

Multiscale Computing: From the desktop to the Exascale

Final Program

Monday 16 April 2018

09:00 – 10:00 Arrival and Registration

Starting Up

plenary, chairperson: Alfons Hoekstra

10:00 – 10:15 Welcome by Lorentz Center

10:15 – 10:30 Kick off by organizers

Setting the Scene

plenary, chairperson: Alfons Hoekstra

10:30 – 10:45 Meet and Greet

10:45 – 11:00 **Alfons Hoekstra** – *Goal of the workshop, exploring Multiscale Computing as a paradigm in Computational Science*

11:00 – 12:00 **Bastien Chopard** – *Multiscale Modelling and Simulation*

12:00 – 14:00 Lunch

The Application Pull I

plenary, chairperson: Simon Portegies Zwart

14:00 – 14:30 **David Coster** – *Making ITER burn, multiscale modelling for fusion*

14:30 – 15:00 **Roeland Merks** – *The scales of life, multiscale modelling in biology*

15:00 – 15:30 **Ute Ebert** – *Multiscale Dynamics in Electrical Discharges*

15:30 – 16:00 Coffee and tea break

Planning in detail

16:00 – 16:30 Organizers will present the details of the next days, including the composition of the working sessions and study groups.

Speed Session I

plenary, chairperson: Alfons Hoekstra

16:30 – 17:00 Poster presentation by 6 participants (5 minutes each)

17:00 Wine and Cheese Welcome Party

Tuesday 17 April 2018

Multiscale Computing (the organizers provide their vision)

plenary, chairperson: Bastien Chopard

09:00 – 09:45 **Alfons Hoekstra** – *The MMSF and MUSLCE story (DMC, HPMC)*

09:45 – 10:30 **Simon Portegies Zwart** – *The AMUSE story*

10:30 – 11:00 Coffee and tea break

Work session on Multiscale Computing I

11:00 – 12:00 Guided discussion in smaller groups, taking as input specific viewpoints and questions formulated by the organizers and participants

12:00 – 14:00 Lunch

Work session on Multiscale Computing II

14:00 – 14:30 In same groups, formulate conclusions of discussions

Discussion on Multiscale Computing

plenary, chairperson: Alfons Hoekstra

14:30 – 15:00 Reporting back from discussions, formulating conclusions, issues, open questions.

Speed Session II

plenary, chairperson: Alfons Hoekstra

15:00 – 15:30 Poster presentation by 6 participants (5 minutes each)

15:30 – 16:00 Coffee and tea break

Multiscale Modelling and Simulation

plenary, chairperson: Ute Ebert

16:00 – 16:30 **Jannis Teunissen** - *Simulating multiscale electric discharges: computational techniques and challenges*

16:30 – 17:00 **Maxime Vassaux** - *Heterogeneous Multiscale Modelling for polymer nanocomposites*

17:00 – 17:30 **Gabor Zavodszky** - *The virtual artery, a multiscale model for vascular pathophysiology*

Common Room Session

17:30 – 18:30 No agenda

Wednesday 18 April 2018

The Application Pull II

plenary, chairperson: Gabor Zavodszky

09:30 – 10:00 **Philipp Neumann** – *From Convergence of Weather and Climate Simulations to a Coupling Software for Massively Parallel Molecular-Continuum Flows*

10:00 – 10:30 **Lucas Visscher** – *Multiscale Modelling for Complex Molecular Systems*

10:30 – 11:00 Coffee and tea break

Multiscale Computing Patterns

plenary, chairperson: David Coster

Lecture and live demonstrations organized by delegates from the ComPat project

11:00 – 11:20 **James Suter** – *Multiscale Computing Patterns for High Performance Multiscale Computing, the ComPat story*

11:20 – 12:00 **Onnie Luk, Olivier Hoenen, James Suter, Saad Alowayyed and Derek Groen** – *Live demonstration of Pattern software*

12:00 – 14:00 Lunch

Work session on Multiscale Computing and Multiscale Computing Patterns

14:00 – 15:00 Guided discussion in smaller groups, taking as input specific viewpoints and questions formulated by the organizers and participants

Discussion on Multiscale Computing Patterns

plenary, chairperson: Alfons Hoekstra

15:00 – 15:30 Reporting back from discussions, formulating conclusions, issues, open questions.

15:30 – 16:00 Coffee and tea break

Special session followed by Workshop Dinner

plenary, chairperson: Simon Portegies Zwart

16:00 – 16:45 **Ben Haring**, from the University Leiden, expert in social, economic, administrative and legal aspects of ancient Egypt will give a guest lecture on a conspiracy against Ramses III

17:00 – 17:30 Bus to Katwijk

17:30 – 20:30 BBQ at the beach, Restaurant Zilt Katwijk (also for vegetarians)

20:30 – 21:00 Bus back to Lorentz Center, Leiden Central Station and Van der Valk hotel

Thursday 19 April 2018

The Application Pull III

plenary, chairperson: Derek Groen

09:30 – 10:00 **Henk Dijkstra** – *Multiscale Modelling in Ocean Circulation and Climate*

10:00 – 10:30 **Stefan Lüding** – *Multiscale Mechanics of Complex Materials*

10:30 – 11:00 Coffee and tea break

Frameworks and Software for Multiscale Computing

plenary, chairperson: James Suter

11:00 – 11:30 **Derek Groen** – *Generic Software for Multiscale Computing, can this become a Reality?*

11:30 – 12:00 **Kenneth Leiter** – *A Distributed Multiscale Computing Framework for Modeling Materials*

12:00 – 14:00 Lunch

Work session on Frameworks and Software for Multiscale Computing

14:00 – 15:00 Guided discussion in smaller groups, taking as input specific viewpoints and questions formulated by the organizers and participants

15:00 – 16:30 Coffee / tea break plus demo session on existing frameworks for Multiscale Computing
Live demos of software frameworks, e.g. AMUSE, FABSIM, ComPat stacks, etc.

Discussion on Frameworks and Software for Multiscale Computing

plenary, chairperson: Alfons Hoekstra

16:30 – 17:00 Reporting back from discussions, formulating conclusions, issues, open questions.

The Application Pull IV

plenary, chairperson: tbd

17:00 – 17:30 **Jeroen Bedorf** – *Multiscale Computing in Astrophysics*

Common Room Session

17:30 – 18:30 No agenda

Friday 20 April 2018

The Application Pull V

plenary, chairperson: Kenneth Leiter

09:30 – 10:00 **Anna Nikishova** – *Uncertainty Quantification for Multiscale Models*

10:00 – 10:30 **Robin Richardson** – *Multiscale Modelling for Cerebral Blood Flow*

10:30 – 11:00 Coffee and tea break

HPC towards the exascale

plenary, chairperson: Lucas Visscher

11:00 – 11:30 **Peter Coveney** – *Challenges for Multiscale Computing towards the Exascale*

12:00 – 13:00 Lunch

Work Session on Drafting White Paper

13:00 – 14:00 In groups, each on a specific topic, taking as input the notes from the whole week

Plenary Wrapping Up Session

plenary, chairperson: Alfons Hoekstra

14:00 – 15:00 Plenary discussions on workshop conclusions, white paper, special issue, follow up activities.

15:00 End of Workshop