SPECIAL SECTION

SIMULATION OF MULTIPHYSICS MULTISCALE SYSTEMS: GOING NANO

GUEST EDITOR

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PREFACE

Reflecting the ever-growing interest and need in advanced multiscale modeling, a series of mini-symposia on Simulation of Multiphysics Multiscale Systems (SMMS) annually brings together experts from fundamental and applied sciences to push forward this challenging multidisciplinary research field and to foster cross-fertilization between different areas of applications [1]. The topics traditionally addressed by the symposium include modeling of multiphysics and/or multiscale systems on different levels of description, novel approaches to combine different models and scales in one problem solution, advanced numerical methods for solving multiphysics multiscale problems, new algorithms for parallel distributed computing specific to the field, and challenging multiphysics multiscale applications from industry and academia. A good tradition of the SMMS workshop is to publish the best papers in a special issue of the International Journal for Multiscale Computational Engineering. With this preface, I am opening the fifth edition of the special issue on simulation of multiphysics multiscale systems. This time, it will be split in two journal issues to speed up the publication and to adapt to the individual pace of the authors.

A large collection of rigorously reviewed papers presented at the past six workshops highlight modern trends and recent achievements [2]. A number of selected papers have been published in special issues of the *International Journal for Multiscale Computational Engineering*, describing state-of-the-art methods for multiscale multiphysics applications [3]. These publications demonstrate the progress made in generic methodologies and mathematical analysis, and introduce novel software systems that facilitate efficient simulation of multiphysics multiscale systems. Special attention was paid to the approaches for coupling different models and scales, such as continuous and discrete models; quantum and classical approaches; deterministic and stochastic techniques; nano, micro, meso and macro descriptions. In addition, a number of advanced computational methods have been developed for coupling the models, e.g. homogenization techniques, multigrid and nested grids methods, variational multiscale methods; embedded, concurrent, integrated or hand-shaking multiscale methods, domain bridging methods, etc.

Following the trend of modern high-tech devices to grow ever smaller, computational engineering is shifting its attention towards the smallest known scales, where quantum effects must be properly taken into account while modeling end-user devices. The task of modeling nanoscale processes while designing and optimizing the macroscale equipment is far from trivial, but thanks to the nanotechnology boom experienced in the past few years, the research into modeling nanomaterials and nanodevices has matured enough to start giving fruit of novel modeling approaches. The two papers presented in this section, show the advances in multiscale modeling of nanodevices [4,5].

I would like to thank my colleague Alfons Hoekstra for his help in organizing the SMMS workshops; the authors for their inspiring contributions; and the Program Committee for their diligent work, which led to the very high quality of the conference and formed the basis for the selection of papers for this special section.

We invite you to visit the workshop website http://staff.science.uva.nl/~valeria/SMMS/ and to participate in the forthcoming events. SMMS-2010 will take place in Amsterdam, celebrating the 10th Anniversary of ICCS.

REFERENCES

1. Simulation of Multiphysics Multiscale Systems, a series of International Workshops http://www.science.uva.nl/~valeria/SMMS
2. LNCS V. 5544/2009. ICCS-2009 Proceedings, Part I. Soon available online; LNCS V. 5102/2008. http://dx.doi.org/10.1007/978-3-540-69387-1, pp. 165-340; LNCS V. 4487/2007. http://dx.doi.org/10.1007/978-3-540-72584-8, pp. 755-954; LNCS V. 3992/2006. http://dx.doi.org/10.1007/11758525, pp. 1-138; LNCS V. 3516/2005. http://dx.doi.org/10.1007/b136575, pp. 1-146; LNCS V. 3039/2004. http://dx.doi.org/10.1007/b98005 , pp. 540-678.
3. Simulation of Multiphysics Multiscale Systems. Special Issues of the International Journal for Multiscale Computational Engineering::
   http://dx.doi.org/10.1615/IntJMultCompEng.v6.i1, **6**(1), 2008.
   http://dx.doi.org/10.1615/IntJMultCompEng.v5.i1, **5**(1), 2007.
   http://dx.doi.org/10.1615/IntJMultCompEng.v4.i2, **4**(2), 2006.
   http://dx.doi.org/10.1615/IntJMultCompEng.v4.i3, **4**(3), 2006.
4. Fedoseyev, A. I. et al. Simulation of Quantum Dot Based Nanodevices for Photovoltaic Applications with Multiscale Model. *Int. J. Multiscale Computational* Eng. **7**:1–7, 2009.
5. Fedoseyev, A. I. et al. Multiscale Simulation Models for Transient Radiation Effects with 3D Ionizing Tracks in Semiconductor Nanodevices. *Int. J. Multiscale Computational Eng*. **7**:9–16, 2009.

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