerful tool for time series modeling. The system dynamics operate in a regime that can be stable or can exhibit chaotic behavior. Over the past few years, several studies concerning the network stability have been carried out using Lyapunov exponents and the computation of the edge of chaos. These works shown the significant impact of the eigenvalues modulus on the system stability. In recurrent topologies computing the spectrum could be not-robust and computational expensive. Below the converge rate is determinate by how close certain eigenvalues are to zero. In this work, we analyze the impact of the $\epsilon-$pseudospectrum on the stability of the RNNs, which is robust and cheaper than the computation of the eigenvalues. We explore the relationship between the pseudospectra and stability of the RNNs on a set of widely used supervised learning problems.

Isogeometric Analysis for Navier-Stokes Equations

B. Bastl, M. Brandner, J. Egermaier, K. Michálková, E. Turnerová

This contribution is devoted to the simulation of viscous incompressible fluid flow described by Navier-Stokes equations. The numerical model is based on the isogeometrical approach. This is a part of the project devoted to the shape optimization of water turbines. Typically in engineering practice, design is done in CAD systems and meshes, needed for the finite element analysis, are generated from CAD data [1]. Primary goal of using isogeometric analysis is to be geometrically exact, independently of the discretization. Then we do not need to create any other mesh - the mesh of the so-called "NURBS elements" is acquired directly from CAD representation.

The numerical solution of Navier-Stokes equations by the standard finite element method is reasonable only for relatively low Reynolds numbers. Therefore, it is necessary to use stabilization methods (e.g. SUPG, PSPG, see [2]). Other problems with oscillations can be solved by the SOLD methods [3]. The following steps of this project will be focused on turbulence modelling and transient case described by non-stationary Navier-Stokes equations.

Acknowledgement: This work has been supported by Technology agency of the Czech Republic through the project TA03011157 Innovative techniques for improving utility qualities of water turbines with the help of shape optimization based on modern methods of geometric modeling.

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Shape Optimization in 3D Contact Problems with Coulomb Friction

P. Beremlijski, A. Markopoulos

We study the discretized problem of the shape optimization of 3D elastic bodies in contact. Mathematical modeling of the Coulomb friction problem leads to an implicit variational inequality. It has been shown that for small coefficients of friction the discretized contact problem with Coulomb friction has a unique solution and this solution is Lipschitzian as a function of a control variable describing the shape of the elastic body. The uniqueness of the equilibria for fixed controls enables us to apply the so-called implicit programming approach. Its main idea consists in minimization of a nonsmooth composite function generated by the objective and the (single-valued) control-state mapping. For the solution of this nonsmooth problem we use our Matlab implementation of bundle trust method proposed by Schramm and Zowe. In each step of the iteration process, we must be able to find the solution of the state problem (contact problem with Coulomb friction) and to compute one arbitrary Clarke subgradient. To get subgradient information needed in the used numerical method we use the differential calculus of Mordukhovich.

For solving a state problem we use the method of successive approximations. We use domain decomposition technique for speed-up of the computation of a solution of the state problem. We apply a modification of FETI that we call Total FETI, which imposes not only the compatibility of a solution across the subdomain interfaces, but also the prescribed displacements.

Numerical examples illustrate the efficiency and reliability of the suggested approach.

Hydro-mechanical Modelling of SEALEX Experiments

R. Blaheta, M. Hasal, Z. Michalec

This contribution describes the on-going modelling of the SEALEX experiments within Decovalex 2015 project. The concerned models are based on coupling Richards model of flow in variable saturated porous media and mechanical deformation modelled by elasticity or plasticity. The aim is to show how these models can be implemented within

the COMSOL Multiphysics software, discuss a bit the computed results and possible numerical techniques for future development of the models.

Parallel Processing of High Resolution FEM Systems in Micromechanics

R. Blaheta, O. Jakl, J. Starý

Our aim is to determine effective (homogenized) material properties from tests on small material samples with relatively complicated inner structure. Such testing means solution of boundary value problems on test domains involving the microstructure with loading provided by suitable boundary conditions. This leads to the solution of high resolution FE systems.

In our case, we investigate geomaterials, which are handled by X-ray CT scanning of small rock samples. Those scans provide 3D information on the structure of the samples. Material properties of the individual material constituents are additional input.

For the FE solution of the high resolution boundary value problems of tens or hundreds million degrees of freedom we make use of parallel computers at the Institute of Geonics and the IT4Innovations supercomputer centre in Ostrava. We describe efficiency of the in-house GEM solvers exploiting the Schwarz domain decomposition method with aggregation by performing computational experiments on the computing platforms above.

Efficient solution of these systems is necessary for successful solution of inverse material identification problems.

Mindlin-Timoshenko Beam in a Dynamic Contact with a Rigid Obstacle

I. Bock

The dynamic contact problems are not frequently studied comparing with static or quasistatic problems. The abstract theory of variational inequalities cannot be applied in the dynamic case. The main problem is the change of the sign of the velocity vector after hitting the rigid obstacle by the structure under consideration. Simultaneously the acceleration of the movement can be expressed only in a generalized distributive form. There are two ways of solving hyperbolic variational inequalities modeling dynamic contact problems. The authors [1] substitute the nonstationary initial-boundary value problem by a sequence of stationary problems in chosen time moments after applying finite differences instead of time derivatives. Another approach is the penalization method applied by authors in the paper [2]. This method leads to the sequence of nonlinear hyperbolic partial differential equations. In [2] the viscoelastic Reissner-Mindlin plate was considered. Solving a dynamic contact problem for an elastic Reissner-Mindlin plate is an open problem.

In the case of an elastic Mindlin-Timoshenko beam problem one can apply both approaches mentioned above. We apply the substitution of time and space derivatives by

finite differences and finite elements respectively enabling to solve the problem numerically. The convergence of the method will be investigated.

Acknowledgement: The paper is supported by the Grants APVV-0246-12 and VEGA 1-0426-12 of the Slovak Republic.

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BEM-based Domain Decomposition for Polygonal Subdomains

J. Bouchala, D. Lukáš, L. Malý, P. Vodstrčil

We propose and analyze a parallel solver based on primal domain decomposition for two-dimensional elliptic partial differential equations with highly varying material coefficients. While the standard theory has been developed only for triangular or quadrilateral subdomains, where harmonic base functions are available, the practical mesh-partitioners generate complex polygonal subdomains. We aim at bridging this gap. Being inspired by [3] we generalized the method originally proposed and analyzed in [2], so that the coarse solver can treat rather general polygonal subdomains. To this goal we employ boundary element discretizations of Steklov-Poincare operators on subdomains.

Our method enjoys the parallel scalability $O((1+\log\frac{H}{h})^2\frac{n}{N})$, where h, H, n, and N denote the fine discretization parameter, coarse discretization parameter, number of DOFs, and number of processes, respectively. This is documented with numerical results. In [1] we also give details of the standard analysis.

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Flow123d - Modeling Tool for Processes in Fractured Media

J. Březina, J. Stebel

Modeling underground water flow and transport processes on domains of regional scale has to deal with presence of spatially localized features (e.g. cracks and channels) with

material properties significantly different compared to the surrounding continuum. One of possible solutions is integration of governing equations in the normal direction, derivation of the equations on 2D or 1D domains corresponding to the localized features, and introduction of coupling between the equations on domains of different dimension. This approach stood at the origin of the Flow123d software about ten years ago. Same approach was considered independently by several other authors, e.g [1].

The aim of this contribution is twofold. First, we present derivation of the equations and their couplings in the multi-dimensional approach from the general advection-diffusion equation. Second, we overview main features of the Flow123d software[2]. These include models for: steady and unsteady water flow in saturated porous media, transport of substances due to advection, diffusion and hydrodynamic-dispersion, adsorption, dual porosity model, first order reactions and heat transfer. Multi-dimensional approach is used consistently in all models allowing simultaneous coupling of the equations on 1D, 2D, and 3D domains. The software has very flexible input interface; almost all parameters in the equations as well as in the boundary conditions can be given as a general function of both time and space with values including integers, scalars vectors and tensors. The function can be specified in several ways: piecewise constant on regions, as a run-time parsed formula, via Python script, or using GMSH data file for arbitrary values on individual elements of the computational mesh.

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Robust Discontinuous Galerkin Method for Transport Processes in Fractured Porous Media

J. Březina, J. Stebel

Mathematical models of solute transport and heat transfer in a fractured rock massif have the form of an advection-diffusion equation. We aim to develop a robust method for the numerical solution of these processes taking into account the geometrical complexity and material inhomogeneity of the model.

In the talk we shall present a mathematical model for the advection-diffusion equation in a system of domains with different spatial dimensions, which results from the dimensional reduction of fractures, and establish it well-posedness. Further, we will describe the weighted interior penalty discontinuous Galerkin method [1] adopted to the model, and show its approximation properties. The method will be demonstrated by example computations done with help of the computational code Flow123d [2].

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Coupled Model of Flow-through Experiment in Novaculite Fracture

I. Bruský, J. Šembera

The talk focuses on a coupled mechanical-geochemical model of the laboratory experiment. The experiment is as follows: water is injected into a single fracture in novaculite rock sample under moderate effective stresses. There are measurements of fractures surfaces, pH and SiO_2 concentration of outlet solution. The model simulates closing of fracture and chemical composition of outlet solution. Using the model, we try to understand all of the processes that taking place in the experiment. Conceptual model will be introduced. The results will be discussed.

Acknowledgement: The work of I. Bruský was supported by the Ministry of Education of the Czech Republic within the SGS project No. 21066/115 on the Technical University of Liberec. J. Šembera was supported by Technology Agency of the Czech Republic via project No. TA02021132.

On Modelling of Non-Newtonian Free Surface Flows Using the Lattice Boltzmann Method

O. Bublík, J. Vimmr, A. Jonášová

This work is focused on the numerical simulation of non-Newtonian free surface fluid flow using the lattice Boltzmann method, which has become very popular during the last decade. The method is based on the mesoscopic fluid description unlike the classical methods that utilise the macroscopic description. Because of this approach, the lattice Boltzmann method is simpler and less computationally demanding than the finite element and finite volume methods. The lattice Boltzmann method originates from the lattice gas cellular automata (LGCA), which represents a simplified molecular dynamics. Compared to the LGCA, the lattice Boltzmann method operates with virtual particles, which make it possible to solve various complex flow problems such as free surface flow and multiphase flow.

To capture the free surface of the fluid in this study, we adopt the algorithm based on the volume of fluid method established by Thürey (Thürey, Ph.D. thesis, 2007). This algorithm is able to simulate the free surface of the fluid in a natural way. For the

simulation of non-Newtonian effects, the power-law viscosity model is used. The rate of deformation tensor is computed with the help of the finite difference method.

The developed computational algorithm is used for the simulation of the moulding process in the "Z" test geometry by considering a non-Newtonian fluid (polyurethane). The obtained results show that the developed algorithm is well suited for the modelling of free surface flows.

Acknowledgement: This work was supported by the the project TA03010990 of the Technology Agency of the Czech Republic.

Analytical Solution for Singularities of Rotationally Symmetric Stokes Flow and Applications to Finite Element Solution

P. Burda, M. Hanek, J. Šístek

We present analytical solution of the Stokes problem in rotationally symmetric domains. We analyze the singularities arizing in rotationally symmetric tubes with nonsmooth walls, e.g. with forward and/or backward steps, or jumps in diameter. We get the asymptotic behaviour of the Stokes flow near 'corners' of the rotationally symmetric tubes.

In [1] we described the way how to make use of the asymptotics of the solution near the singular points. The results obtained in [1] may be applied to axisymmetric flows, using the 2D domain as a cross section of the axisymmetric tube. In the paper we show the singularity in pressure in the hydrostatic cell.

Acknowledgement: This work was supported by the IT4Innovations Centre of Excellence project, reg. no. CZ.1.05/1.1.00/02.0070 and partly by the Czech-American Cooperation Program of the Ministry of Education, Youth and Sports of the Czech Republic under research project LH11004.

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Solving Elastoplastic Problems with the FLLOP Solver

M. Čermák, V. Hapla, D. Horák

We present here our novel package FLLOP for quadratic programming and FETI domain decomposition, built on top of PETSc (similarly to TAO and SLEPc packages). Currently tested applications include mainly engineering problems of structure mechanics: linear elasticity, contact problems, elastoplasticity, and shape optimization.

Here we will focus on the elastoplastic problems. Model of elastoplasticity is time dependent model where the history of loading is taken into account. We consider the

associated elastoplasticity with von Mises plastic criterion and isotropic or kinematic hardening law. Elastoplastic problems are nonlinear, thus some linearization scheme is needed; we use the Newton method with a line search implemented in the PETSc SNES package as the SNESNEWTONLS type. The pseudo-timestepping needed for time depending problems is implemented with the PETSc TS package. The linear problem in each Newton iteration is finally solved by our FLLOP package. FLLOP is compatible with the formulation resulting from the TFETI domain decomposition where the subdomains are all floating, corresponding stiffness matrices assembled independently, and continuity as well as Dirichlet boundary conditions enforced with the Lagrange multipliers. Numerical and parallel scalability and efficiency of our implementation will be illustrated on several elastoplastic benchmarks in 3D.

Isogeometric Analysis in Electronic Structure Calculations

R. Cimrman, M. Novák, R. Kolman, M. Tůma, J. Vackář

We develop a new software for ab-initio calculations of electronic states within the density-functional framework, based on the open source finite element package SfePy (http://sfepy.org). The code should allow computing various material properties by means of computing the total energy of a system as well as derivatives of the total energy w.r.t. atomic positions. The derivatives, also known as Hellman-Feynman forces, require, from practical computation reasons, that the discretized charge density and wave functions have continuous derivatives in the whole solution domain. In the contribution we describe our use of isogeometric analysis (IGA), a spline modification of finite element method (FEM), to achieve the needed continuity. The technique of Bezier extraction is used for adding the IGA capabilities to our FEM based code.

Acknowledgement: The work was supported by the Grant Agency of the Czech Republic, project P108/11/0853. R. Kolman's work was supported by the grant project of the Czech Science Foundation (GACR), No. GAP 101/12/2315, within the institutional support RVO:61388998.

The Projected Barzilai-Borwein Method for Solving Quadratic Programming Problems with Separable Elliptic Constraints

Z. Dostál, L. Pospíšil

The Barzilai-Borwein method for solving minimizing problems without constraints was firstly presented in [1] and afterwards, the projected version of the algorithm was sucessfully used in the development of Spectral Projected Gradient Method [2] for solving minimizing problems of general function on convex sets.

In this paper, we present the modification without additional line-search step. We control the descend of quadratic cost function using additional decrease control. In the

case the value of object function did not decrease during last few iterations, we return back and use more conservative constant step-size, which always induces the sufficient descend. The phenomena of monotone descend of projected gradient method with constant step-size was introduced in [4].

The performance of our algorithm is demonstrated on the solution of a contact problem with anisotropic Tresca friction discretized by finite element method. Our experiments are compared with recent results [3].

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Calibration Methods for Rainfall-runoff Simulations inside FLOREON+ System

D. Fedorčák, M. Theuer, R. Vavřík, Š. Kuchař, V. Vondrák

One of the primary goals of the FLOREON+ project is creation of flood monitoring & prediction system. During its development, the project evolved into various aspects of the disaster management support including air-pollution modelling or traffic monitoring and analysis. However, the rainfall-runoff simulation is a core module which must be continually improved and maintained in order to provide best possible predictions.

There are many problems which must be faced when the rainfall-runoff simulation is deployed for practical and automated usage and most of them are connected with the parameterization of the modelling task. Results of the simulation are heavily influenced by the river basin abstraction which is based on many empirical attributes (e.g. CN values). It is difficult to set all the attributes consistently with the reality and some level of generalization is necessary. Unfortunately, the model verification indicates that there are locations where the lack of correct river basin description increases the simulation error high above negligible levels.

This article targets the problem of calibration of various rainfall-runoff (RR) models incorporated into the FLOREON+ system. The calibration is based on inverse problem techniques and extensive usage of HPC capabilities available at the IT4I center of excellence. The calibration process includes a variety of approaches starting with simple semi-analytic gradient methods where applicable (own RR model implementation) up to

global optimization methods for black boxed RR models. Moreover, specific issues may arise when dealing with the RR model calibration. For example, the parallelization of such process is handicapped by the hierarchic nature of the model (channels must be evaluated according to the river flow). Another issue lays in the input data (precipitations, measured runoff levels etc.) where fundamental differences between investigated events (e.g. season of the year) may lead to difficulties with construction of the consistent data set.

Searching for Local Contact Constraints in the Finite Element Procedures for Contact Problems

D. Gabriel, J. Kopačka, J. Plešek

In the context of the finite element method, a frictionless three-dimensional contact algorithm using pre-discretization penalty formulation was proposed [1]. The method was shown to be consistent with the variational formulation of a continuum problem, which enabled easy incorporation of higher-order elements with midside nodes to the analysis. Local search and the penalty constraint enforcement were performed on the Gausspoint level of quadratic serendipity elements rather than the nodal level of a finite element mesh. Owing to a careful description of kinematics of contacting bodies when the non-linearized definition of penetration has been introduced, the displacement increments in the course of one load step were permitted to be large. Thus, the extension of the algorithm to geometrically nonlinear problems was straightforward. The algorithm proved to be robust, accurate and symmetry preserving-no master/slave surfaces had been introduced.

In this work, we focused on one particular task at hand-measuring penetration of a Gauss point through the counterparts object surface. It is necessary first to define the outward normal and then to compute its intersection with a curved surface, establishing distance. Although appearing trivial at first glance the numerical solution process is far from being easy, especially when dealing with severely distorted surfaces. Several methods for the solution of non-linear algebraic systems were thoroughly tested: the Newton-Raphson procedure, the least square projection, the steepest descent method, Broyden's method, BFGS method and the simplex method.

The effectiveness of these methods was tested by means of proposed benchmark problems, which involves the bending of two rectangular plates over a cylinder and the contact-impact between two tubes. It is concluded that it is the simplex method that significantly increases the robustness of the local contact search procedure and, consequently, even improves the effectiveness of the global solution [2].

Acknowledgement: GAP101/12/2315 with institutional support RVO:61388998.

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Comparison Results of Running of an Eulerian Computer Model for Long Range Air Pollution on Different High-performance Computers

K. Georgiev, Z. Zlatev

The Danish Eulerian Model (DEM) is an Eulerian model for studying the transport of air pollutants on large scale. Originally, the model was developed at the National Environmental Resarch Institute (NERI) of Denmark (Roskilde, Denmark). The model computational domain covers Europe and some neighbour parts belong to the Atlantic Ocean, Asia and Africa. If DEM model is to be applied by using fine grids, then its discretization leads to a huge computational problem. If the space domain is discretized by using a (480×480) grid, which corresponds to cells with dimensions $(10\,\text{km} \times 10\,\text{km})$ and the number of chemical species studied by the model is 35, then several systems of ordinary differential equations containing 8 064 000 equations have to be treated at every time-step (the number of time-steps being typically several thousand). If a three-dimensional version of the same air pollution model is to be used, then the figure above must be multiplied by the number of layers. This implies that such a model as DEM must be run only on high-performance computer architectures. The implementation and tuning of such a complex large-scale model on each different computer is a non trivial task.

Here, the unified parallel version of DEM (UNI-DEM) will be used and some comparison results of running of this computer model on different kind of vector, parallel computers with distributed memory, parallel computers with shared memory and parallel computers with two level of parallelism will be presented. The main idea in the parallel version of DEM is the domain partitioning approach. Discussions according to the effective use of the cache and hierarchical memories of the modern computers as well as the performance, speed-ups and efficiency achieved will be done. The parallel code of DEM, created by using MPI standard library, appears to be highly portable and shows good efficiency and scalability on different kind of vector and parallel computers.

Diffusion Wavelet Based Space - time Adaptive Numerical Method

K. Goyal, M. Mehra

The paper presents a diffusion wavelet based space-time adaptive numerical method to solve partial differential equations. The diffusion wavelet is used for spatial as well as time adaptivity. The time steps are adapted to the spatial resolution such that CFL

like stability conditions are satisfied. The beauty of the method lies in the fact that the same operator is used for the approximation of differential operators and for the construction of the diffusion wavelet. The numerical results show that the method can accurately capture the emergence of the localized patterns at all the spatial and temporal scales. The convergence of the method is verified. The method is applied to a couple of test problems. For each test problem, the CPU time taken by the proposed method is compared with the CPU time taken by traditional methods. It is observed that the diffusion wavelet based space-time adaptive numerical method is highly efficient.

FLLOP: A Massively Parallel QP Solver Compatible with the TFETI Substructuring Scheme

V. Hapla

We present here our novel FLLOP package for quadratic programming, built on top of the PETSc framework. FLLOP is compatible with the TFETI substructuring scheme (domain decomposition method) where the subdomains are all floating, corresponding stiffness matrices assembled independently, and continuity as well as Dirichlet boundary conditions enforced with the Lagrange multipliers. Employing this scheme we can solve real world problems discretized to huge numbers of elements on large distributed memory machines. Currently tested FLLOP applications are dominated with engineering problems of elasticity including contacts, elasto-plasticity, shape optimization and their combinations.

On Parameter Dependent Static Contact Problems

J. Haslinger, V. Janovský, R. Kučera

Let us consider the static contact problem with Coulomb friction on two planar domains assuming a standard finite element approximation. Under generic assumptions the problem has always a solution.

The aim is to construct examples of *non-unique* solutions. We exploit the *continuation* with respect to a given parameter. Changes of the parameter of the problem correspond to solution changes. The resulting *solution path* is continuous, piecewise smooth. It consists of oriented smooth branches connected by transition points. The particular transition points called *folds* are responsible for the emergence of non-unique solutions.

We developed a) a predictor-corrector algorithm to follow oriented smooth branches, b) branching and orientation indicators to detect transition points and the folds, in particular. The techniques incorporate semi-smooth Newton iterations and inactive/active set strategy on the contact zone.

Acknowledgement: Supported by the grant P201/12/0671 of the Grant Agency of the Czech Republic.

Solution of Contact Problems Using FLLOP Library

D. Horák, V. Hapla, L. Říha, A. Markopoulos

The poster deals with the ingredients helping us to reach better scalability of the solvers for systems of linear equations and contact problems. For their solution we develop at IT4Innovations at VSB-TU Ostrava novel software package FLLOP (FETI Light Layer On top of PETSc). It is an extension of PETSc, which is a suite of data structures and routines for the parallel solution of scientific applications modelled by PDE. These solvers can employ direct, iterative or hybrid (combining both previous) methods. Our team has a longterm experience with design and implementation of the scalable domain decomposition methods of FETI type, especially for contact problems, combining iterative a direct solvers. Each method has its pros and cons. We will present bottlenecks of these methods including the strategies for their elimination.

Typical example is the coarse problem solution appearing in TFETI method or in deflated conjugate gradient method (DCG). We are able to reach significant improvements using parallel direct solvers in subcommunicators formed by CPUs only or by CPUs accelerated by GPUs/MICs, or using iterative pipelined CG solver applied to the coarse problem matrix better conditioned because of the orthonormalization of the rows of the constrained matrix or the columns of the null space of the stiffness matrix. For contact problems solved by FETI, once the dual solution is computed, to get the primal solution it is necessary to exclude rows in the constraint matrix with inequalities corresponding to zero Lagrange multipliers, compute new coarse space matrix and solve new coarse problem. We will present the new efficient reconstruction formula for the amplitudes of the rigid body modes in FETI for contact problems avoiding this computation using part of the residuum and the multipliers generated by SMALSE algorithm. Numerical experiments illustrate the efficiency of these approaches.

Rendering and Post-processing of OpenFOAM CFD Simulations

M. Jaroš

In this talk we deal with the rendering and post-processing of OpenFoam data. OpenFoam is open source software for computational fluid dynamics (CFD) simulations. There are few possibilities to extract result from OpenFOAM such as IsoSurfaces, StreamLines or Particles. The visualization of the generated results is done by the Visualization Toolkit (VTK) of the open source application ParaView. But the rendering options provided by this toolkit are limited. More advanced post-processing results can be achieved by using of Blender (one of the most popular open source 3D graphics applications, which provides a wide spectrum of modeling, lighting, animation, and video post-processing functions in one package), MaxwellRender (a render engine based on the physics), and VTK together. The whole process will be illustrated on a few examples of CFD simulations.

The Monotonic Algorithm for the Solution of the Variational Equations with Bound Constrains Exploiting Weakly Feasible Steps

M. Jarošová, Z. Dostál

In this talk we propose a modification of our MPGP algorithm for the solution of bound constrained quadratic programming problems. The algorithm is based on active set strategy and explores the faces by conjugate gradients and changes the active sets and active variables by gradient projections. By the theory the MPGP algorithm converges fast when it generates long chains of CG iterations, thus it can be advantageous to continue the CG iterations even if the trial CG step is unfeasible. The modification of MPGP proposed here is based on the observation that the convergence of MPGP is preserved when we insert between the last feasible iteration and the expansion step a number of unfeasible iterations. We examine the conditions for accepting the unfeasible steps and the convergence of the resulting algorithm. We compare the behavior of both algorithms on the academic and engineering benchmarks.

Black-box Eigenvalue Solver for the 3D Integro-differential Hartree-Fock Equation by Tensor Numerical Methods

V. Khoromskaia

The Hartree-Fock eigenvalue problem governed by the 3D integro-differential operator is the basic model in *ab initio* electronic structure calculations. Several years ago the idea to solve this equation by fully 3D grid based numerical approach seemed to be unfeasible, and tensor-structured methods did not exist. In fact, they evolved during the work on this challenging problem [1,2,4]. We present a Hartee-Fock solver by the tensor numerical methods based on the rank-structured calculation of the 3D Laplace and nuclear potential operators, and of the 3D two-electron integrals tensor (TEI), using a general, well separable basis discretized on $n \times n \times n$ 3D Cartesian grids. The arising 3D convolution integrals with the Newton kernel are replaced by algebraic operations in 1D complexity [1,2]. This enables usage of 3D grids with routine size of 10^{15} entries in accurate calculations of the 3D integral operators [5]. The quantics tensor approximation is used to evaluate the 3D Laplace operator in $O(\log n)$ complexity [3]. The performance of our "black-box" solver in time and accuracy is compatible with the benchmark packages in quantum chemistry based on analytical precalculation of involved multidimensional integrals [5]. We present on-line demonstrations of our solver (in Matlab) on a laptop in *ab initio* calculations for the ground state energy of compact molecules including Glycine and Alanine amino acids.

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Parallel Solution of Elasticity Problems using Aggregations

R. Kohut

The contribution is devoted to a FE solution of elasticity problems. For the solution of the corresponding system of linear equations we use preconditioned CG method with overlapping Schwarz type preconditioners. The efficiency of the preconditioner decreases with an increasing number of subproblems and for avoiding this problem it is necessary to involve a coarse mesh correction. We use the algebraic coarse space created by aggregation.

The aggregation used in the contribution is based on the idea that the basis functions for the coarse grid space are given by a linear combination of the basis functions for the fine grid space in the case of fully compatible FE spaces. The corresponding coefficients are given by the function values of the coarse grid basis function in the corresponding fine grid nodes. Using these relations between basis functions for the coarse grid and the fine grid spaces we obtain formulae for relations between the coarse matrix elements and the fine matrix elemenst.

If the grids are nonrectangular and nonuniform the determination of the coefficients can be difficult and time consuming. In some problems the fine grid is such complicated that the fully compatible coarse grid space doesn't exist. In our codes we use FE with structural grids. It means that the position of each node is given by the triplet of indices (i, j, k) and the corresponding nodal coordinates $(x(i, j, k), y(i, j, k), z(i, j, k))$. The general structural grid with $n_x \times n_y \times n_z$ nodes corresponds to the rectangular uniform "index" grid where the node in the position (i, j, k) has the coordinates (i, j, k). So we use the presented formulae for these index coordinates. The numerical tests are presented at the end of the contribution.

On Homogenization-based Models for Fresh Concrete Flow through Reinforcing Bars

F. Kolařík, J. Zeman, B. Patzák

Mechanical performance and durability of concrete structures is to a significant extent influenced by the casting process. Predicting the flow behavior of concrete in the formwork has thus become an important part of the design procedure of concrete mixes. The present contribution is concerned with the so-called homogeneous models [1], augmented with computational homogenization procedures to account for sub-scale phenomena arising e.g. from the presence of an array of reinforcing bars.

In the most simple steady-state case, we decompose the domain into two parts corresponding to a homogeneous fluid and porous medium. In the first sub-domain, the flow is governed by the Stokes model, whereas in the second sub-domain we employ the Darcy law with permeability determined from the homogenized Stokes flow [2]. At the interface, the Beavers–Joseph–Saffman conditions are adopted. Accuracy of the homogenized formulation is investigated by comparing its predictions to the fully resolved simulations.

Acknowledgement: This work was supported by the Czech Science Foundation through project No. 13-23584S.

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Goldberg-like Decompositions and Voxel Representation of 3D Space

A. Kolcun

Space decomposition methods represent an important part of numerical modelling process. Using current methods, creating 3D models is an extremely time-consuming, unreliable, and labour-intensive process. So, when the geometry information is obtained e.g. from computer tomograph or similar devices, i.e. in the form of pixel/voxel grid, it is reasonable to create the space decomposition in the same or similar way. Different raster concept, based on regular hexagonal mesh, is analyzed e.g. in [3]. There are several methods how to decompose 3D space into the set of the same tetrahedra [1], [2], [4]. In the paper the discretization scheme based on Goldberg's one is introduced: we find tetrahedral element which is close to equilateral (regular) one and which can be used as a 3D space filler. Mutual realtionshis betwee voxel decomposition and our approach is presented.

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On an Accurate Explicit Time Integration Algorithm for Wave Propagation Problems in Solids

R. Kolman, S.-S. Cho, K. C. Park

The paper reports algorithmic treatments and numerical experiments an accurate explicit time integration algorithm [1, 2] with a time step size adjustment for finite element computations of wave propagation problems in solids. The resulting algorithm traces different waves with different intermediate time steps, which makes use not only of the different critical time steps for different waves. In addition, the partition of unity properties of the finite element shape functions is exploited to realize the component-wise partition of equations of motion to longitudinal and shear parts such that the partitioned equations for each wave component can be integrated in accordance with their different wave speeds. The algorithm is implemented with a diagonal mass matrix, second-order accurate, and conditionally stable. We remark that the algorithm produces excellent histories not only of displacements, stresses and velocities, but also of accelerations.

A predictor-corrector form of the present algorithm, its implementation details, and performance of the three-time step scheme, is reported. In that paper, we describe how we have implemented the algorithm in terms of an equivalent predictor-corrector form with a critical time step size estimator for the both components of equations of motion into standard finite element codes exploited quadrilateral and hexahedral finite elements.

The contribution is concluded with some numerical examples, as applied to linear and non-linear wave propagation and contact problems, to verify and validate the proposed time integration method.

Acknowledgement: GACR project GAP101/12/2315 under support RVO:61388998, WCU Program through KOSEF project R31-2008-000-10045-0, NRF project 2013M2B9A1024419, Radioactive Waste Manag. Technology Development project MOTIE 20111710200011.

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Influence of Mass Lumping Techniques on Contact Pressure Oscillations in Explicit Finite Element Contact-impact Algorithm Based on Isogeometric Analysis with NURBS

J. Kopačka, D. Gabriel, R. Kolman, J. Plešek

The main difficulty in the contact analysis is a non-smoothness of contacting surfaces. It arises from inequality constraints as well as from geometric discontinuities induced by spatial discretization. A remedy to the geometric discontinuity may be provided by isogeometric formulation. Recently, two penalty-based isogeometric contact algorithms were proposed in the reference [1]. The former is the so-called knot-to-surface (KTS) algorithm and the second algorithm is called the mortar-KTS algorithm.

Our symmetry preserving FE contact algorithm, originally proposed in [2], was extended for explicit transient dynamics in [3]. Further, beside the existing classic FE version of the contact-impact algorithm, the isogeometric NURBS based variant has been implemented.

Both versions of the algorithm are studied by means of a numerical example, which involves 2D frictionless dynamic Hertz contact problem of two equally shaped cylinders. The attention was paid to the influence of different lumping techniques, such as the row sums and HRZ method, on the oscillations of contact force and contact pressure. The comparison of the quadratic Lagrange shape functions with the second order NURBS basis functions demonstrate ambiguous results. Although contact pressure for IGA is smoother than for FEA, higher oscillations of contact force and contact pressure was observed for IGA. This is the case when the mass matrix was lumped by the HRZ algorithm for both IGA and FEA. The investigation reveals that oscillations are minimal for the consistent mass matrix.

Acknowledgement: GAP101/12/2315 with institutional support RVO:61388998.

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Acceleration of Direct and Iterative Solvers Used in Domain Decomposition Based Algorithms by Novel Techniques and Novel Many-cores Accelerators

T. Kozubek

The contribution describes acceleration of direct and iterative solvers used in FETI (Finite Element Tearing and Interconnecting) domain decomposition based algorithms applied to the solution of extremely large and complex problems arising in computational mechanics.

FETI type domain decomposition methods are powerful tool for constructing numerically and parallel scalable solvers. A great deal of research effort has been devoted worldwide to studying this topic. The reason is that FETI methods can dramatically increase potential and reliability of significant applications of FEM (Finite Element Method). The new FETI classes of methods and their applications represent a novel solution to many challenging problems with great impact to computational sciences.

First, we briefly describe ideas of the hybrid FETI domain decomposition method enabling massive parallelization until tens of thousands of cores. Then we say a few words about the Krylov subspace methods and preconditioners used in FETI solvers and how to accelerate them using communication avoiding and hiding techniques. The coarse problem solution is accelerated using MAGMA LU factorization based on many-cores accelerators GPU Nvidia Tesla K20m and Intel Xeon Phi 5110P. Finally, the performance of the resulting algorithms are demonstrated on mechanical engineering benchmarks and compared with standard FETI algorithms.

Incomplete Factorization by Local Exact Factorization (ILUE)

J. Kraus, M. Lymbery

This study explores a preconditioning technique referred to as incomplete factorization by local exact factorization (ILUE) in the framework of auxiliary space preconditioning. It employs an exact LU factorization of the local matrices corresponding to the overlapping or non-overlapping subdomains of a decomposition of the domain. The proposed preconditioner is analyzed and condition number estimates are derived. A comparison to standard one-level additive Schwarz methods is drawn. Finally, a representative collection of numerical experiments is conducted revealing the efficiency of the ILUE method, in particular, for problems with highly varying coefficients such as flows in highly heterogeneous porous media.

Moisture Transport in Partially Damaged Materials

J. Kruis, T. Koudelka

Moisture transport in concrete or masonry has strong influence on its durability and reliability. The moisture influences long-term behaviour of concrete. Moreover, the moisture

can transport chemical species which usually destroy mechanical properties of concrete or masonry.

Moisture transport in building materials is described by Künzel model introduced in 1995. The model is based on the balance equations for moisture and heat where the relative humidity and temperature appear. The moisture transport depends on the level of damage caused by mechanical or thermal load. The higher level of damage, the higher hydraulic conductivity.

Damage of concrete or rock material is very often described by an isotropic model with a single damage parameter although behaviour of concrete and rock in tension and compression is different. For complex loading paths, damage models with two damage parameters or orthotropic damage models have to be used. Nevertheless, the isotropic model is a suitable starting point for coupling of damage mechanics and moisture transport. The hydraulic conductivity depends on the damage parameter.

Acknowledgement: Financial support for this work was provided by project number 13-18652S of Czech Science Foundation. The financial support is gratefully acknowledged.

Modeling of Ferro/paramagnetic Transition

M. Kružík, J. Valdman

A recently developed model of temperature/external field–driven evolution of magnetization by Benešová-Kružík-Roubíček is fully discretized and tested on examples in 2D.

Partitioned and Monolithic Approaches for Fluid-structure Interaction Simulation

U. Langer, H. Yang

In this talk, we will discuss two strongly coupled approaches, partitioned and monolithic, to solve the fluid-structure interaction problems with applications in hemodynamics. The conventional partitioned approach is built on the coupling of existing fluid and structure sub-problem solvers. The fixed-point method using Dirichlet-Neumann or Robin-Neumann iterations on the interface equations, and the partitioned Newton's method applied to the Poincaré-Steklov operator fall into this type of approach. We will present a unified algebraic multigrid solver for the mixed formulation arising from stabilized discretization for both sub-problems, which shows the robustness with respect to mesh size and material parameters, in particular to the near incompressibility constraint of biological tissues. Although it is relatively easy to realize the algorithm by combining both sub-problem solvers, we may suffer from low convergence rate due to the added-mass effect in hemodynamics. Recently, a monolithic approach for the coupled fluid-structure interaction system becomes more and more interesting in order to gain

more robustness and effiency. Compared to the partitioned one, this approach solves the large coupled system in an all-at-once fashion. More precisely, we apply Newton's method in the outer iteration dealing with nonlinearities of the coupled system coming from the moving domains, convection terms, material laws, and transmission conditions, that usually converges in two or three iterations. As a price to pay, at each Newton iteration, a large linearized system is to be solved efficiently in order to reduce the overall cost. For this purpose, we will present some Krylov sub-space methods combined with robust and efficient preconditioners applied to the whole system, that altogether outperforms the partitioned approach.

Thin Film Flows of Piezoviscous Fluids in Lubrication Problems

M. Lanzendörfer

Hydrodynamic lubrication (or elastohydrodynamic lubrication, EHL) describes the formation of a thin film of lubricant in between two nonconforming (elastic) solid mechanical elements in relative motion. The model reduction due to the thin film flow assumptions, leading to Reynolds lubrication approximation and its many generalizations, is fundamental to both theory and computations in this field.

We will briefly review the classical concepts and comment on some recent results, focusing on the question of how justifiable and inevitable it is to use the Reynolds approach, and why the CFD approach proved to be limited so far, bringing forward some unexpected questions.

Our point of view will be related to the following equations:

$$\begin{aligned} \operatorname{div} \boldsymbol{v} &= 0, \\ \operatorname{div}(2\mu(p,|\boldsymbol{D}|^2)\boldsymbol{D}) &= \nabla p \end{aligned} \qquad \text{in } \Omega \subset \mathbb{R}^3, \tag{1}$$

governing the flow of an incompressible fluid with the viscosity $\mu(p,|\boldsymbol{D}|^2)$ increasing with pressure and decreasing with $|\boldsymbol{D}|^2$ (here $\boldsymbol{D} = \frac{1}{2}(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T)$).

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Parallel Fast BEM

D. Lukáš, P. Kovář, T. Kovářová, M. Merta, M. Kravčenko

We propose a method of a parallel distribution of densely populated matrices arising in boundary element discretizations of partial differential equations. In our method the underlying boundary element mesh consisting of n elements is decomposed into N submeshes. The related $N \times N$ submatrices are assigned to N concurrent processes to be assembled. Additionally we require each process to hold exactly one diagonal submatrix, since its assembling is typically most time consuming when applying fast boundary elements. We obtain a class of such optimal parallel distributions of the submeshes and corresponding submatrices by cyclic decompositions of undirected complete graphs. It results in a method the theoretical complexity of which is $O((n/\sqrt{N})\log(n/\sqrt{N}))$ in terms of time for the setup, assembling, matrix action, as well as memory consumption per process. Nevertheless, numerical experiments up to $n = 3145728$ and $N = 133$ document that the method exhibits superior parallel scalability $O((n/N)\log n)$ of the overall time, while the memory consumption scales accordingly to the theoretical estimate.

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Termodynamics of Rate-type Fluid Models and Their Applications to Deformations of Apshalt Binders

J. Málek

For the description of complicated behavior and response of viscoelastic materials we derive a new thermodynamically compatible rate-type fluid model. We show that this new model is capable of capturing two non-linear relaxation responses observed in the available experiments concerning asphalt binder; it is notable that the standard linear models such as Maxwell, Oldroyd and Burgers are not capable of capturing these experimental data. Finally, we use this model for the simulations in the deforming domains. Specifically, we compute two problems. In the first one we show the influence of the material parameters on the behavior of viscoelastic material. The other problem describes the rolling of incompressible asphalt binder with the real material parameters. This talk is based on the PhD thesis of Karel Tůma, it also reflects some results obtained jointly with K. R. Rajagopal and K. Tůma.

Spectral Diagonal Covariance in EnKF

J. Mandel, I. Kasanický, M. Vejmelka

Ensemble Kalman filter (EnKF) is one of the most common solutions to data assimilation problems, when observations are incorporates into a complex physical model with a hidden state. The EnKF is a sequential application of Bayesian update, when the prior distribution of ensemble (usually called forecast) is processed to accomplish the best estimate of the posterior, often called analysis, distribution of the hidden state. The analysis ensemble is then evolved in time. Since the EnKF relies only on the simple linear algebra, usually large ensembles are required to achieve reasonable level of error and its covergence is very slow. Tapering or other type of localization could notably increase the accuracy of the analysis, but it also significantly increases computation costs and usually a large ensemble is still needed.

We have proposed a new approach to the forecast covariance estimation based on transforming the ensemble to a spectral space (Fourier or wavelet) and estimating the covariance using only diagonal elements of the sample covariance matrix. This technique provides a natural localization of the covariance since it is well known, that diagonal covariance in Fourier space is equivalent with weak sense stationarity of the random field in spatial domain. The use of specific types of wavelets allows the covariance function to vary spatially and to be locally stationary.

We will provide a very efficient implementation of the proposed method in case when the whole state is observed on a finite dimensional regular grid, and we will also show that this algorithm could be easily extended to the case, when only a subset of the grid is observed. We will also show some simulation results using ideal nonlinear models, such as Lorenz 96 dynamic system or shallow water equations, which will show that the method rapidly decrease the analysis error and the required number of ensemble members.

Acknowledgement: This research was supported by GA CR grant 13-34856S and NSF grant DMS-1216481.

Domain Decomposition Method, Plasticity, Krylov Subspace Method with Multiple Search Directions

A. Markopoulos

FETI is an efficient tool for solving large-scale problems. We are focusing on the reduction of the cost of data transfer as well as on the improvement of performance for the local forward-backward substitutions during FETI iterations. This can be realized for instance via suitable modification of conjugate gradient method or another Krylov subspace method, by working with several search direction vectors at the same time. Then the solution time can be non-negligibly lesser compared with the standard approach.

BEM4I - parallel BEM Library with Applications

M. Merta, J. Zapletal

In this talk a newly developed library of parallel solvers based on the boundary element method (BEM) will be presented. Since the BEM reduces the problem to the boundary of the computational domain, it is fairly suitable, e.g., for sound scattering problems modelled by the wave or Helmholtz equations. Considering the fact that the volume of the domain does not need to be discretized, BEM is also well suited for shape optimization problems. In the first part of the talk we give a short overview of the library and present results of performance and scalability benchmarks. In the second part we present the application of the library for solving time-dependent wave equation or shape optimization problems.

A Comparative Study on Iterative Solvers for FFT-based Homogenization of Periodic Media

N. Mishra, J. Vondřejc, J. Zeman

We are concerned with an FFT-based numerical homogenization method proposed by Moulinec and Suquet in 1994 for problems characterized by high-resolution microstructural scans. Recently [1], we have interpreted the method as a Galerkin scheme generating a system of linear equations for an unknown $x \in \mathbb{E} \subset \mathbb{R}^n$ in the form

$$GAx = GAb \text{ with } G = F^{-1}\widehat{G}F. \tag{1}$$

Here, $G \in \mathbb{R}^{n\times n}$ is an orthogonal projection from $\mathbb{R}^n$ to $\mathbb{E}$, expressed in terms of the inverse and forward Fourier transform matrices F^{-1} and $F \in \mathbb{R}^{n\times n}$ and a block-diagonal matrix $\widehat{G} \in \mathbb{R}^{n\times n}$, block-diagonal $A \in \mathbb{R}^{n\times n}$ stores the problems coefficient, and $b \notin \mathbb{E}$ is a given vector. In the present contribution, we benchmark the performance of several Krylov solvers when applied to (1).

Acknowledgement: This work was supported by the European Union under the project No. CZ.1.07/2.3.00/30.0034.

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A Parallel Space -time Multigrid Solver for the Stokes Equations

M. Neumüller

For evolution equations we present a space-time method based on Discontinuous Galerkin finite elements. Space-time methods have advantages when we have to deal with moving

domains and if we need to do local refinement in the space-time domain. For this method we present a multigrid approach based on space-time slabs. This method allows the use of parallel solution algorithms. In particular it is possible to solve parallel in time and space. Furthermore this multigrid approach leads to a robust method with respect to the polynomial degree which is used for the DG time stepping scheme. Numerical examples for the Stokes equations will be given which show the performance of this space-time multigrid approach.

Mathematical Modelling of the Spread and Control of Onchocerciasis in Nigeria

I. Ch. Oguoma, T. M. Acho

Onchocerciasis, also known as river blindness and Robles disease is a parasitic disease caused by Onchocerca volvulus, a nematode (roundworm) and it is endemic in Nigeria. The reason of this paper is to discuss the mathematical formulation underpinning the spread and control of this disease on one hand. On the other hand, we make use of some new analytical methods to derive the solution of this set of equations. The numerical results are presented to test the efficiency and the accuracy of both methods. The techniques used for solving these problems are friendly, very easy, and less time consuming. The numerical solutions in both cases display the biological behaviour of the real world situation.

Efficient In-core Sparse Direct Solution of Large Finite Element Problems

P. Pařík, J. Plešek

Direct solution methods are particularly important in the Finite Element Method (FEM) since they enable the factorization (the most time demanding part of the solution) to be performed only once for a given problem and subsequently to solve it for any number of right-hand sides (or load cases), which is especially useful in the solution of dynamic and non-linear problems.

Sparse direct solvers represent one of the possible approaches to the solution of large problems in FEM. However, the definition of a large problem in FEM changed significantly in the past decades. For example, in the Harwell - Boeing Sparse Matrix Collection, which is still used for solver benchmarks, there are only a few matrices of order $> 10^4$ and none of order $> 10^5$. As of today, we can assume that a large problem has an order $10^6 \sim 10^7$.

Our approach focuses on minimizing the amount of storage space and computational time required for the solution of a large problem. This is achieved particularly by using a modified minimum ordering algorithm to reduce the fill-in, therefore, reducing the

number of numerical operations needed to compute the solution. Both the factorization and the backsubstitution algorithms are parallelized using the OpenMP library to fully exploit today's multi-core and multi-processor computers. The global stiffness matrix is assembled and stored in-core throughout the computation, using an efficient sparse matrix storage format; although that leads to considerably high memory requirements, in practice, it does not present a significant problem for today's computers.

We present the details of our sparse direct solver implementation, realized within the framework of our in-house finite element code PMD. We show the performance results for several large real-world problems taken from the engineering practice and assess the scalability of the solver. Finally, we make an attempt at comparing our solver to other available codes, both commercial and free.

SVM Regression Parameters Optimization Using Parallel Global Search Algorithm on Intel Xeon Phi

A. Polovinkin, K. Barkalov, I. Meyerov, A. Sysoyev, N. Zolotykh

The problem of reconstructing a functional dependency of a given value on measurement results (regression problem) is often met in applied studies. In practice the nature of dependence is usually unknown, therefore the regression function is chosen from a certain pre-determined class which depends on the selected model. Support Vector Machine (SVM) is a widely used method for solving the regression reconstruction problem. Its main advantages are possibility of efficient nonlinear dependencies modelling and independence of generalization capability on the feature space dimension. Though, in some cases practical application of the SVM is limited due to the fact that accuracy of the method depends strongly on choice of parameters. The most frequently used approaches to optimal selection of parameters eventually reduce to solving a global optimization problem.

This work introduces a novel approach to SVM regression parameters selection based on optimization of the cross-validation error function. It is well known that global optimization problems usually are hard to solve. One of the strategies for dealing with them is the development of parallel algorithms and their implementation on high performance computing systems. We suggest to use the global search method presented in studies of R. Strongin, V. Gergel, V. Grishagin, Ya. Sergeev. Our previous work considered several modifications of the parallel global search algorithm and evaluated efficiency of the modifications on cluster systems. It has been shown that the proposed algorithm achieves a linear speedup in the number of used nodes and cores (up to 24 threads). In this work we extend parallel implementation to the class of modern manycore coprocessors, namely, the Intel Xeon Phi with 60 cores and up to 240 threads. We present performance and scalability analysis and describe software optimization techniques for Intel Xeon Phi.

Application of the 3D Numerical Model in the Control and Predictions during the Underground Rock Heating Experiment

P. Rálek, M. Hokr

This work is a part of the project of in-situ rock heating experiment in Josef gallery, testing the granite rock properties for geothermal application (heat, energy storage). The experiment is of meter scale, with the heater installed in a large borehole from end of a tunnel, with months to years duration. The area, surrounding the borehole, is covered by many temperature and stress sensors.

The thermal-stress model, developed in COMSOL software and combining the unsteady heat conduction and the linear elasticity, has been used for comparison with measured data, to check the validity of parameters determined in laboratory and possible other effects. Moreover, after the validation, the predictions from the model have been used for the control of the experiment.

The model results have been used as quantitative estimations of the quasi steady-state, both in terms of time and in terms of temperature and stress distribution. From the measurement, we can observe the level of attainment of the steady-state and use those estimations as stopping criteria for particular phases of the experiment ("switching" between heating and cooling phase). The results for two actually realized phases of the experiment (one run of heating and one run of cooling phase) will be presented.

Fine Resolution Modelling of Meteorological Conditions and Air Quality in Urbanized Areas

J. Resler, P. Juruš, K. Eben, J. Liczki, M. Belda, I. Kasanický, E. Pelikán, J. Karel, R. Jareš, O. Vlček, N. Benešová, M. Kazmuková

Both air quality and meteorological conditions constitute an important part of quality of life, particularly in urban areas where the impact is higher due to high population density. On the other hand, urban environment has a considerable influence on meteorology and air quality and any attempts to model pollutant concentrations and meteorological quantities should account for the effect of urbanization.

Traditionally, global and mesoscale Eulerian models do not have sufficient resolution to model urban areas. Considering the air quality, they are used mostly for the modelling of background concentrations and additional steps are required to model the urban environment, e. g. statistical postprocessing and downscaling. Similar situation is in meteorology where the effects of urban heat island are not well captured by generic numerical weather prediction models. The increase of computational power in recent years however allows a refinement of the resolution of the models to the order of hundreds of meters. New parameterizations of atmospheric processeses suitable for high resolution simulations have been developed together with special models of effects of the urban

surface. Thus urban modelling systems based on Eulerian meteorological and chemical transport models have arisen, with all advantages of this approach.

Our goal is to test the performance of a very detailed model (both in resolution and in description of its inputs) for the urban area by means of a long-term simulation, so as to capture the statistical behaviour of the model during different seasons of the year and different modes of weather. In particular, we investigated the effect of going down to very fine scale and the effect of urban meteorology parameterization on weather and air quality. The present study shows the results of one year simulation of a coupled meteorological and air quality model for the year 2010. The modelling system consists of the meteorological model WRF-ARW v.3.5.1 and the chemical transport model CMAQ v.5.0.1. The models are configured on five nested domains with horizontal resolutions 27km, 9km, 3km, 1km and 333m covering areas from Europe to Prague. Special data sets (landuse, statistical characteristics of urban surface, etc.) have been prepared so that urban parameterizations of the WRF model uses could be used, especially the BEM (Building Energy Model). Also, detailed emission inventories including special models for transportation have been used.

As a reference, a simulation with a standard model configuration has been run. The two simulations, one with the model of urban surface BEM enabled and the other one without it, have been compared. The meteorological data (T2, wind speed, âĂę) and air pollution concentrations (NO, NO2, O3, CO, NH3, PM10, PM25) were compared with observations. First results indicate a strong positive impact of the urban parameterizations on accuracy of wind speed modelling. In other variables the effect is not so pronounced and may differ according to the type of meteorological situation.

Acknowledgement: This work was supported by the Urban Heat Island, a Central Europe Project No. 3CE292P3 and by the long-term strategic development financing of the Institute of Computer Science RVO:67985807. Simulations were partly performed in National Supercomputing Centre at VSB-TU Ostrava with support of the program IT4Innovations CZ.1.05/1.1.00/02.0070 as well as the project Large Research, Development and Innovations Infrastructures LM2011033.

Model of the Water Balance of a Lake Created by Hydrological Recultivation of an Open Pit Coal Mine

J. Říha, J. Šembera

This contribution aims to describe the topic of calculation of the water balance of the Chabarovice (Milada) lake which was created by hydrological recultivation of an open pit coal mine. The catchment area of the lake is strongly anthropogenically influenced hence the use of existing models would be problematic. A creation of model concept based on available data will be discussed. Model parameters will be calibrated using the values of water level in the lake measured during its filling when the lake had no outflow.

Then, the model will be validated on the rest of the simulation period. Eventually, the calibrated model will be used for the computation of scenarios of the future development of the water balance of the lake with an aim to answer the question whether the lake that has no tributary is endangered by drying out.

Acknowledgement: The work of J. Riha was supported by the Ministry of Education of the Czech Republic within the SGS project No. 21066/115 on the Technical University of Liberec. J. Sembera was supported by Technology Agency of the Czech Republic via project No. TA02020177.

Waves in Large Contrast Fluid-saturated Porous Deformable Media

E. Rohan

Wave propagation in fluid-saturated porous media presents a classical but still extremely challenging area of research due the complexity of the problem studied and its obvious applicability in geosciences and material engineering. In the paper the homogenization approach is applied, which is based on asymptotic analysis of periodic structure w.r.t. $\varepsilon \to 0$, the scale of heterogeneities. We consider the Biot compressible model relevant to the mesoscopic structure characterized by the *periodic representative cell* $Y \in \mathbb{R}^n$, $n = 2, 3$. The dynamic problem formulation involving displacements $\boldsymbol{u}$, seepage velocity $\boldsymbol{w}$ and pressure p is constituted by the following equations

$$\begin{aligned} -\nabla \cdot (\mathbb{D}\boldsymbol{\epsilon}(\boldsymbol{u})) + \nabla(\boldsymbol{\alpha} p) + \overline{\rho}\ddot{\boldsymbol{u}} + \rho^f \dot{\boldsymbol{w}} = \boldsymbol{f} \ , \\ \rho^f \ddot{\boldsymbol{u}} + \rho^w \dot{\boldsymbol{w}} + \boldsymbol{K}^{-1}\boldsymbol{w} + \nabla p = 0 \\ \boldsymbol{\alpha} : \boldsymbol{\epsilon}(\dot{\boldsymbol{u}}) + \mathrm{div}\boldsymbol{w} + \mu^{-1}\dot{p} = 0 \ . \end{aligned} \tag{1}$$

where $\boldsymbol{\epsilon}(\boldsymbol{u})$ is the strain, $\rho^f, \rho^w, \overline{\rho}$ are densities, $\boldsymbol{K}$ is the permeability and coefficients $\mathbb{D}, \boldsymbol{\alpha}, \mu$ determine the poroelasticity properties.

As the main result, a homogenized model describing the wave propagation in the double porous structure is derived. All material coefficients involved in (1) are defined with respect to the decomposition of $Y = Y_c \cup Y_m$ into the primary and the dual porosities, Y_c and Y_m, respectively. Large contrasts in the permeability and the elasticity coefficients are respected by ε^2 scaling:

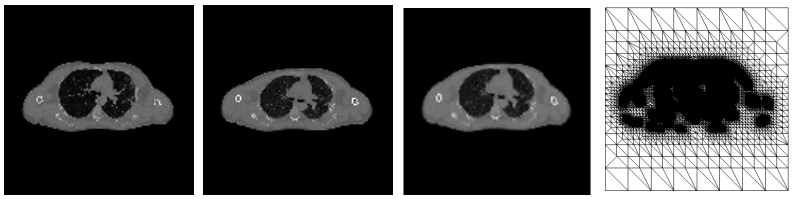
$$\boldsymbol{K}^\varepsilon(y) = \begin{cases} \boldsymbol{K}_c & \text{if } y \in Y_c \ , \\ \varepsilon^2 \widehat{\boldsymbol{K}_m} & \text{if } y \in Y_m \ , \end{cases} \qquad \mathbb{D}^\varepsilon(y) = \begin{cases} \varepsilon^2 \widehat{\mathbb{D}}_c & \text{if } y \in Y_c \ , \\ \mathbb{D}_m & \text{if } y \in Y_m \ . \end{cases} \tag{2}$$

The resulting homogenized model consists of the global macroscopic equations, involving the homogenized coefficients, and of the local problems which describe the characteristic responses of the primary and dual porosities.

Elastic Image Registration with Mesh Adaptation

A. Ronovský, A. Vašatová

Medical images are increasingly being used within healthcare for diagnosis, planning treatment and monitoring disease progression. These images are acquired at different times, with different imaging modalities, from different subjects etc. Thus it often yields that additional clinical information are not apparent in the separate images. The spatial relation between the images has to be found and this process is called image registration. In our contribution, we use elastic registration which supposes that the images are two different observations of an elastic body which is discretized by the finite element method. Because medical images usually contain large area of background and even only small area of changes, regular discretization results in waste of computational resources due to the fine refinement of the space outside the region of interest (especially in 3D). To avoid this, we use coarser grid with local refinement that takes into account specific features of the images and their differences. The related elasticity problems are solved by TFETI, which is a variant of the FETI domain decomposition method for massively parallel numerical solution of elliptic PDE with optimal complexity. At the end we present some examples of possible use of elastic image registration.



(a) Image R. (b) Image T. (c) Image T_φ. (d) Mesh.

Figure 1: Registration example.

The Two Steps Optimization of Plunger Cooling in the Glass Forming Process

P. Salač

In the contribution we present two problems of shape optimization of the plunger cooling which come from the forming process in the glass industry. Firstly, we optimize the shape of the inner surface of the plunger cavity and then the outward surface optimization of the regulation current body follows. A rotationally symmetric system composed of the mould, the glass piece, the plunger and the plunger cavity is considered. The state problem is given as multiphysics problem where solidifying molten glass is cooled from

inside by water flowing through the plunger cavity and from outside by the environment surrounding the mould.

The cost functional is defined as the squared L_r^2 norm of the difference between a prescribed constant and the temperature on the outward boundary of the plunger. The temperature distribution is controlled by changing the wall thickness of the plunger in the first optimization problem and by water velocity changing in the second problem.

Existence and uniqueness of the state problem solution and existence of a solution of the optimization problem for plunger cavity optimization are proved in [1].

The numerical results of the optimization to required target temperature 800 $[°C]$ of the outward plunger surface together with the distribution of temperatures along the interface between the plunger and the glass piece before and after the optimization process are presented for both problems.

Acknowledgement: This work was realized with financial support by the Technological Agency of the Czech Republic, project No. TA03010852.

[1] P. Salač: Optimal Design of the Cooling Plunger Cavity. Appl. Math., 58 (2013), 405 - 422.

A Stock-recruitment Relationship Derived from a Slow-fast Population Dynamic Model

U. Schaarschmidt, S. Subbey, T. Steihaug

The Beverton-Holt and Ricker functions are two distinct ecological descriptions of the link between a parental population size and subsequent offspring that may survive to become part of the fish stock.

This paper presents a model consisting of a system of ordinary differential equations (ODEs), which couples a pre-recruit stage with several adult stages. Elements of slow-fast dynamics capture the different time-scales of the population dynamics and lead to a singular perturbation problem.

The novelty of the model presented here is its capability to replicate a broad spectrum of the stock-recruitment relationship, including the Beverton-Holt and Ricker dynamics. The results are explained using geometric singular perturbation theory and illustrated by numerical simulations.

Geochemical Model of Calcite Dissolution in Column Experiments

J. Šembera, V. Žabka

The contribution presents 1D reactive transport model of the column experiment. Tested porous material is a calcite. The model includes kinetic dissolution of calcite, transport of multispecies components and dissolution of atmospheric carbon dioxide. The outcomes

from several types of models will be compared with the values measured in laboratory experiments.

Acknowledgement: The authors are supported by Technology Agency of the Czech Republic via project Nr. TA02021132 and by Student Grant Competition of Technical University of Liberec.

Heat Transfer of an Impinging Jet on a Plane Surface

J.-J. Shu

A cold, thin film of liquid impinging on an isothermal hot, horizontal surface has been investigated. An approximate solution for the velocity and temperature distributions in the flow along the horizontal surface is developed, which exploits the hydrodynamic similarity solution for thin film flow. The approximate solution may provide a valuable basis for assessing flow and heat transfer in more complex settings.

In response to the abundance of practical applications the heat transfer associated with impinging jets has been the subject of numerous theoretical and experimental research studies reported in the literature. This is particularly true in the context of condensers, as used in power generation. Here the draining fluid is accumulated condensate.

An approximate and the elements of engineering practice, namely the skin friction and heat transfer coefficients for the flow of a cold two-dimensional jet against a hot, horizontal plate have been presented. Although at this stage a comparison between theory and experiment is unavailable, the work provides the basis for re-assessing condensation.

Parallel Performance of Iterative Solvers for Pressure-correction Methods for Incompressible Flows

J. Šístek

We deal with a pressure-correction method for solving unsteady incompressible flows. In this approach, five subsequent equations are solved within each time step. These correspond to three scalar convection-diffusion problems, one for each component of velocity, a pure Neumann problem for the correction of pressure, and a problem of the L2 projection for pressure update. We present a comparative study of several paralle preconditioners and Krylov subspace methods from the PETSc library and investigate their suitability for solving the arising linear systems after discretizing by the finite element method. The target application are large-scale simulations of flows around wings of insects. This is joint work with Fehmi Cirak.

On Control of the Loading Process in Hencky's Perfect Plasticity

S. Sysala

The Hencky elastic-perfectly plastic problem is formulated depending on the load parameter (ζ) to describe the loading process up to the limit load. For the discretized problem with the von Mises yield criterion, the parameter α representing the work of external forces is introduced and mutual relation between ζ and α is described. The curve describing this relation represents a global material response and can be used for stable control of the loading process up to the limit load. It is shown that the relation between ζ and α can be generalized even for continuous formulation of the problem and for an abstract yield criterion.

[1] S. Sysala, J. Haslinger, I. Hlaváček, and M. Cermak. *Discretization and numerical realization of contact problems for elastic-perfectly plastic bodies. PART I – discretization, limit analysis.* ZAMM - Z. Angew. Math. Mech., 1–23, 2013. doi 10.1002/zamm.201300112.

BEM for Homogenization in 2D

M. Theuer, D. Lukáš, J. Bouchala

Numerical realization of mathematical homogenization of elliptic equations is based on homogenization theorem which is unfriendly to boundary element methods. Homogenized coefficients of a periodic material are given by an integral formula that includes derivation of a function - the solution of an auxiliary periodic equation on a unit cell. It turns out that for some composite materials the volume variational formulation of the auxiliary problems can be reduced to the interface between the parts of the composite material and periodic boundary by means of Steklov-Poincaré operator. Furthermore the homogenized coefficient matrix can be computed directly using the auxiliary function values only on the interface.

In our talk we present derivation of boundary formulation for the problem of mathematical homogenization. The resulting problem is discretized by a Galerkin direct boundary element method and efficiency of the method is documented for various shapes periodic inclusions.

On Incomplete Symmetric Decompositions

M. Tůma

Our aim is to design and develop a new robust and efficient general-purpose incomplete factorization package that uses a limited memory approach. The talk will summarize some of the results obtained on this way to solve not only the positive definite systems

but to cover also sparse and symmetric indefinite systems and possibly also linear least-squares problems. We intend to discuss selected implementation features and dropping strategies. We expect to present results of extensive experiments.

Acknowledgement: This work was partially supported by the projects 13-06684S and 108/11/0853 of the Grant Agency of the Czech Republic and the EPSRC grant EP/I013067/1. The results come from the joint work with Jiří Kopal, Miroslav Rozložník and Jennifer Scott.

Identification of Moisture Distribution in Porous Building Materials from Microwave Measurements

J. Vala

The traditional methods of determination of moisture content in porous building materials rely on measurements of sample weight before and after drying in an oven. This approach takes a long time (because of necessity of drying a sample in hot air or vacuum) and is not able to obtain sufficiently large database for reliable identification of such material characteristics as the (temperature-variable) capillary transfer factor κ in problems of evolution, coming from the thermomechanical mass conservation principle and from the (at most) semilinear Fick law; moreover, the dependence of its effective value on available microstructural data cannot be taken into consideration.

The research for the indirect moisture measurement approaches using electromagnetic waves of high frequency or microwaves started after World War II and is still not closed. These approaches can generate fast nondestructive and contactless time-dependent moisture profiles including moisture included in the inner part of material. The identification of κ and similar macroscopic parameters needs non-trivial computational simulations, respecting the assessment of material permittivity from the two-phase mixture models, or applying the theory of quasi-periodic homogenization.

Unlike the historical approach of Matano (1933), based on the Boltzmann transform (1894), suggested for weighting methods, advanced computational algorithms must handle large 3-dimensional time-variable data from indirect measurements. This contribution shows the common basis for various ad hoc identification approaches from the literature, as two different 3-dimensional integration methods, the so-called double integration method, etc., covering the formula of Matano as a very special case. The new measurement methodology, developed at the Faculty of Civil Engineering of Brno University of Technology, partially supported from the project of specific university research FAST-S-14-2346, contains the original numerical approach, including its software implementation in MATLAB; some application results are available.

Thermomechanical Contact Problems in MatSol

O. Vlach

In our work, we used the mortar approach for discretization of the interface conditions in dynamical contact problems with Coulomb friction including the coupling with heat, i.e. the effects of thermal softening, heat transfer on the contact interface and heat generation caused by friction. In each timestep is solved the strictly convex bound constrained quadratic programming problem optionally preconditionined by the conjugate projector to the subspace defined by the trace of the rigid body motions on the artificial subdomain interfaces.

Accurate Guaranteed Bounds on Homogenized Matrix by FFT-based Methods

J. Vondřejc, J. Zeman, I. Marek

FFT-based homogenization algorithm has become a popular numerical method for evaluating an effective (homogenized) matrix of periodic heterogeneous materials. Originally, the method was based on a solution of the Lippmann-Schwinger type of an integral equation with the Green function derived from an auxiliary homogeneous problem. A numerical solution proposed by Moulinec and Suquet in 1994 is based on the Neumann series expansion corresponding to a simple iteration procedure.

We explain the algorithm by the Galerkin method of corresponding variational formulation with an approximation space composed of trigonometric polynomials. Techniques of numerical integration, that leads to different numerical schemes, are also discussed.

Moreover, the primal and the dual variational formulation, according to Dvořák (1995), serve to evaluate arbitrary accurate guaranteed bounds on homogenized matrix. We explain this approach by the FFT-based Galerkin methods and show its behavior on numerical examples.

[1] J. Vondřejc, J. Zeman, and I. Marek, *An FFT-based Galerkin method for Homogenization of Periodic Media*. arXiv preprint arXiv:1311.0089, (2013).

[2] J. Vondřejc, J. Zeman, and I. Marek, *Accurate Guaranteed bounds on Homogenized matrix by FFT-based Galerkin method*, Submitted for publication in 2014.

A Coupling Method for the Parallel Solution of Vibro-acoustic Problems

A. Y. Wang, F.-X. Roux

The objective of this paper is to present a novel fast parallel iterative method for solving the linear system arising from the finite element discretization of vibro-acoustic problems.

One of the main diffculties in solving the coupled linear system arising from the finite element discretization of a vibro-acoustic problem is due to the discrepancy between the spectrums of the two uncoupled systems. In such a case, the global coupled system becomes very ill-conditioned and is difficult to solve with classical iterative methods. To overcome this challenge it is possible to use a domain decomposition approach that consists in solving a condensed problem associated with auxilliary degrees of freedoms on the coupling interface. The condition number of the condensed system can be significantly decreased by choosing the right interface unknowns.

In the proposed method, the fluid and structure domains themselves are decomposed into non-overlapping subdomains. Then, new degrees of freedom are introduced into the system by designing an artificial Robin condition on the coupling interface. Afterwards, the original degrees of freedom are eliminated from the system. The resulting condensed coupling system contains only the coupling interface unknowns. A General Conjugate Residual (GCR) iteration is used to solve the reduced linear system. At each iteration, the method requires the solution of one independent local problem per physical medium, that can be performed in parallel using a domain decomposition method.

The implementation of this method is relatively simple and preserves the existing codes of the two uncoupled systems. The iterations for solution of the degrees of freedom on the interface are managed by an additional solver outside the two exisitng codes. The results obtained for various problems show that the proposed interface method is significantly faster than the GCR method applied to the global system.

BEM4I - Parallel BEM Library and its Applications

J. Zapletal, M. Merta

We present a newly developed parallel library based on the boundary element method. The aim of the library is to utilize modern techniques of programming with the main focus on deployment on HPC architectures. To effectively exploit the vector instructions (SSE, AVX) of nowadays CPUs we use explicit vectorization of analytical and numerical evaluation of the boundary integral operators and the representation formula. To speed up the assembly of Galerkin matrices and to reduce memory consumption we employ the fast multipole method. OpenMP shared memory parallelism is used to assemble both admissible and non-admissible blocks efficiently on multicore CPUs. The distributed memory parallelism by MPI is to be added in the near future.

The possible applications of the library include shape optimization problems, where BEM has clear advantages over the finite element method, or sound scattering problems modelled both by the Helmholtz equation and the evolutionary wave equation discretized by the time-domain BEM.

ODE's for Description of Reactive Transport Including Equilibrium Reactions

L. Zedek, J. Šembera

In my contribution I will introduce an original ODE description of reactive transport including kinetic as well as equilibrium chemical reactions. It is a kind of description which enables to put together PDE description of groundwater transport with algebraic equations describing chemical equilibrium. Resulting ODE formulation consists of n ordinary differential equations defining the change in concetration of n species in each mesh node. The only and sufficient condition for equilibrium to be held is "consistency" of initial conditions. Potential inconsistency does not make the problem unsolvable, but it results in unreasonable results.

Set of models has been prepared and solved for evaluation and validation of proposed approach. Mentioned models have been solved using various kinds of mathematical tools such as a symbolic solver Sage or numerical solver CVODE which is a part of a package sundialsTB. Simulation times have been noted and theirs dependency on number of mesh nodes has been evaluated.

Results achieved from our ODE models agree with reference results from widely used software The Geochemist's Workbench.

Acknowledgement: This work was supported by Student Grant Competition of Technical University of Liberec. The authors of this contribution were supported by Technology Agency of the Czech Republic via project Nr. TA02021132.

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