

Summer School on Distributed Multiscale Computing

Barcelona, 3-4 June 2013

Agenda

Monday, June 3rd 2013

9.00 Registration at PL-Grid (assisted by instructors)

9.30 Welcome (Alfons Hoekstra, University of Amsterdam/The Netherlands)

9.45 **General Session: Introduction to Multiscale Modeling and Simulation**

- Multiscale modeling and simulation (Alfons Hoekstra, University of Amsterdam/The Netherlands)
- Distributed Multiscale Computing (Alfons Hoekstra, University of Amsterdam/The Netherlands)

Includes a coffee break at about 10.45

12.00 Lunch Break

13.00 **Hands On Session 1: How to Develop Loosely Coupled Multiscale Applications?**

- Development using MAPPER Memory (MaMe), Multiscale Application Designer (MAD) and GridSpace (Katarzyna Rycerz, Eryk Ciepiela, Maciej Pawlik; Institute of Computer Science and CYFRONET, AGH, Cracow/Poland)
 - Multiscale modeling of polymer electronics using Unicore (Ivan Kondov; Karlsruhe Institute of Technology/Germany, and Luca Grisanti; University of Mons/Belgium)
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15.45 Coffee Break

16.00 **Community Presentation**

- MAPPER (Alfons Hoekstra; University of Amsterdam/The Netherlands)
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16.30 **General Session: Tools and Services for Distributed Multiscale Modeling**

- QosCosGrid and Application Hosting Environment (AHE) (Derek Groen; University College London/United Kingdom, and Mariusz Mamonski; Poznan Supercomputing and Networking Center, Poznan/Poland)
 - includes a demonstration of a Nanomaterial application (Derek Groen; University College London/United Kingdom)
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18.30 End of Day 1

Tuesday, June 4th 2013

9.15 Community Presentation

- MMM@HPC (Ivan Kondov; Karlsruhe Institute of Technology/Germany)
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9.45 Hands On Session 2: How to Develop Tightly Coupled Multiscale Applications?

- Development using the Multiscale Coupling Library and Environment (MUSCLE) (Joris Borgdorff; University of Amsterdam/The Netherlands, and Derek Groen; University College London/United Kingdom, and Mariusz Mamonski; Poznan Supercomputing and Networking Center, Poznan/Poland)
- Development using the MPWide communication library (Derek Groen; University College London/United Kingdom)

Includes a coffee break at about 10.45

12.15 Lunch Break

13.15 Community Presentation

- ScalaLife (Agusti Emperador; Institute for Research in Biomedicine, Barcelona/Spain)
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13.45 Hands On Session 3: How to Turn an Application into Multiscale?

- Demonstration using ScalaLife applications DALTON and GROMACS (Zilvinas Rinkevicius; Royal Institute of Technology, Stockholm/Sweden, and Mariusz Mamonski; Poznan Supercomputing and Networking Center, Poznan/Poland)
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15.45 Coffee Break

16.00 Hands On Session 4: How to Deploy Multiscale Applications on European e-Infrastructures?

- An assessment of deployment procedures for the European Grid Infrastructure (EGI) and the Partnership for Advanced Computing in Europe (PRACE) (Ilya Saverchenko; Ludwig-Maximilians-University, Munich/Germany and Leibniz Supercomputing Centre, Garching/Germany, and Mariusz Mamonski; Poznan Supercomputing and Networking Center, Poznan/Poland)
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17.00 Wrap Up, Feedback, End of School
