SPOMECH

Workshop 2013

on Supercomputing and computational solid and fluid mechanics

Ostrava, November 13–15, 2013

Lecture hall of the Institute of Geonics AS ČR

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Preface

SPOMECH Workshop 2013 on Supercomputing and computational solid and fluid mechanics is the third workshops organized annually from 2011. SPOMECH stands for the Czech abbreviation "SPOLEHLIVÁ MECHANIKA" meaning "RELIABLE MECHANICS". SPOMECH project runs between July 2011–June 2014 as a joint activity of the VŠB-Technical University of Ostrava (VŠB-TU Ostrava) and the Institute of Geonics AS ČR (IGN AS ČR). The project is supported by the ESF and the Government of the Czech Republic.

The project employs one project coordinator (T. Kozubek), two scientific leaders recruited abroad (J. Valdman and M. Kwasniewski), seven researchers (postdocs), and three Ph.D. students working in fields of numerical mathematics and experimental mechanics. Apart from organized workshops there are also one day courses for students in the Czech Republic and series of lectures by Czech and foreign scientists on given topics including domain decomposition methods, a posteriori error estimates, contact problems, geometrical and material nonlinearities and nonlinear behavior of rock and building materials.

More about SPOMECH activities can be found on the official project website http://spomech.vsb.cz/.

We are delighted that you have accepted our invitation to the workshop.

On behalf of the organizers

Tomáš Kozubek, Vít Vondrák, Jan Valdman, Dalibor Lukáš, Marta Jarošová (VŠB-TU Ostrava), Radim Blaheta (IGN AS ČR)

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Programme

Wednesday, November 13, 2013

9.00 - 13.00	Registration of participants, discussion, coffee
13.00 - 13.50	Lunch
13.50 - 14.00	Opening
14.00 - 15.45	**Radek Tezaur**: Toward solving smaller problems for Helmholtz - Interpolatory model order reduction for frequency sweeps and the discontinuous enrichment method I
	Nicole Spillane: Robust domain decomposition methods for symmetric problems I
	Tomáš Karásek: Supercomputing for industry - From cube to airplanes
15.45 - 16.15	Coffee break
16.15 - 17.45	**Michal Merta**: BEM4I - Preview of the new BEM library
	Lukáš Malý: Boundary element based vertex solver for polygonal subdomains
	Jan Valdman: Verification of functional a posteriori error estimates for obstacle problem in 2D
17.45	Dinner

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Thursday, November 14, 2013

9.00 - 11.00	**Nicole Spillane**: Robust domain decomposition methods for symmetric problems II **Radek Tezaur**: Toward solving smaller problems for Helmholtz - Interpolatory model order reduction for frequency sweeps and the discontinuous enrichment method II **Petr Vaněk**: Exact interpolation scheme with approximation vector used as a column of the prolongator I
11.00 - 11.30	Coffee break
11.30 - 13.00	**Leszek Marcinkowski**: Mortar finite element and some of its domain decomposition methods **Jakub Šístek**: Parallel performance of iterative solvers for pressure-correction methods for incompressible flow
13.00 - 14.30	Lunch
14.30 - 15.30	**Pavel Burda**: Rotationally symmetric Stokes flow near corners **Tomáš Ligurský**: A continuation problem for computing solutions of quasi-static contact problems with friction
15.30 - 17.00	Discussion

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Friday, November 15, 2013

9.00 - 11.00	**Petr Vaněk**: Exact interpolation scheme with approximation vector used as a column of the prolongator II
	Leszek Marcinkowski: Some linear and nonlinear domain decomposition methods
	Zdeněk Dostál: Mortar discretization of non-penetration conditions in TFETI based domain decomposition
11.00 - 11.30	Coffee break
11.30 - 13.00	**Michal Kuráž**: Solving nonlinear Richards equation with adaptive domain decomposition
	Stanislav Sysala: On control of loading process in perfect plasticity with contact
	Matyáš Theuer: Boundary element method in mathematical homogenization
13.00 - 14.30	Lunch
14.30 - 17.00	Discussion, coffee, closing

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Abstracts

Pavel Burda: Rotationally symmetric Stokes flow near corners

We present analytical solution of the Stokes problem in rotationally symmetric domains using polar coordinates and separation of variables. This is then used to find the asymptotic behaviour of the solution in the vicinity of corners, also for Navier-Stokes equations. We also present alternative solution based on the Fourier transform. We apply the result to construct very precise numerical finite element solution.

Zdeněk Dostál: Mortar discretization of non-penetration conditions in TFETI based domain decomposition

This is joint work with T. Brzobohatý, T. Kozubek, O. Vlach.

The variationally consistent discretization of the non-penetration condition that was introduced by B. I. Wohlmuth became an important ingredient of effective algorithms for the solution of multibody contact problems of elasticity, especially when it is necessary to deal with the non-matching grids on contact interface or when the contact interface is large and curved. Here we discuss the problems related to the application of this discretization method in the FETI based algorithms. We first show that the resulting constraint matrices with normalized normals are well conditioned under mild conditions. The estimates are then used to extend the optimality results obtained earlier for simple node-to-node description of non-penetration to the mortar discretization. The results are illustrated by numerical solution of 2D and 3D academic benchmarks and of some realistic the problems.

Tomáš Karásek: Supercomputing for industry - From cube to airplanes

Demand from end users who need to solve their problems which are in many cases very complex is and always has been driving force for developing new efficient algorithms. This is even more apparent in era of supercomputers. Nowadays high performance computers give their users computational power unimaginable few years ago. Demand for algorithms able to tame and utilize this power has been lately driving force for parallelization of existing and development of new parallel

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algorithms. In this talk overview of algorithms and codes deployed on Anselm used for solving real industrial problems together with their scalability will be presented.

Michal Kuráž: Solving nonlinear Richards equation with adaptive domain decomposition

Modeling the transport processes in a vadose zone plays an important role in predicting the reactions of soil biotopes to anthropogenic activity, e.g. modeling contaminant transport, the effect of the soil water regime on changes in soil structure and composition, etc. Water flow is governed by the Richards equation, while the constitutive laws are typically supplied by the van Genuchten model, which can be understood as a pore size distribution function. Certain materials with dominantly uniform pore sizes (e.g. coarse-grained materials) can exhibit ranges of constitutive function values within several orders of magnitude, possibly beyond the computer real numbers length. Thus a numerical approximation of the Richards equation often requires the solution of systems of equations that cannot be solved on computer arithmetic. An appropriate domain decomposition into subdomains that cover only a limited range of constitutive function values, and that will change adaptively, reflecting the time progress of the model, will enable an effective and reliable solution of this problem. This presentation focuses on improving the performance of a nonlinear solver by locating the areas with abrupt changes in the solution.

Tomáš Ligurský: A continuation problem for computing solutions of quasi-Static contact problems with friction

A continuation problem for finding successive solutions of discretized plane quasi-static contact problems with friction is proposed and studied. The corresponding first-order system is derived and results of existence and uniqueness of its solutions are obtained. Conditions guaranteeing continuation of a solution curve along a direction from the first-order system are given. Numerical continuation of solution curves is performed on examples with non-smooth folds.

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Lukáš Malý: Boundary element based vertex solver for polygonal subdomains

A boundary-element counterpart of the domain decomposition vertex solver is proposed and tested for a 2-dimensional Poisson's equation. 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 Hofreither, Langer, and Pechstein (2010) we construct the coarse solver on general polygonal subdomains so that the local coarse stiffness matrix is approximated by a boundary-element discretization of the Steklov-Poincaré operator. The efficiency of our approach is documented by a substructuring into L-shape domains, which is robust with respect to material coefficient jumps.

Leszek Marcinkowski: Some linear and nonlinear domain decomposition methods

Domain Decomposition Methods (DDMs) is a research area which offers one of the best techniques of constructing effective parallel preconditioners. The term Domain Decomposition refers to the splitting of an original differential equation problem on a given domain or an approximation thereof into a collection of coupled subproblems on subdomains forming decomposition of the original domain. In this talk we discuss some basic linear DDMs frameworks like multiplicative Schwarz method (MSM), additive Schwarz method (ASM) and some substructuring methods like e.g. Neumann-Neumann type of DDMs.

In the second part of the talk we also present nonlinear DDM namely Nonlinearly Preconditioned Inexact Newton Methods (ASPIN) for solving the nonlinear systems of equations. The method proved itself to be more efficient than classical inexact Newton algorithms for many problems.

Leszek Marcinkowski: Mortar finite element and some of its domain decomposition methods

Discretizations of differential equation problems usually are constructed on the basis of one global mesh (triangulation) of the domain, in which this differential problem is defined. However, in many applications there is a need to construct discretizations on independent nonmatching meshes in subdomains or to use

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different discretizations methods in the given subdomains (substructures) of the original domain. One of the methods of constructing discretizations of differential equation problems on nonmatching meshes is the mortar method proposed by Ch. Bernardi, Y. Madey, and T. Patera. In this talk we will present the construction of mortar discretizations for few types of conforming and nonconforming finite elements for second and fourth order problems. We also present some domain decomposition parallel preconditioners for the arising algebraic systems of equations.

Michal Merta: BEM4I - Preview of the new BEM library

This is joint work with Jan Zapletal.

In this talk we present the first results of our new parallel boundary element library. BEM offers a suitable alternative to FEM especially in the cases when the computational domain is unbounded (e.g. in sound scattering or electromagnetism problems) since it only introduces unknowns on the boundary of the computational area. However the system matrices resulting from BEM are dense with $O(n^2)$ entries requiring $O(n^2)$ operations to assemble. To reduce these main setbacks we combine the vectorization of the computationally most demanding parts with their shared memory parallelization by OpenMP and sparsification of the resulting matrices by the fast multipole method. We present the first scalability results, give the comparison of efficiency obtained by various compilers, and discuss the possibilities of future development.

Nicole Spillane: Robust domain decomposition methods for symmetric problems

This is joint work with Victorita Dolean, Patrice Hauret, Pierre Jolivet, Frédéric Nataf, Clemens Pechstein, Daniel J. Rixen and Robert Scheichl.

Domain decomposition methods are a popular way to solve large linear systems. For problems arising from practical applications it is likely that the equations will have highly heterogeneous coefficients. For example a tire is made both of rubber and steel, which are two materials with very different elastic behaviour laws. Many domain decomposition methods do not perform well in this case, specially if the decomposition into subdomains does not accommodate the coefficient variations. For three popular domain decomposition methods (Additive Schwarz,

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BDD and FETI) we propose a remedy to this problem based on local spectral decompositions. Numerical investigations will confirm robustness with respect to heterogeneous coefficients and automatic (non regular) partitions into subdomains. We will also present large scale computations (over a billion unknowns) conducted by Jolivet in Freefem++ which show that strong scalability is achieved.

[1] F. Nataf, H. Xiang, and V. Dolean. A two level domain decomposition preconditioner based on local Dirichlet-to-Neumann maps. Comptes Rendus Mathématique, 348(21-22) :1163–1167, 2010.

[2] V. Dolean, F. Nataf, N. Spillane, and H. Xiang, A coarse space construction based on local Dirichlet to Neumann maps, SIAM J. on Scientific Computing, 2011, 33:04

[3] V. Dolean, F. Nataf, R. Scheichl, and N. Spillane, Analysis of a two-level Schwarz method with coarse spaces based on local Dirichlet–to–Neumann maps, Computational Methods in Applied Mathematics, 2012, 12:4

[4] N. Spillane, V. Dolean, P. Hauret, F. Nataf, C. Pechstein, and R. Scheichl. Abstract robust coarse spaces for systems of pdes via generalized eigenproblems in the overlaps. Numerische Mathematik, 2013.

[5] N. Spillane, D. J. Rixen, Automatic spectral coarse spaces for robust FETI and BDD algorithms. International Journal for Numerical Methods in Engineering, 2013.

Stanislav Sysala: On control of loading process in perfect plasticity with contact

This is joint work with M. Čermák and J.Haslinger.

The contribution deals with a static case of discretized elasto-perfectly plastic problems obeying Hencky's law in combination with frictionless contact boundary conditions. The main interest is focused on the analysis of the formulation in terms of displacements, limit load analysis and related numerical methods. This covers the study of: i) the dependence of the solution set on the loading parameter ζ, ii) relation between ζ and the parameter α representing the work of external forces, iii) loading process controlled by ζ and by α, iv) numerical methods for solving two different problems, with prescribed values of ζ and α, respectively. The numerical methods are implemented in combination with the Total-FETI domain decomposition method within the MatSol library in Matlab. Some theoretical results and convergence properties are illustrated on numerical examples.

Jakub Šístek: Parallel performance of iterative solvers for pressure-correction methods for incompressible flow

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 parallel 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 applications are large-scale simulations of flows around wings of insects. This is a joint work with Fehmi Cirak.

Radek Tezaur: Toward solving smaller problems for Helmholtz - Interpolatory model order reduction for frequency sweeps and the discontinuous enrichment method

Numerical dispersion, or what is often referred to as the pollution effect, presents a challenge to an efficient finite element discretization of the Helmholtz, Navier equations, and related equations describing acoustic wave propagation in fluids and structures in the medium frequency regime. As a result, a fine discretization is required leading to the solution of large systems of algebraic equations. Two strategies are discussed here to alleviate the difficulty involved in a discretization and a repetitive solution of these equations.

The first part of the talk focuses on frequency sweep problems that arise in many structural dynamic, acoustic, and structural acoustic applications. In each case, they incur the evaluation of a frequency response function for a large number of frequencies. Since each function evaluation requires the solution of an often large-scale system of equations, frequency sweep problems can easily become prohibitively expensive. Interpolatory model order reduction methods have proven to be a powerful tool for reducing their cost. The performance of interpolatory

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MOR methods depends on the location and number of the interpolation frequency points, and the number of consecutive frequency derivatives matched at each frequency point. An automatic adaptive strategy based on monitoring a relative residual in the frequency band of interest is discussed. The robustness, accuracy, and computational efficiency of this adaptive strategy are highlighted with the solution of several frequency sweep problems associated with large-scale structural dynamic, acoustic, and structural acoustic finite element models.

The second part of the talk reviews the discontinuous enrichment method. To alleviate the pollution effect and improve the unsatisfactory pre-asymptotic convergence of the classical Galerkin finite element method with piecewise polynomial basis functions, several discretization methods based on plane wave bases have been proposed. The discontinuous enrichment method is one such method and has been shown to offer superior performance to the classical Galerkin finite element method for a number of constant wavenumber Helmholtz problems and has also outperformed two representative methods that use plane waves - the partition of unity and the ultra-weak variation formulation methods. Applications of DEM ranging from the Helmholtz equation for acoustics in fluids, through the vibration of plates, to the wave equation indicate the potential of such alternative discretization strategies.

Matyáš Theuer: Boundary element method in mathematical homogenization

Numerical realization of mathematical homogenization of elliptic equations is based on homogenization theorem which is in fact quite unfriendly to boundary element methods. Homogenized coefficients of a material are given by an integral formula which includes derivation of a function - solution of an auxiliary periodic equation. In general even if we use BEM for solving this auxiliary problem, we still need values of the solution in volume for computing the homogenized coefficient matrix. Fortunately it can be shown that for some composite materials we can compute the coefficients directly using only values of the auxiliary function at the border between the parts of the composite material. This leads to effective use of indirect BEM in mathematical homogenization.

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Jan Valdman: Verification of functional a posteriori error estimates for obstacle problem in 2D

This is extension of paper of P. Harasim and J. Valdman on Verification of functional a posteriori error estimates for obstacle problem in 1D. Benchmarks with known analytical solutions for contact problem will be implemented numerically and error of discrete approximations will be estimated in energetic norm based on concepts introduced by S. Repin.

Petr Vaněk: Exact interpolation scheme with approximation vector used as a column of the prolongator

This is joint work with Roman Kužel.

Our method is a kind of exact interpolation scheme proposed by Achi Brandt In the exact interpolation scheme, for x being the fine-level approximation of the solution, the coarse-space $V=V(x)$ is constructed so that x satisfies $x \in V$. We achieve it simply by adding the vector x as a first column of the prolongator corresponding to a general purpose coarse-space. (The columns of the prolongator P form a computationally relevant basis of the coarse-space $V=\mathrm{Im}(P)$.) The advantages of this construction become obvious when solving non-linear problems. The cost of enriching the coarse-space V by the current approximation x is a single dense column of the prolongator that has to be updated each iteration. Our method can be used for multilevel acceleration of virtually any iterative method used for solving both linear and non-linear systems. The method is tested, with excellent results, on nuclear reactor criticality computations.

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