Program

Monday, 26 June 2023

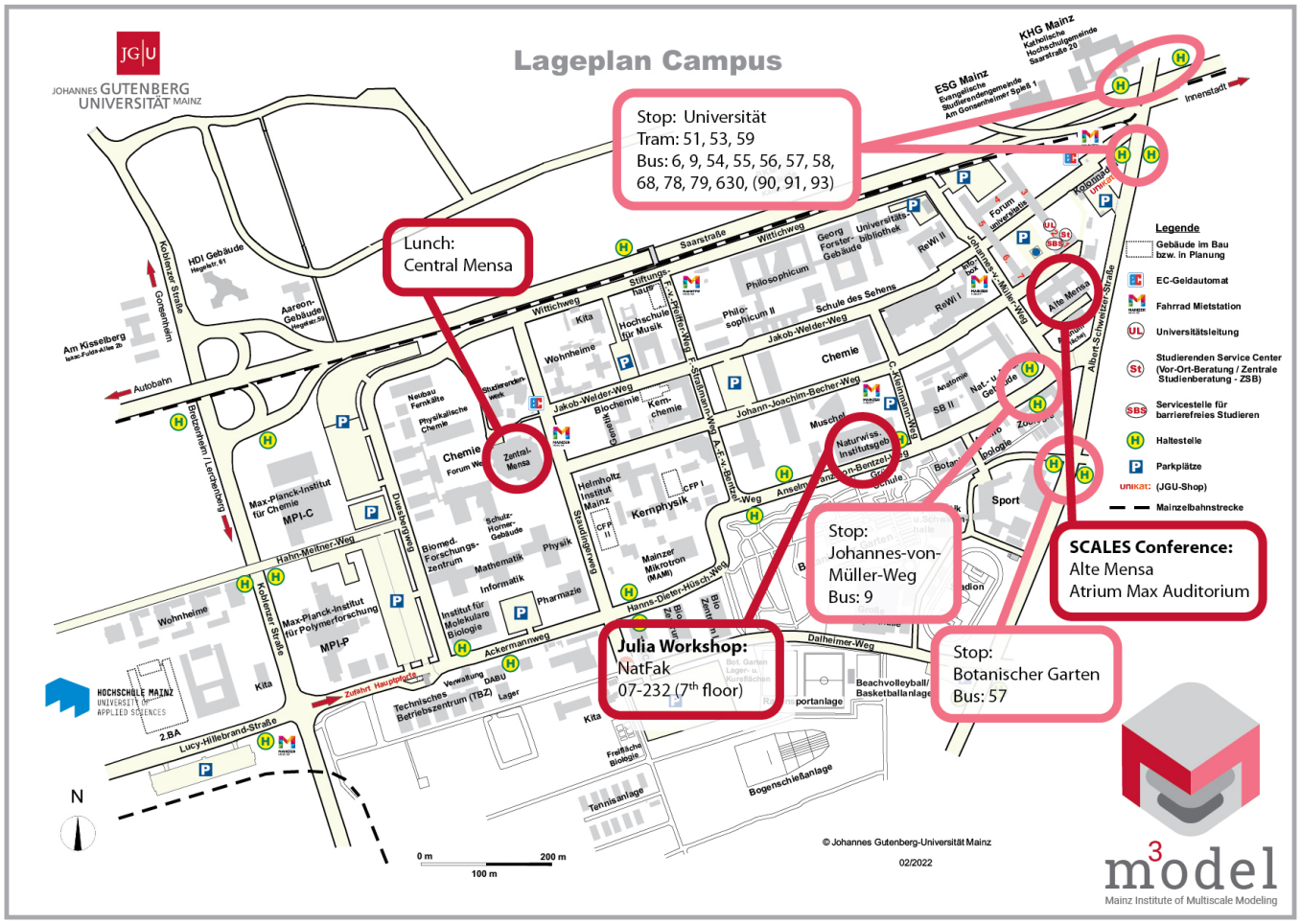
Pre-conference Workshop HPC Using julia

Organizers: Dr. Ludovic Räss & Dr. Ivan Utkin – ETH Zurich Prof. Dr. Boris Kaus – JGU Mainz

Time: 9:00 – 17:00

Place: Senatssaal 7th floor, NatFak Building, J.-J.-Becher-Weg 21 D-55128 Mainz

Participants will do hands-on exercises on how to use julia with a GPU based cluster. The Paderborn Center for Parallel Computing (PC2), part of the NHR, is providing access to 40 A100 GPU's on their NOCTUA 2 supercomputer for training purposes.



Tuesday, 27 June 2023

scales Multiscale Modeling of Complex Systems

Johannes Gutenberg University Mainz
Alte Mensa
55099 Mainz
26 – 30 June 2023

7:45–8:15	**Registration**		
8:20–8:30	**Welcome remarks**		
8:30–9:10	IS	**Gerhard Hummer** MPI-Biophysics Frankfurt	Molecular simulations in the era of AI and exascale computing
9:10–9:30	CT	**M. Mazzucchelli** JGU Mainz	Effect of nonhydrostatic stress on mineral-fluid equilibria assessed by molecular dynamics
9:30–9:50	CT	**S. Boisserée** RWTH Aachen	An adaptive space-time method for transient porous media flow models
9:50–10:20	**Coffee break**		
10:20–11:00	IS	**Ludovic Räss** ETH Zurich	Parallel inverse modelling on GPUs combining automatic differentiation and the adjoint method
11:00–11:40	IS	**Maribel Núñez Valdez** GFZ Potsdam	Ab initio quest for materials for technological and energy applications employing atomistic theory and modeling
11:40–13:10	**Lunch**		
13:10–13:30	CT	**D. Gomes Albuquerque** University of Warsaw	Investigating the role of sub-grid turbulence in mixed-phase clouds with a stochastic Lagrangian microphysics model
13:30–13:50	CT	**M. del Razo** FU Berlin	Data-driven dynamical coarse-graining for condensed matter systems
13:50–14:10	CT	**Lukas Stelzl** JGU & IMB Mainz	Resolving hierarchical interactions of proteins in phases separated condensates by multi-scale simulations
14:10–14:50	IS	**Albert Cohen** Sorbonne University, Paris	Stable nonlinear inversion application and application to interface reconstruction from cell-averages
14:50–15:20	**Coffee break**		
15:20–16:00	IS	**Taras Gerya** ETH Zurich	New i3elvis: Robust 3D geodynamic modelling code based on staggered finite differences and marker in cell
16:00–19:30	**Poster session & refreshments**		

IS: Invited Speaker, CT: Contributed Talk

Topics:

- Uncertaintly Quantification & Inverse Methods
- Multiscale Methods
- High Performance Computing & Machine Learning
- Interdisciplinary Applications

Wednesday, 28 June 2023

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8:30–9:10	IS	**Eitan Tadmor** University of Maryland	Swarm-based gradient descent method for non-convex optimization
9:10–9:30	CT	**Juliane Rosemeier** University of Exeter	Multi-level Parareal method with averaging
9:30–9:50	CT	**Emily Butler** University of Leeds	An investigation of the fluid structure interaction in articular cartilage across disparate scales
9:50–10:20	**Coffee break**		
10:20–11:00	IS	**Markus Deserno** Carnergie Mellon University	Differential stress in asymmetric membranes
11:00–11:40	IS	**Dave May** UC San Diego	Non-intrusive reduced order models for geophysics applications
11:40–13:10	**Lunch**		
13:10–13:30	CT	**Lukas Holbach** JGU Mainz	A Bayesian level set method for identifying subsurface geometries and rheological properties in Stokes flow
13:30–13:50	CT	**Jan Glaubitz** MIT	The power of joint sparsity: A hierarchical Bayesian learning approach
13:50–14:10	CT	**Janina Bender** University of Kassel	Entropy-conservative and well-balanced discontinuous Galerkin methods for the shallow water equations with uncertainty
14:10–14:50	IS	**Benjamin Gess** Bielefeld University	Fluctuations in conservative systems and SPDEs
14:50–15:20	**Coffee break**		
15:20–15:40	CT	**Oded Farago** Ben Gurion University	Multiscale lattice modeling and simulations of heterogeneous membranes
15:40–16:00	CT	**Thomas Berkemeier** MPI-Chemistry Mainz	Multiscale and multiphase modelling in atmospheric chemistry
16:00–16:40	IS	**Paola Gallo** Roma Tre University	Simulations of water and aqueous solutions under extreme conditions: the important role of molecular dynamics simulations
16:40–18:30	**Poster session & refreshments**		

IS: Invited Speaker, CT: Contributed Talk

Topics:

- Multiscale Methods
- Uncertaintly Quantification & Inverse Methods
- Stochastic Models
- Interdisciplinary Applications

Thursday, 29 June 2023

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8:30–9:10	IS	**Alexandre Tkatchenko** Univ. of Luxembourg	Fully quantum (bio)molecular simulations enabled by Machine Learning and HPC: Dream or reality?
9:10–9:30	CT	**Tom Dörffel** FU Berlin	Matched asymptotics of a hurricane boundary layer
9:30–9:50	CT	**Sabin Roman** Univ. of Cambridge	Emergence of chaos in coupled socio-environmental systems
9:50–10:20	**Coffee break**		
10:20–11:00	IS	**Robert Scheichl** Heidelberg University	Multilevel delayed acceptance Markov chain Monte Carlo
11:00–11:20	CT	**Simon-Christian Klein** TU Braunschweig	Dafermos' entropy rate criterion in simulations
11:20–11:40	CT	**Gottfried Hastermann** University of Potsdam	Interpolation and stability of a DG-FEM projection on staggered quadrilateral and cuboid meshes for compressible, (pseudo)-incompressible and hydrostatic fluid flow
11:40–13:10	**Lunch**		
13:10–14:50	**Poster session**		
14:50–15:20	**Coffee break**		
15:20–16:00	IS	**Wojciech Grabowski** NCAR, Boulder	Multiscale modeling of atmospheric processes: from cloud microphysics to climate
16:00–16:40	IS	**Virginie Ehrlacher** École des Ponts ParisTech	Multi-center decomposition of molecular densities: a mathematical perspective
17:00–22:00	**Social event & dinner at Schloss Vollrads**		

IS: Invited Speaker, CT: Contributed Talk

Topics:

- High Performance Computing & Machine Learning
- Uncertaintly Quantification & Inverse Methods
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Friday, 30 June 2023

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8:30–9:10	IS	**Nikki Vercauteren** University of Oslo	Stochastic parameterization of unsteady turbulence for weather and climate models
9:10–9:30	CT	**Simon Schneider** JGU Mainz	Integrable neural networks and their application to scalar hyperbolic conservation laws
9:30–9:50	CT	**Sothea Has** Univ. Paris Cité	Estimating balloon-observed gravity wave momentum Fluxes using Machine Learning with inputs from reanalyses
9:50–10:20	**Coffee break**		
10:20–11:00	IS	**Marcin Dabrowski** Polish Geological Inst.	Analytical and numerical modelling of deformation structures in anisotropic viscous media
11:00–11:20	CT	**Georg Voelker** Goethe Univ. Frankfurt	The Multi Scale Gravity Wave Model - MS-GWaM: A 3D transient parameterization for atmospheric models
11:20–11:40	CT	**A. Brunk** JGU Mainz	Multiscale model for viscoelastic phase separation: Modelling and existence
11:40–11:50	**Closing remarks**		
11:50–14:00	**Lunch, optional**		

IS: Invited Speaker, CT: Contributed Talk

Topics:

- Stochastic Models
- High Performance Computing & Machine Learning
- Interdisciplinary Applications
- Multiscale Methods

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