Multiscale Modelling, Uncertainty Quantification and the Reliability of Computer Simulations

11th-12th June 2020, Online Conference (time zone: CEST/BST+1)

Programme

Key: MMS   UNEQUIvOCAL/SIAM

Day 1 – Thursday 11th June

Time	Title	Speaker	Chair
09:45 – 09:55	*Login to Zoom*		
09:55 – 10:00	Welcome	Derek Groen	
10:00 – 10:20	Projective Integration for Moment Models of the BGK Equation	Julian Koellermeier	Derek Groen
10:20 – 10:40	Modeling and Simulation of the Spread of Messages in Social Networks	Robert Elsaesser	
10:40 – 11:00	Multilevel Monte Carlo with improved correlation for kinetic equations in the diffusive scaling	Emil Løvbak	
11:00 – 11:20	VECMAtk demo	Wouter Edeling	
11:20 – 11:50	Coffee Break		
11:50 – 12:10	Running Coupled Simulations on HPC and Cloud Resources with Enhanced TOSCA Workflows	Francisco Javier Nieto	David Coster
12:10 – 12:30	Open Boundary Modeling in Molecular Dynamics with Machine Learning	Philipp Neumann	
12:30 – 12:50	Easing multiscale model design and coupling with MUSCLE 3	Lourens Veen	
12:50 – 13:10	Time bridging techniques for multiscale fusion plasma simulations	Onnie Luk	
13:10 – 13:30	Development and application of the Statistically Similar Representative Volume Element for numerical modelling of multiphase materials	Łukasz Rauch	
13:30 – 14:30	*Lunch Break*		
14:30 – 14:50	Inverse Uncertainty Quantification of a cell model using a Gaussian Process metamodel	Anna Nikishova	Wouter Edeling
14:50 – 15:10	Uncertainty Quantification for Epidemic Models	Georgios Arampatzis	
15:10 – 15:30	Intrusive Polynomial Chaos for CFD using OpenFOAM	Jigar Parekh	
15:30 – 15:50	MCMC for Bayesian uncertainty quantification from time-series data	Philip Maybank	
15:50 – 16:10	Future Proofing a Building Design Using History Matching Inspired Level Set Techniques	Evan Baker	
16:10 – 16:40	*Coffee Break*		
16:40 – 17:00	Distributions of a general reduced-order dependence measure and conditional independence testing	Jan Mielniczuk	Anna Nikishova

17:00 – 17:20	Deriving reduced subgrid scale models from data	Wouter Edeling	
17:20 – 17:40	Verification, Validation & Uncertainty Quantification for Molecular Dynamics Simulation	Shunzhou Wan	
17:40 – 18:00	Markov Chain Monte Carlo Methods for Fluid Flow Forecasting in the Subsurface	Arunasalam Rahunanthan	
18:00 – 18:20	A bluff-and-fix algorithm for polynomial chaos methods	Laura Lyman	
18:20 – 18:40	Sensitivity analysis of soil parameters in crop model supported with high-throughput computing	Mikhail Gasanov	

Day 2 – Friday 12th June

Time	Title	Speaker	Chair
11:15 – 11:25	*Login to Zoom*		
11:25 – 11:30	Welcome	Peter Coveney	
11:30 – 11:50	VECMAtk: Towards a Full Release of a Verification & Validation and Uncertainty Quantification toolkit for Multiscale and HPC Simulations	Derek Groen	Peter Coveney
11:50 – 12:10	Uncertainty quantification for multiscale fusion plasma simulations with VECMA toolkit	Jalal Lakhlili	Peter Coveney
12:10 – 12:30	Sensitivity-guided simulation development: A case study in forced migration	Diana Suleimenova	
12:30 – 12:50	Semi-intrusive Uncertainty Quantification for Multiscale Simulation	Dongwei Ye	
12:50 – 13:10	Assessing uncertainties in an atmospheric model with EasyVVUQ	Fredrik Jansson	
13:10 – 14:10	*Lunch Break*		
14:10 – 14:30	Towards Accurate Simulation of Global Challenges on Data Centers Infrastructures via Coupling of Models and Data Sources	Sergiy Gogolenko	Stefano Casarin
14:30 – 14:50	Improving accuracy of multi-scale urban air pollution simulation via coupling with sensor data and meteorological forcasts	Zoltán Horváth	
14:50 – 15:10	Building cloud-based data services to enable earth-science workflows across HPC centres	Milana Vuckovic	
15:10 – 15:30	An Agent-based Multiscale Simulation of Forced Migration: A case study of South Sudan	Imran Mahmood	
15:30 – 16:10	*Coffee Break*		
16:10 – 16:30	A heterogeneous multi-scale model for blood flow	Ben Czaja	Philipp Neumann
16:30 – 16:50	A statistical mean-field model for bridging the scale gap between cell resolved and continuum blood flow mechanics	Gabor Zavodszky	
16:50 – 17:10	UrbanAir - modelling air quality over complex urban areas	Michal Kulczewski	
17:10 – 17:30	Formation of morphogenetic patterns in cellular automata	Bakhti Vasiev	
17:30 – 17:50	Microtubule Biomechanics and the Effect of Degradation of Elastic Moduli	Roderick Melnik	
17:50 – 18:10	Coupled Microstructure-Resolved Simulation of Metal Additive Manufacturing Processes	John A. Turner	