WP3: Finite Element Computer Simulation of Strongly Heterogeneous Media

1. Major Activities and Results

<u>Task 3.1</u>: Robust discretization methods for highly heterogeneous media. The finite volume method, the Galerkin finite element method (FEM) and the mixed FEM are the basic advanced tools for discretization of mathematical models of highly heterogeneous (including porous) media. Each of these methods has its advantages and disadvantages. For applications related to highly heterogeneous media, the finite volume and mixed FEM have proven to be accurate and locally conservative. It is shown that after the elimination of the unknowns representing the pressure and the velocity from the algebraic system, the resulting Schur system for the Lagrange multipliers is equivalent to a discretization by Galerkin method using linear non-conforming finite elements. This is the strong motivations for further development, tuning and implementation of non-conforming FEM and Discontinuous Galerkin (DG) methods, algorithms and software tools, included in the task. Fore instance, new robust and locally conservative non-conforming and DG discretizations are obtained for: a) parabolic problems (see Fig. 1); b) almost incompressible materials in linear elasticity; c) Navier-Stokes equations with high Reynolds numbers. This task has a particular focus on locally conservative approximations applicable to complex voxel structures (see Fig. 2). New specialized numerical homogenization methods are developed. Some of the obtained results are published in the papers [KMV_09c, BMN_09s, HP_09a] coauthored by N. Kosturski, P. Boyanova, S. Petrova and Y. Vutov.

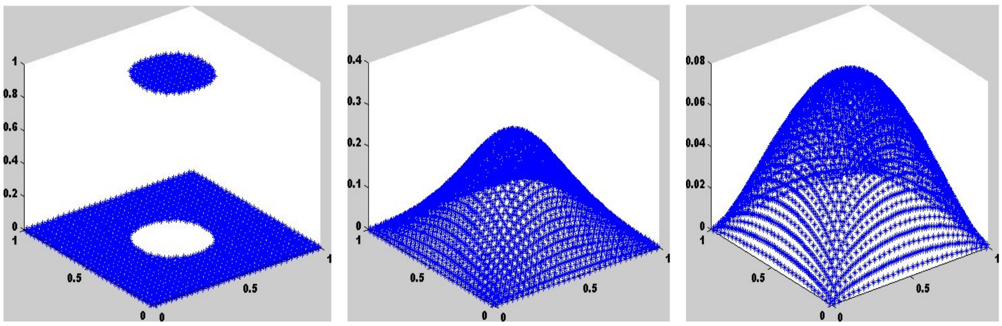

Fig.1 Numerical solution of a parabolic problem discretized by non-conforming finite elements: t = 0 (left), t = 2 (center), t = 10 (right) [BMN_09s]

<u>Task 3.2</u>: Parallel iterative solution methods, algorithms and software tools for FEM linear systems. This task includes development, adaptation, tuning and testing of algorithms and programming tools. Efficient projection iterative methods of the type of conjugate gradients in Krylov subspaces are applied for solution of the FEM linear systems. The deep knowledge of the properties and the sparsity structure of the matrices are to be taken into account for these methods. New results in the field of parallel preconditioning using MIC(0) (modified incomplete factorization) and AMG (algebraic multigrid) are obtained. In the case of nonlinear problems, projection decupling schemes and/or the Newton method are applied. The construction of efficient (including parallel) iterative methods and algorithms for complex and strongly coupled composite problems is based on balanced block partitioning of the matrix. The domain decomposition is an important issue in the block representation. Another general approach for construction of efficient partitioning of the stiffness matrix is based on analysis of the graph representing the sparsity structure. To get more realistic theoretical estimates of the parallel efficiency, the communication times are studied taking into account the architecture of the parallel computer system including the characteristics of its connectivity. Originally developed parallel MIC(0) preconditioners as well as composite algorithms using Boomer AMG (developed at Lawrence Livermore National Laboratories of USA) are implemented and tested on the supercomputer IBM Blue Gene/P. The team working on this task includes G. Bencheva, I. Lirkov, N. Kosturski, S. Margenov and Y. Vutov. Some of the obtained results are published in [V_09, GPDSLIOT_09a, KM_09a, LVGP_09a, V_09p, K_09p].

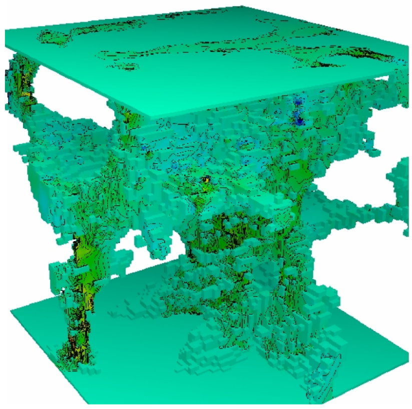

Fig.2 Reference volume element: voxel microstructure of a trabecular bone

<u>Task 3.3</u>: Multiscale simulation of bone tissues and (geo)composites. This task concerns two advanced real life applications of the supercomputers: a) μFEM analysis of microstructure of human bone; b) μFEM analysis of (geo)composite materials. Specialized methods for numerical upscaling of the elastic (poroelastic) properties of strongly heterogeneous and highly porous materials are developed and implemented. The microstructure of the reference volume element (see Fig. 2) is obtained using high resolution computer tomography. In many cases these problems lead to FEM systems with 10^8 -10^9 degrees of freedom. The use of supercomputers is the only way for practical solution of such kind of problems. New results characterizing the process of development of osteoporoses in trabecular bone tissues are obtained. The anisotropy level as well as the influence of the fluid phase for different porosities is studied in the frame of linear elasticity models at micro and macro scales. Pilot numerical tests for analysis of the bone structure are performed where the Biot's model of poroelasticity at macro level and fluid-structure interaction at micro level are used. The development and implementation of a parallel algorithm for multiscale simulation of fluid flows in a porous (geocomposite) media is in progress. New results in the analysis of microfluids concerning shape optimization are obtained which is one important step in the future development of computer simulation of composite materials. The group working on this task includes N. Kosturski, P. Popov, S. Margenov, S. Petrova and Y. Vutov. Part of the results are published in [KM_09a, P_09, HP_09a, P_09a, K_09s].

2. Publications with acknowledgements to the project ДО 02-115/08

a) published:

[V_09] Y. Vutov, Scalability Tests of Two Parallel PCG Solvers on Blue Gene/P, 3rd Annual Meeting of the Bulgarian Section of SIAM, Proceedings (2009), ISSN: 1313-3357, 87-90

[KMV_09] N. Kosturski, S. Margenov, Y. Vutov, Efficient Solution of μFEM Elasticity Problems in the Case of Almost Incompressible Materials, 3rd Annual Meeting of the Bulgarian Section of SIAM, Proceedings (2009), ISSN: 1313-3357, 65-68

[P_09] S. Petrova, Applications of one-shot methods in PDEs constrained shape optimization, Mathematics and Computers in Simulation, 80, No. 3 (2009), ISSN: 0378-4754, 581-597

б) accepted:

[KM_09a] N. Kosturski, S. Margenov, Numerical Homogenization of Bone Microstructure, Large Scale Scientific Computing, Springer LNCS 5910

[P_09a] S. Petrova, On Shape Optimization of Acoustically Driven Microfluidic Biochips, Large Scale Scientific Computing, Springer LNCS 5910

[GPDSLIOT_09a] M. Ganzha, M. Paprzycki, M. Drozdowicz, M. Senobari, I. Lirkov, S. Ivanovska, R. Olejnik, P. Telegin, Information flow and mirroring in an agent-based Grid resource brokering system, Large Scale Scientific Computing, Springer LNCS 5910

[LVGP_09a] I. Lirkov, Y. Vutov, M. Ganzha, M. Paprzycki, Parallel Performance Evaluation of MIC(0) Preconditioning Algorithm for Voxel μFE Simulation, Proceedings of Parallel processing and applied mathematics 2009

[HP_09a] R.H.W. Hoppe and S.I. Petrova, Multi-scale method for the crack problem in microstructural materials, Computational Methods in Applied Mathematics, Volume 10, 2010

в) submitted:

[BMN_09s] Boyanova, S. Margenov, M. Neytcheva, Robust AMLI Methods for Elliptic and Parabolic Crouzeix-Raviart FEM systems, Computational Methods in Applied Mathematics

г) in preparation:

[K_09p] N. Kosturski, Scalable PCG Solution Algorithms for μFEM Elasticity Systems

[V_09p] Y. Vutov, Parallel MIC(0) Preconditioning for Numerical Upscaling of Anisotropic Linear Elasticity Materials

3. Presentations and talks

[1] N. Kosturski, Scalable PCG Solution Algorithms for μFEM Elasticity Systems, Mathematics and Computers in Simulation, Modelling 2009, Roznov pod Radhostem, Czech Republic, June 22 - 26, 2009

[2] N. Kosturski, Scalable PCG Solution Algorithms for μFEM Elasticity Systems, Mathematics and Computers in Simulation, Annual Meeting of BGSIAM'09, Sofia, Dec. 21 – 22, 2009

[3] E. Lilkova, Computer simulation of human interferon-gamma mutants, Meetings in Physics, Sofia University, March 2009

[4] I. Lirkov, Parallel Performance Evaluation of MIC(0) Preconditioning Algorithm for Voxel \u03bcFE Simulation, 8th International Conference on Parallel Processing and Applied Mathematics, Wroclaw, September 13-16, 2009

[5] S. Margenov, Blue Gene in Bulgaria – Center of Excellences on Supercomputing Applications – Joint Project of IPP - BAS, SU, TU - Sofia and MU - Sofia, Opening of the IBM Academic Initiative, Mar. 9, Sofia, 2009

[6] S. Margenov, Parallel PCG algorithms for voxel FEM systems, ComplexHPC Meeting, Universidade Tecnica de Lisboa, Portugal, Oct. 19-20, 2009

[7] S. Margenov, Supercomputing: methods, algorithms and applications (plenary talk), Computer Science'09, Technical University - Sofia, Bulgaria, Nov. 5-6 2009

[8] S. Petrova, Applications of one-shot methods in PDEs constrained shape optimization, Mathematics and Computers in Simulation, ENUMATH 2009, Uppsala, Swiden, June 29-July 3, 2009

[9] Y. Vutov, A Parallel MIC(0) Preconditioning Technique for Elliptic Problems, Bulgarian – Swedish Workshop "Numerical Methods and High Performance Computations – Integrity and Novel Ideas, IPP – BAS, Sofia, February 17 – 18, 2009

[10] Y. Vutov, Parallel MIC(0) Preconditioning for Numerical Upscaling of Anisotropic Linear Elasticity Materials, Minisymposium on HPC-driven Numerical Methods and Applications, ENUMATH 2009, Uppsala, Swiden, June 29-July 3, 2009

4. Others

[1] Organizational and financial activities:
a) Organization of regular meetings of the Operational Board (S. Margenov, S. Grozdanova);
b) Regular meetings of the operational group for organization of the work on WP1, WP3 and WP4 (S. Margenov, K. Boyanov, I. Dimov, V. Lazarov, K. Georgiev);

c) Additional Agreement and Annex to the Additional Agreement (S. Margenov, K. Boyanov).

[2] Development and support of web page of the project: Variant 1 – June 2009; Variant 2 – October 2009 (S. Grozdanova).

[3] Purchasing of equipment for WP1, WP3, WP4 (S. Margenov, K. Boyanov, V. Lazarov, K. Georgiev). Preparation of specification and purchasing of software for WP1, WP3 and WP4 (S. Margenov, I. Dimov, K. Georgiev, V. Lazarov).

[4] Establishment of a new computer lab for education, training and work on project SuperCA: renovation, computer and communication equipment, installation of software under Linux operational system(S. Margenov, V. Lazarov, I. Lirkov, Y. Vutov, N. Kosturski, G. Bencheva, S. Grozdanova).

[5] Adaptation and further development of the curricula of the course on Parallel algorithms, Department of Mathematics and Informatics, Sofia University (S. Margenov, G. Bencheva).

[6] Adaptation and further development of the curricula of the course on Numerical methods for systems with sparse matrices, Department of Mathematics and Informatics, Sofia University (S. Margenov, G. Bencheva).

[7] Additional activities for dissemination and popularization of the obtained results in the frame of:
a) Conference on Large Scale Scientific Computing, Sozopol, June 4-8, 2009 (organized by IPP – BAS);
b) Startup meeting of MC of COST Action IC0805 Open Network for High-Performance Computing on Complex Environments, Brussels, May 7, 2009 (S. Margenov, MC Member);
в) Minisymposium on HPC-driven Numerical Methods and Applications, ENUMATH 2009, Uppsala, June 29 – July 3 (S. Margenov, coorganizer);
г) Meeting of MC of COST Action IC0805 Open Network for High-Performance Computing on Complex Environments, Lisbon, October 20, 2009 (S. Margenov, MC Member).