WP4: Finite Element Computer Simulation of Strongly Heterogeneous Media

1. Major activities and results

Task 4.1: Robust discretization methods for highly heterogeneous media.

The problems described by partial differential equations can be discretaized by the Finite Volume Method (FVM), the Galerkin Finite Element Method (FEM) or the mixed FEM. Each of them has its advantages. New results characterizing the convergence of the Algebraic MultiLevel Iteration (AMLI) methods are obtained. A new survey paper (invited paper for a topical volume of Springer Proceedings in Mathematics & Statistics) on recent advances of multilevel methods for strongly anisotropic elliptic problems is published. New numerical test demonstrating the optimal complexity of the new AMLI methods for strongly heterogeneous media are published. They include cases where the direction of dominating anisotropy is not aligned with the FEM mesh, as well as anisotropic channels. New results for semicoarsening (SC) and balanced SC multilevel methods for strongly anisotropic bicubic FEM systems are constructed. It is important to note that such results are closely related to the efficient solution of highly coupled systems, including the Lamè equations of elasticity in the case of almost incompressible materials, and the Navier-Stokes equations in the case of large Reynolds number. We continued the work on further development of discretization algorithms for time-dependent problems based on stable alternating directions splitting schemes for time-stepping. The published solution algorithm for the Stokes system has optimal computational complexity. New results for numerical solution of classes of nonlinear problems describing the dynamics of beams with complex cross sections are obtained. The efficiency of this kind of algorithms is based on semi analytical approach incorporating the p-version of FEM.

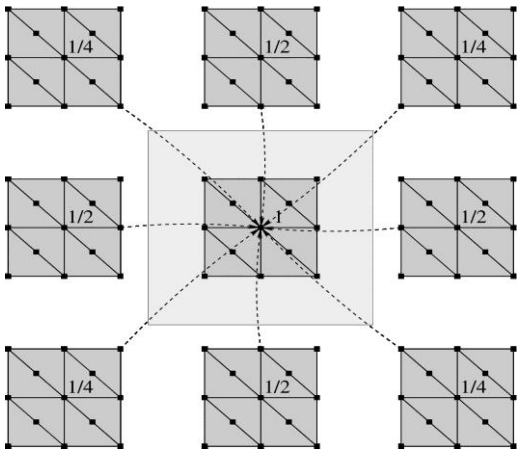

Fig. 1 AMLI preconditioning: additive Schur complement approximation using decomposition of the computational domain by weighted overlapping macroelements

Some results related to this task are presented in [GKL_12], [KLM_12], [KLMa_13], [Sma_1], [L_13a], [SMM_13s], [SM_13p], [SM_13p].

Task 4.2: Parallel iterative solution methods, algorithms and software tools for FEM linear systems.

The recent theory of optimal methods for large-scale sparse linear systems is rather well developed when the coefficient jumps are aligned the interfaces at the coarsest level of the domain partitioning. Such assumptions are usually made in the case of multilevel, multigrid and domain decomposition methods. At the same time, there are a lot of multiscale and multiphysics models of strongly heterogeneous media where the coefficient jumps are resolved on the finest level of the mesh. Such problems are recently referred to as high frequency and high contrast. From other side, certain incomplete factorization methods are more robust with respect to localized coefficient jumps, but their convergence is slower.

In this task we are looking for a balance between robustness and computational complexity issues taking into account the final goal, namely the scalable implementation on high performance clusters and massively parallel machines with distributed memory, such as the IBM Blue Gene/P. The balanced domain decomposition and the proper mapping of the computational graph onto the communication graph of the parallel computer system is of a prime importance for the efficient implementation of the FEM.

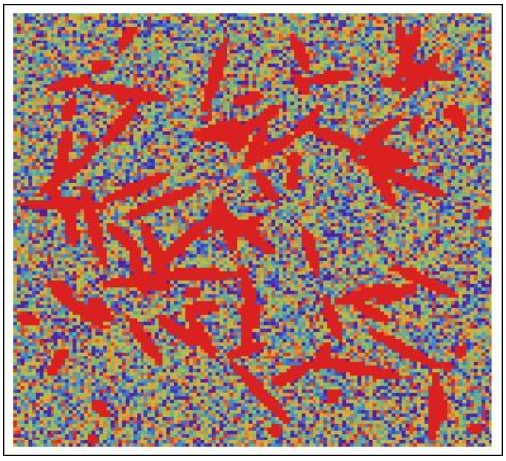

Fig. 2. Test problem for strongly heterogeneous media including stochastic variation of the diffusion coefficient jumps and complex network of channels: the obtained results of numerical tests confirm the optimal computational complexity of the new multilevel iterative methods as well as their robustness with respect to the coefficient jumps and geometry of the interfaces

There are new results for voxel meshes as well as for three dimensional unstructured meshes in a very general setting. They include: a) analysis of the computational complexity; b) analysis of the potential for parallel implementation; c) development of efficient parallel algorithms and their program realization; d) comparative analysis of parallel the speed-up and efficient.

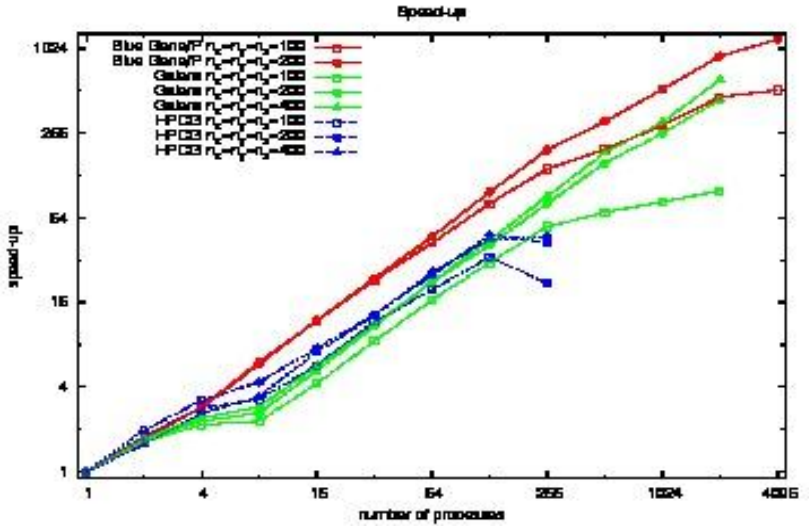

Fig. 3. Comparative analysis of speed-ups for numerical solution of the time dependent Stokes equations on: a) supercomputer IBM Blue Gene/P; b) high performance HP cluster, located at IICT-BAS; c) high performance cluster Galera, located at TU – Gdansk, Polland

Some results concerning this task are published in the papers [GKL_12], [LPG_12], [LPGG_13], [GLP_13a], [SM_13a], [SWGDPFL_13a],[KLM_13p].

<u>Task 4.3</u> Multiscale simulation of human bone tissues and composite materials.

This task continues the work related to micro Finite Element Method (μFEM) analysis and supercomputing applications including: a) μFEM analysis of human bone microstructure; b) μFEM analysis of composite materials. The task is motivated by recent advances in supercomputing technology as well the availability of detailed CT models of the microstructure. It is proposed to upscale Representative Element of Volume (REV) numerically by solving appropriate cell problems and generate macroscopic properties of the homogenized media. New results for determining of the effective bio-mechanical characteristics of trabecular bone tissues are obtained, taking into account the principle directions of dominating anisotropy. We have studied also the effective thermoconductivity of *SiSiC*. This is a special inert material with high porosity, which is used for design of efficient burners. Based on a CT image of a piece of the material, the whole domain of the burner is digitally reconstructed. Then, the time for air cooling is studied in the case of high velocity of the air flow.

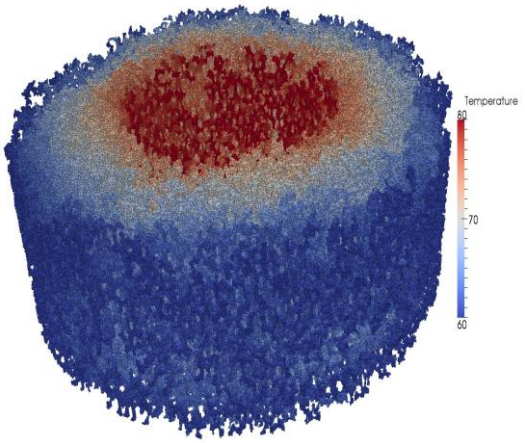

Fig. 4. Supercomputing simulation of processes of combustion and cooling in a porous media based on CT image of the micro-structure of *SiSiC*

Some results concerning this task are published in the papers [MSV_13], [KMV_13], [KMV_13a], [B_13p], [BL_13p].

<u>Task 4.4.</u> Multiscale Modelling of Reactive Flows in Porous Media.

The main focus of this task is the development of multiscale models for porous media including processes of diffusion, convection, reaction, and fluid dinamics. The material characteristics at micro level are strongly heterogeneous and nonlinear. In addition, the processes have different time scales.

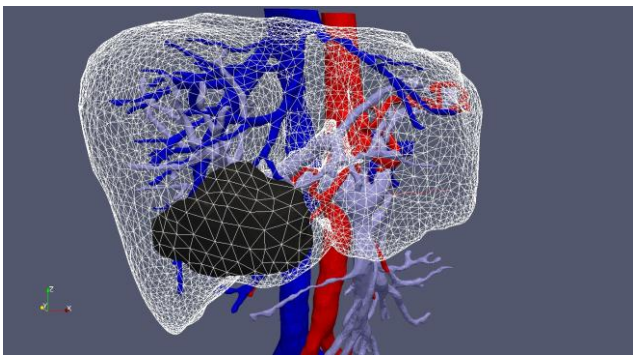

Fig. 5. Supercomputing simulation of radiofrequency hepatic tumor ablation: FEM mesh of the liver, generated using segmented medical image

New results for the following biomedical applications are obtained during the reported period: a) simulation of radiofrequency hepatic tumor ablation; b) modeling of stem cells migration related to blood deceases therapy; c) modeling of the flow in blood vessels with cerebral aneurisms. For instance, in the case of tumor ablation, the developed model includes: the electric field, generated by the electrosurgery instrument; the thermal field generated by the gradient of the electrical field; the loss of heat due to the blood circulation in the capillary network (a mass term) as well as due to the incoming blood thru the portal vane; the destruction of the cell structure of the tissues in the area of ablation.

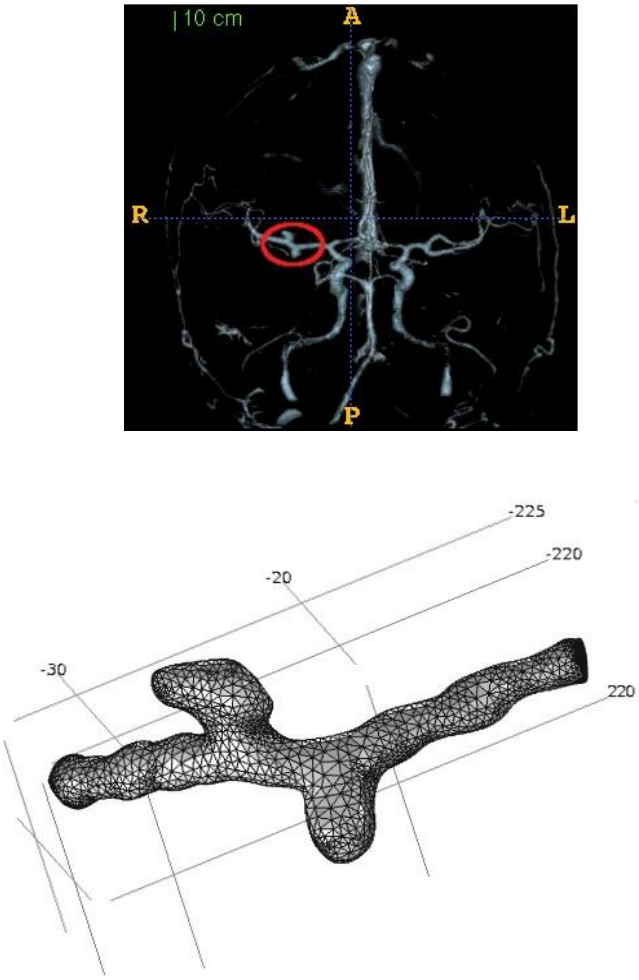

Fig. 6. Supercomputing simulation of cerebral aneurisms: above – segmented medical image; below – FEM mesh of the above indicated part of the blood vessel with aneurisms

Some of the obtained results are presented in [B_11], [KM_11], [KMVa_11a], [KMVc_11a].

2. Publications with acknowledgments to the project DCVP 02/1

(i) published

[GKL_12] M. Ganzha, N. Kosturski, I. Lirkov, Improving the Efficiency of Parallel Alternating Directions Algorithm for Time Dependent Problems, AIP Conference Proceedings, 1487 (2012), 322-328

[KMV_13] N. Kosturski, S. Margenov, Y. Vutov, Computer Simulation of RF Liver Ablation on an MRI Scan Data, AIP Conf. Proc. 1487 (2013), 120-126

[KLM_12] J. Kraus, M. Lymbery, S. Margenov, Semi-Coarsening AMLI Preconditioning of Higher Order Elliptic Problems, AIP Conference Proceedings, Vol. 1487 (1) (2012), 30-41

[KLM_13] J. Kraus, M. Lymbery, S. Margenov, Robust Algebraic Multilevel Preconditioners for Anisotropic Elliptic Problems, In: Numerical Solution of Partial Differential Equations: Theory, Algorithms and their Applications, Springer Proceedings in Mathematics & Statistics (2013), 217-246

[KLMa_13] J. Kraus, M. Lymbery, S. Margenov, Robust Multilevel Methods for Quadratic Finite Element Anisotropic Elliptic Problems, Numerical Linear Algebra With Applications (2013), DOI: 10.1002/nla.1876 (**IF 1.202**)

[LPG_12] I. Lirkov, M. Paprzycki, M. Ganzha, Performance Analysis of Parallel Alternating Directions Algorithm for Time Dependent Problems, Springer LNCS, 7203 (2012), 173-182

[LPGG_13], I. Lirkov, M. Paprzycki, M. Ganzha, P. Gepner, Performance Evaluation of MPI/OpenMP Algorithm for 3D Time Dependent Problems, Preprints of Position Papers of the Federated Conference on Computer Science and Information Systems (2013), 27-32

[SM_13] S. Stoykov, S. Margenov, Nonlinear Vibrations of Rotating 3D Tapered Beams with Arbitrary Cross Sections, Proceedings of the 4th ECCOMAS Thematic Conference on Computational Methods in Structural Dynamics and Earthquake Engineering, M. Papadrakakis, P. Papdopoulos (eds.), Kos, Greece (2013), Paper id.: 1479, 15 p.

[SMa_13] S. Stoykov, S. Margenov, Nonlinear Free Vibrations of 3D Composite Beams, Proceedings of the 11th International Conference on Vibration Problems, Z. Dimitrovova, J. Almeida, R. Goncalves (eds.), Lisbon, Portugal (2013), Paper id: 164, 10 p.

(ii) accepted

[GLP_13a] M. Ganzha, I. Lirkov, M. Paprzycki, Comparative Analysis of High Performance Solvers for Solving Stokes Equation, AIP Conf. Proc.

[GKV_13a] K. Georgiev, N. Kosturski, Y. Vutov, On the Adaptive Time-Stepping in Radio-Frequency Liver Ablation Simulation: Some Preliminary Results, Springer LNCS

[KMV_13a] N. Kosturski, S. Margenov, Y. Vutov, Calibration of Parameters for Radio-Frequency Ablation Simulation, Springer LNCS

[L_13a] M. Lymbery: Robust Balanced Semi-Coarsening Multilevel Preconditioning of Bicubic FEM Systems, Springer LNCS

[MSV_13] S. Margenov, S. Stoykov, Y. Vutov, Numerical Homogenization of Heterogeneous Anisotropic Linear Elastic Materials, Springer LNCS

[SM_13a] S. Stoykov, S. Margenov, Nonlinear Forced Vibration Analysis of Elastic Structures by Using Parallel Solvers for Large-Scale Systems, Springer LNCS

[SWGDPFL_13a] P. Szmeja, K. Wasielewska, M. Ganzha, M. Drozdowicz, M. Paprzycki, S. Fridanova, I. Lirkov, Reengineering and Extending the Agents in Grid Ontology, Springer LNCS

(iii) submitted

[SMM_13s] S. Stoykov, E. Manoach, S. Margenov, An efficient beam model based on the p-version finite element method and preliminary cross sectional analysis, Finite Elements in Analysis and Design

(iv) in preparation

[B_13p] G. Bencheva, Computer Modelling of Cerebral Aneurysm Hemodynamics

[BL_13p] G. Bencheva, I. Lirkov, High-Performance Computer Modelling of Patient Specific Cerebral Aneurysm Hemodynamic

[KLM_13,] J. Kraus, M. Lymbery, S. Margenov, Auxiliary Space Multigrid Method for Elliptic Boundary Value Problems

[SM_13p] S. Stoykov, S. Margenov, Nonlinear Forced Vibrations of 3D Laminated Composite Beams, Journal of Applied Mathematics

[Sma_13p] S. Stoykov, S. Margenov, Geometrically Nonlinear Vibrations of Elastic Structures by Parallel Computations

3. Presentations and talks

I. Lirkov, Improving the efficiency of parallel alternating directions algorithm for time dependent problems, Application of Mathematics in Technical and Natural Sciences, St.St. Constantine and Helena, Varna, Bulgaria, June 11-16, 2012

M. Lymbery, Semi-coarsening AMLI preconditioning of higher order elliptic problems, Application of Mathematics in Technical and Natural Sciences, plenary talk, St.St. Constantine and Helena, Varna, Bulgaria, June 11-16, 2012

S. Margenov, Multilevel preconditioning of anisotropic heterogeneous problems, Application of Mathematics in Technical and Natural Sciences, St.St. Constantine and Helena, Varna, Bulgaria, June 11-16, 2012

S. Margenov, Multilevel preconditioning of strongly anisotropic elliptic problems, 21st International Conference on Domain Decomposition Methods, INRIA, Rennes, France, June 25-29, 2012

S. Margenov, Robust multilevel methods for strongly heterogeneous anisotropic problems and simulations in porous media, plenary talk, Annual Conference of the European Consortium for Mathematics in Industry, ECMI 2012
, Lund, Sweden, July 23-27, 2012

S. Margenov, On the robustness of multilevel preconditioners for quadratic FE discretizations of anisotropic elliptic problems, European Congress on Computational Methods in Applied Science and Engineering, ECCOMAS 2012, Vienna, Austria, September 10-14, 2012

M. Lymbery, On the robustness of multilevel preconditioners for quadratic FE discretizations of elliptic problems, European Congress on Computational Methods in Applied Science and Engineering, ECCOMAS 2012, Vienna, Austria, September 10-14, 2012

S. Margenov, Robust solution methods for strongly heterogeneous problems and supercomputing applications in porous media, plenary talk, SPOMECH, Workshop on Supercomputing for computational solid and fluid mechanics, Ostrava, Czech Republic, November 19-23, 2012

S. Margenov, Robust multilevel mthods for strongly heterogeneous problems, Numerical Methods for PDEs, Texas A &M University, College Station, Texas, USA, January 25-26, 2013

Г. Бенчева, Паралелни пресмятания с MPI, Еднодневен курс "Въведение в паралелно програмиране с MPI и CUDA", ИИКТ-БАН, София, България, Февруари 25, 2013

S. Margenov, Supercomputing Support of the Researches and Education, First Europe – China HPC Conference: Partnership for Supercomputing Applications in Science and Industry, Sofia, Bulgaria, April 8-10, 2013

Г. Бенчева, Компютърно моделиране хемодинамиката на церебрален аневризъм, Workshop: Информационни и комуникационни технологии за човешко здраве и качество на живот (ICT-HuHeQuL), Старозагорски минерални бани, 15-17 Май, 2013

S. Margenov, Robust multilevel methods for strongly heterogeneous problems and supercomputing applications in porous media, plenary talk, 5th International Conference on Porous Media, Prague, Czech Republic, May 21-24, 2013

Y. Vutov, Numerical simulation of the cooling process in a porous media gas burner, 5th International Conference on Porous Media, Prague, Czech Republic, May 21-24, 2013

G. Bencheva, On the High-Performance Computer Modelling of Patient Specific Cerebral Aneurysm Hemodynamics, Large-Scale Scientific Computations, Sozopol, Bulgaria, June 3-7, 2013

I. Lirkov, Reengineering and extending the Agents in Grid Ontology, Large-Scale Scientific Computations, Sozopol, Bulgaria, June 3-7, 2013

M. Lymbery, Robust balanced semi-coarsening multilevel preconditioning of bicubic FEM systems, Large-Scale Scientific Computations, Sozopol, Bulgaria, June 3-7, 2013

S. Stoykov, Nonlinear forced vibration analysis of elastic structures by using parallel solvers for Large-Scale Systems, 9th International Conference on "Large-Scale Scientific Computations", Sozopol, Bulgaria, June 3-7, 2013

Y. Vutov, Numerical Homogenization of Heterogeneous Anisotropic Linear Elastic Materials, 9th International Conference on "Large-Scale Scientific Computations", Sozopol, Bulgaria, June 3-7, 2013

S. Stoykov, Nonlinear vibrations of rotating 3D tapered beams with arbitrary cross sections, COMPDYN 2013, Kos, Greece, June 12-14, 2013

I. Lirkov, Comparative analysis of high performance solvers for solving Stokes equation, Application of Mathematics in Technical and Natural Sciences, Albena, Bulgaria, June 24-29, 2013

S. Margenov, Multilevel methods for strongly anisotropic problems, plenary talk, Preconditioning of Iterative Methods, Prague, Czech Republic, July 1-5, 2013

I. Lirkov, Performance Evaluation of MPI/OpenMP Algorithm for 3D Time Dependent Problems, 6th workshop "Computer Aspects of Numerical Algorithms", Federated conference on Computer science and information systems, Krakow, Poland, September 8-11, 2013

S. Stoykov, Nonlinear free vibrations of 3D composite beams, ICOVP, Lisbon, Portuga, September 9-12, 2013

4. Others

[1] Management activities:

a) Organization periodic meetings of the Operational Committee (S. Margenov, S. Grozdanova);

b) Periodic meetings of the Operational Group for management of WP1, WP3, WP4 and WP5 (S. Margenov, V. Lazarov, E. Atanasov, I. Dimov, K. Georgiev С. Маргенов);

[2] Dissemination of the results of the project in mass media (С. Маргенов);

[3] Development and maintenance of the project web site (S. Grozdanova);

[4] Coordination activities related to delivery of equipment and specialized software for WP1, WP3, WP4 and WP5 (S. Margenov, E. Atanasov, V. Lazarov);

[5] Adaptation and further development of curricula of the lecture courses on Numerical Methods for Sparse Matrices, and Parallel Algorithms, Department of Mathematics and Informatics, Sofia University (S. Margenov, G. Bencheva);

[6] Additional dissemination activities within the frame of:

a) Conference on Large Scale Scientific Computing, Sozopol, June 6-10, 2013 (S. Margenov, S. Grozdanova, I. Lirkov, G. Bencheva, M. Lymbery, S. Stoykov);

b) Annual Meeting and Information Days: SuperCA++, Tryavna, March 31 – April 2, 2013 (S. Margenov, S. Grozdanova).