EXTENDED SUMMARY

1. Published works

We have made considerable progress in all of the tasks summarized in Section 1. In particular we have developed two different Multiscale Finite Element algorithms for Fluid-Structure interaction problems with multiple length scales [2, 5]. The methods incorporate nonlinear macroscopic equations for conservation of mass and momentum into an iterative homogenization framework. The coarse scale quantities are the average pressure and displacement. The homogenization process is written in an iterative form at the macroscale with appropriately defined downscaling operators. The downscaling operators project the coarse quantities to define fine-scale velocity, pressure and displacement fields. During every macroscale iteration we first project the coarse pressure and displacements to the fine-scale. This defines a porous microstructure based on the macroscopic parameters (pressure and displacement) from the previous iteration. Then, macroscopic properties are computed, based on the downscaled microstructure and those change the macroscopic model, allowing for a next iterative approximation of the macroscopic parameters. The proposed methods were applied to a series of model problems involving flow past deformable elastic obstacles made of a linear isotropic elastic material [2, 5]. In all cases our iterative multiscale algorithm provided accurate approximation of the fine-scale reference solution in terms of pressure and displacement. They also showed good convergence properties in terms of the length-scales parameter (ε). That is, the downscaling map produces fields which converge to the “real” velocity, pressure and displacements, which were generated using direct numerical simulations. With this, all objectives of Task 1.1 were fulfilled. Moreover, we have analyzed rigorously one of the algorithms for convergence with respect to the length-scale parameter (ε). This is done by comparing the downscaled fields at a given iteration of our MsFEM with a comparable approximation obtained by an iterative direct numerical simulation algorithm. We have demonstrated that the two remain close in terms of ε under certain assumptions, establishing convergence (Taks 3) [2].

We have also implemented our methods on a distributed cluster environment [2, 5]. We have run the codes on both traditional high-performance clusters and on distributed computing environments. In particular, the macroscopic discretization is run on a single workstation and the downscaling tasks on a heterogeneous computing grid. The communication between the macro solver and the downscaling tasks is done via TCP sockets using a CORBA-like interface (Common Object Reference Brokerage Architecture is a software standard for remote execution of object-oriented code). This resulted in a flexible implementation, suitable to a variety of heterogeneous computing architectures. With this we have combined Tasks 2.1. and 2.2 and provided a very scalable implementation [2, 5].

We have also developed tools for processing voxel-based data and reconstructing the fluid-solid interface of complex CAT (Computed Axial Tomography) images of human femur [4]. With this we have enabled the use of realistic CAT data into our multiscale algorithms. We have made preliminary computations of cell problems on realistic bone tissue samples, recovering both macroscopic mechanical and flow properties [4]. With this, we have fulfilled the requirements stated in Task 4.1. The developed tools are capable to perform complex simulations of general geometries (Task 1.4).

In addition to the explicitly planned activities we have also executed a number of complimentary activities, directly related to our iterative multiscale framework for fluid-structure problems. First, in collaboration with Prof. Yalchin Efendiev (Texas A&M University) and Prof. Viktoria Savatorova (Moscow Engineering Physics Institute) we have extended our framework to Stokes-Brinkman equations [1]. This equation models flow in media with porous and free flow domains. It can be very useful in multiscale fluid-structure problems as well, the main topic of our grant. In particular, it allows extending in a natural way our multiscale fluid-structure algorithms by replacing the elastic skeleton with a poroelastic one, thus adding one more scale. In such a setting the Stokes-Brinkman equation allows a natural coupling between fluid in the free-flow regions and the poroelastic skeleton. This complements mechanical coupling, which is already implemented. This research direction will be pursued both as part of the current project and beyond its planned duration. In performing this work we developed a new class of preconditioners for solving medium-sized cell problems based on the Navier-Stokes-Brinkman (NSB) equation [6]. We note that when the permeability tensor is highly oscillatory, existing approaches utilizing iterative linear solvers to tackle the linear system resulting from discretizations of the NSB equations perform very poorly. Our preconditioner allows for efficient solution of intermediate sized cell problems (up to 1M DOF) utilizing Krylov based iterative methods. This in turn enables large scale MsFEM computations, where many such local solved are required.

In a separate development we have also successfully developed analytical tools which allow very fast approximation of cell solutions. While these analytical approximations to cell solutions do not yield very accurate downscaled solutions, they turned to be extremely useful in an MG context. When one is interested in the actual fine-scale solution, rather then homogenization based approximations, a very large system of equations needs to be solved. The natural approach is to use a MG method. We tested several highly heterogeneous diffusive flow problems, where standard MG approaches do not work well and we obtained excellent acceleration when computing the actual fine-scale solution. The work was also extended to using (and comparing) a number of robust of two-level domain decomposition preconditioners for high-contrast anisotropic flows in multiscale media [7]. A complementary global smoother was introduced to handle the case of a network of highly anisotropic channels. The proposed approach is based on robust multilevel (AMLI) constructions for highly anisotropic elliptic problems in the case of nonconforming FEM approximations.

Finally we have also developed a fine-scale solver for numerical simulations of electrochemical diffusion processes in Li-Ion batteries [3,8]. This was done in collaboration with our partners at Fraunhofer ITWM (Prof. Oleg Iliev and Prof. Arnulf Latz) and was partially supported by the current grant. This activity can be combined with fluid-structure problems, for example in modeling processes in fuel cells, as well as other multifunctional devices.

2. Dissemination Activities

As part of this reintegration project, we have also engaged in various transfer of knowledge activities. Dr. Peter Popov taught a course on Theory of Finite Element Methods at the Dept. of Mathematics and Informatics, Sofia University in the Spring of 2010. This allowed him to teach aspects of MsFEM such as the use of oscillatory basis functions to graduate level students. He was also able to recruit two MS students (Mr. Maxim Taralov and Ms. Vasilena Nakova) who were supported by this grant. We have also made efforts to maintain positive gender balance in the sense that one of the students is female. As part of our ongoing collaboration with the Dept. of Flow and Material Simulation at Fraunhofer ITWM (K. Steiner, A Latz, O. Iliev), Fraunhofer ITWM provided co-funding for a summer internship for Mr. Taralov and Ms. Nakova at their facility (Aug.-Oct., 2010). Since the autumn of 2011 they both got PhD positions at ITWM.

Two cycles of invited lectures at the Department of Civil Engineering, Ruhr University of Bochum (Collaborative Research Center 837, Interaction Modeling in Mechnized Tunneling) were taught within the frame of this project, namely: (i) Homogenization Theory and Multiscale Methods (Dr. Popov, Oct. 2010) and (ii) Large-scale Scientific Computing in FEM Simulations (Prof. Margenov, Dec. 2010).

Dr. Popov has also engaged in number of discussions with Mr. Yavor Vutov and Mr. Nikola Kosturksi, PhD students at the host institution. Mr Vutov and Mr, Kosturksi were trained in deriving cell problems for the Biot system poroelastic equations, which is important for their ongoing research on modeling the human femur. This also resulted in the design of new schemes for interpreting CAT based information which is also instrumental in their research. For their part, Mr. Vutov and Mr. Kusturksi provided valuable information on utilizing Blue Gene/P supercomputing systems which is important for the career development. Dr. Popov.

3. List of Papers

[1] V. Savatorova, P. Popov, Y. Efendiev, *Upscaling of the Stokes-Brinkman Equation for Essentially non-Darcy Flows* (in preparation)

[2] P. Popov, Y. Gorb and Y. Efendiev, Multiscale Finite Element Methods for Fluid-Structure Interaction Problems (submitted)

[3] P. Popov, Y. Vutov S. Margenov O. Iliev, *Finite Volume Discretization of Equations Describing Nonlinear Diffusion in Li-Ion Batteries*, Numerical Methods and Applications, Springer Lecture Notes in Computer Science, Vol. 6046, 2011, 338-346.

[4] P. Popov. U*pscaling of Deformable Porous Media with Applications to Bone Modelling*, 4th Annual Meeting of the Bulgarian Section of SIAM, BGSIAM'09 Proceedings, Demetra, 2010, 105-110.

[5] P. Popov, Y. Efendiev, and Y. Gorb, *Multiscale Modeling and Simulation of Fluid Flows in Highly Deformable Porous Media*, Large-Scale Scientific Computing, Springer Lecture Notes in Computer Science, Vol. 5910, 2010, 148-156.

[6] P. Popov, *Preconditioning of Linear Systems Arising in Finite Element Discretizations of the Brinkman Equation*, Large-Scale Scientific Computing, Springer Lecture Notes in Computer Science, Vol. 7116, 2012, 381–38.

[7] Y. Efendiev, J. Galvis, R.D. Lazarov, S.D. Margenov, J. Ren, *Robust Two-level Domain Decomposition Preconditioners for High-contrast Anisotropic Flows in Multiscale Media*, Computational Methods in Applied Mathematics, Vol. 12, 2012, 1–22.

[8] M. Taralov, V. Taralova, P. Popov, O. Iliev, A. Latz, J. Zausch, Report on Finite Element Simulations of Electrochemical Processes in Li-ion Batteries with Thermic Effects, Fraunhofer ITWM, Bericht 221, 2012, 33

4. List of Conferences

We have presented results obtained within the frame of this project in a number of international conferences, workshops and seminars including:

1. P. Popov, *Multiscale Modeling of Poroelasticity in Highly Deformable Fractured Reservoirs*, 7th International Conference on Numerical Methods and Applications, Aug. 20 - 24, 2010, Borovets, Bulgaria.

2. P. Popov, *Coupling Core-scale Fluid-Structure Interaction Problems with Field-scale Geomechanics*, Invited Talk at ExxonMobil Upstream Research Company, Jul. 15, 2010, Houston, Texas, USA.
3. S. Margenov, *Large-Scale Scientific Computing of Engineering and Environmental Problems*, Invited Plenary Talk, Mathematics in Industry Conference in Cooperation with Annual Meeting of European Mathematical Society, Jul. 11-13, 2010, Sofia, Bulgaria.
4. N. Kosturski, Y. Vutov, *Efficient Parallel Solution Algorithms for μFEM Elasticity Systems*, 6th International Workshop on Parallel Matrix Algorithms and Applications, Jun. 29 – Jul. 2, 2010, Basel, Switzerland.
5. Y. Vutov, *Large Scale Finite Element Modeling on Unstructured Grids*, 6th International Workshop on Parallel Matrix Algorithms and Applications, Jun. 29 – Jul. 2, 2010, Basel, Switzerland.
6. S. Margenov, *Robust AMLI Methods for Time-Dependent FEM Systems*, Joint SIAM/RSME-SCM-SEMA Conference on Emerging Topics in Dynamical Systems and Partial Differential Equations, May 31- Jun. 4, Barcelona, Spain, 2010.
7. P. Popov. *Multiscale Modeling and Simulation of Fluid Flows in Highly Deformable Porous Media,* 4th Annual Meeting of the Bulgarian Section of SIAM, BGSIAM'09, Dec. 21-22, 2009, Sofa, Bulgaria.
8. P. Popov. *Multiscale Modeling and Simulation of Fluid Flows in Highly Deformable Porous Media*, 11-th National Congress on Theoretical and Applied Mechanics, Sept. 2-5, 2009, Borovets, Bulgaria.
9. N. Kosturski, Scalable PCG Solution Algorithms for μFEM Elasticity Systems, Modelling, Jun. 22 - 26, 2009, Roznov pod Radhostem, Czech Republic.
10. Y. Vutov, Scalable PCG Algorithms for Numerical Upscaling of Voxel Structures, The eighth European Conference on Numerical Mathematics and Advanced Applications, Sweden, Jun. 29 – Jul. 3, 2009, Uppsala, Sweden.
11. P. Popov. *Multiscale Modeling and Simulation of Fluid Flows in Highly Deformable Porous Media*, 7th International Conference on Large-Scale Scientific Computing, Jun. 4 – 8, 2009, Sozopol, Bulgaria.
12. P. Popov, *Preconditioning of Linear Systems Arising in Finite Element Discretizations of the Brinkman Equation*, 8th International Conference on Large-Scale Scientific Computing, Sozopol, Jun. 5 – 9, 2011, Bulgaria.
13. S. Margenov, *Multilevel Preconditioning of Anisotropic Heterogeneous Problems,*Invited Plenary Talk, Conference on Modelling Storage in Deep Layers, Schwetzingen Castle, Oct. 11 – 13, 2011, Germany.
14. Y. Vutov, *Computer simulation of RF liver ablation on an MRI scan data*, PPAM'11, Sept. 11-14, 2011, Torun, Poland.
15. S. Margenov, *Robust Multilevel Methods for Strongly Heterogeneous Anisotropic Problems and Simulations in Porous Media*, Invited Plenary Talk, Annual Conference of European Consortium for Industrial Mathematics (ECMI), Jul. 23 – 27 2012, Lund, Sweeden.

In addition to that, the IRG researcher, Dr. Peter Popov organized, together with Prof. Oleg Iliev a special session on Modelling And Simulation of Electrochemical Processes at the 7th International Conference on Numerical Methods and Applications, Aug. 20 - 24, 2010, Borovets, Bulgaria. He was also in the organizing committee of the 8th International Conference on Large-Scale Scientific Computing in Sozopol, Bulgaria, 2011, organizing together with Prof. Oleg Iliev a special session on Multiscale Industrial, Environmental and Biomedical Problems.

5. Collaboration

In addition to the usual conference activities, as part of this project we have held four fruitful discussion with our colleagues from Fraunhofer ITWM (K. Steiner, A Latz, O. Iliev) on the topic of the grant as well as on modeling electrochemical processes in LiIon batteries at the micro scale. Three of these meetings were held at Fraunhofer ITWM and one in the host institution. Dr. Peter Popov has also made two visits to the Institute for Scientific Computation, Texas A&M University in College Station discussing extensions to the ongoing research to Stokes-Brikman flows coupled with mechanical deformations.

6. Other Activities

During the reporting period, the researcher, Dr. Peter Popov has completed his habilitation and is presently employed as associate professor at the host institution.