Challenges and Solutions in Simulation of Multiphysics Multiscale Systems

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Simulation of multiphysics and multiscale systems poses a grand challenge to computational and computer science, with vast applications in engineering, plasma physics, material science, biophysics, neuroscience, aerospace and automotive sectors. Most real-life systems involve interactions amongst **a wide range of physical phenomena**. In addition to that, the **time and length scales** of the individual processes often differ by many orders of magnitude. Numerical simulation of such complex systems requires development of sophisticated models and methods for their integration, as well as efficient numerical algorithms and advanced computational techniques.

In this talk, I will give an overview of the recent trends and open issues in the field of multiphysics multiscale simulation, as I observed it in the *Workshops on Simulation of Multiphysics Multiscale Systems* organized in the past 7 years http://staff.science.uva.nl/~valeria/SMMS/ and in the ASME IDETC/CIE *Symposia on Computational Multiphysics Applications* http://www.science.uva.nl/~valeria/IDETC-CIE-Multiphysics/.

As an example of multiphysics multiscale simulations, I will describe my own research in modeling semiconductor technologies and flood defense systems:

- Plasma chemical deposition (PECVD) is one of the key technologies in manufacturing solar cells and semiconductor electronics. A number of intertwined processes occur in PECVD reactors: plasma discharge processes, convective and diffusive transport, homogeneous and heterogeneous chemical reactions, adsorption and desorption, film defect formation, etc. Several models and codes have been developed to simulate all the processes, along with the interfacing algorithms for their coupling. I will give some details of the modeling approach and present the Virtual Reactor problem-solving environment that harnessed Grid technologies by adaptive load balancing of parallel solvers on heterogeneous computing resources.

- Flood defense and early warning systems are a very hot topic in view of global warming -in spite of the very cold winter 2009/2010. One of the main goals of the *UrbanFlood* EU FP7 project is modeling flood protection systems, such as river embankments, sea dikes, dams and levees. The models shall go all the way from the scale of a sand grain, via the scale of the ocean tides, to the scale of seasonal and global changes. Full 3D transient simulation of dike failure with subsequent inundation will require tremendous computing resources. The project started only 2 months ago; I will describe our preliminary ideas and present the modeling cascade we foresee.

Related links

1. *Simulation of Multiphysics Multiscale Systems*, annual workshops within the International Conference on Computational Science http://www.science.uva.nl/~valeria/SMMS
2. *Computational Multiphysics Applications*, annual symposia within ASME Computers and Information in Engineering Conference http://www.science.uva.nl/~valeria/IDETC-CIE-Multiphysics
3. *ICCS proceedings*:
   Procedia Computer Science, will be available online in May 2010;
   LNCS V. 5544/2009. DOI: http://dx.doi.org/10.1007/978-3-642-01970-8 , pp. 653-806;
   LNCS V. 5102/2008. DOI: http://dx.doi.org/10.1007/978-3-540-69387-1 , pp. 165-340;
   LNCS V. 4487/2007. DOI: http://dx.doi.org/10.1007/978-3-540-72584-8 , pp. 755-954;
   LNCS V. 3992/2006. DOI: http://dx.doi.org/10.1007/11758525 , pp. 1-138;
   LNCS V. 3516/2005. DOI: http://dx.doi.org/10.1007/b136575 , pp. 1-146;
   LNCS V. 3039/2004. DOI: http://dx.doi.org/10.1007/b98005 , pp. 540-678.
4. *Special Issues of the International Journal for Multiscale Computational Engineering*:
   V. 8, Issue 2, 2010. In preparation.
   V. 6, Issue 1, 2008. DOI: http://dx.doi.org/10.1615/IntJMultCompEng.v6.i1;
   V. 5, Issue 1, 2007. DOI: http://dx.doi.org/10.1615/IntJMultCompEng.v5.i1;
   V. 4, Issue 2, 2006. DOI: http://dx.doi.org/10.1615/IntJMultCompEng.v4.i2;
   V. 4, Issue 3, 2006. DOI: http://dx.doi.org/10.1615/IntJMultCompEng.v4.i3.

Dr. Valeria Krzhizhanovskaya is a researcher at the University of Amsterdam, The Netherlands and an assistant professor at St. Petersburg Polytechnic University, Russia. In the past three years, she has been also working as a consultant for Applied Materials, USA, leading several R&D projects in simulation of multiphysics processes in semiconductor industry. Valeria received her Ph.D. degree in Computational Science from the University of Amsterdam and M.Sc. degree in Applied Mathematics and Physics from St. Petersburg Polytechnic University. She has published over 60 papers; worked as an editor of the Elsevier Journal of Computational Science, and a guest editor of 7 special issues of the International Journal of Multiscale Computational Engineering; organized 7 international symposia on Simulation of Multiphysics Multiscale Systems http://www.science.uva.nl/~valeria/SMMS/ and three ASME IDETC/CIE Special Topic Symposia on Computational Multiphysics Applications http://www.science.uva.nl/~valeria/IDETC-CIE-Multiphysics/. Valeria served as a program committee member and a reviewer in over 20 conferences and 10 international journals; participated in more than 40 conferences; and worked in about 20 international projects. Her research interests include modeling multiphysics multiscale processes, with special emphasis on plasma chemical technologies; numerical methods; parallel distributed computing; Grid applications; problem solving environments and ICT.