

Workshop IV: Uncertainty Quantification for Stochastic Systems and Applications

Monday November 13, 2017

- 8:00–8:55 *Check-In/Light Breakfast (Hosted by IPAM)*
- 8:55–9:00 *Welcome and Opening Remarks*
- 9:00–9:40 **Michele Ceriotti** (École Polytechnique Fédérale de Lausanne (EPFL))
Learning and Correcting Static and Dynamic Properties of Materials in Atomistic Simulations
- 10:00–10:15 *Break*
- 10:15–10:55 **Youssef Marzouk** (Massachusetts Institute of Technology)
Couplings for sequential Bayesian inference
- 11:15–11:30 *Break*
- 11:30–12:10 **Josselin Garnier** (Ecole Polytechnique)
Uncertainty in wave propagation and imaging in random media
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:10 **Stefan Engblom** (Uppsala University)
Bridging the scales between the single cell and the cell population - computational considerations
- 3:30–3:45 *Break*
- 3:45–4:25 **Sebastian Reich** (Universität Potsdam)
Data assimilation as an optimal control problem and applications to uncertainty quantification
- 4:45–5:15 *Lightning Poster Presentations*
- 5:15–6:30 *Poster Session & Reception (Hosted by IPAM)*

Tuesday November 14, 2017

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–9:40 **Kurt Lejaeghere** (Ghent University)
Six Inconvenient Truths about Dft Uncertainty Quantification
- 10:00–10:15 *Break*
- 10:15–10:55 **Francesca Tavazza** (National Institute of Standards and Technology)
UQ associated to controlled approximation choices in DFT
- 11:15–11:30 *Break*

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- 11:30–12:10 **Luc Rey-Bellet** (University of Massachusetts Amherst)
Uncertainty Quantification for Complex Stochastic Systems
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:10 **Tim Sullivan** (Free University of Berlin and Zuse Institute Berlin)
Bayesian Probabilistic Numerical Methods
- 3:30–4:00 *Break*
- 4:00–4:40 **Matthew Dunlop** (California Institute of Technology)
Robust MCMC for high dimensional Bayesian inversion with non-Gaussian and hierarchical priors

Wednesday November 15, 2017

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–9:40 **Shi Jin** (University of Wisconsin-Madison)
Stochastic Asymptotic-Preserving Schemes and Hypocoercivity Based Sensitivity Analysis for Multiscale Kinetic Equations with Random Inputs
- 10:00–10:15 *Break*
- 10:15–10:55 **Udo von Toussaint** (Max Planck Institute for Plasma Physics)
Uncertainty Quantification for computer simulations of the interaction of energetic particles with amorphous solids
- 11:15–11:30 *Break*
- 11:30–12:10 **Roger Ghanem** (University of Southern California (USC))
Multiscale probabilistic models for manufacturing, performance and failure of composites
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:10 **Virginie Ehrlacher** (École Nationale des Ponts-et-Chaussées)
Tensorized Adaptive Biasing Force method for molecular dynamics (joint work with Pierre Monmarché and Tony Lelièvre)
- 3:30–4:00 *Break*
- 4:00–4:40 **Frederic Legoll** (École Nationale des Ponts-et-Chaussées (ENPC))
Model reduction in stochastic dynamics and applications to MD

Thursday November 16, 2017

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–9:40 **Paul Dupuis** (Brown University)
Competing sources of variance in parallel replica Monte Carlo, and optimization in the low temperature limit
- 10:00–10:15 *Break*
- 10:15–10:55 **Petr Plechac** (University of Delaware)
Accelerated sampling and sensitivity analysis for stochastic reaction networks
- 11:15–11:30 *Break*
- 11:30–12:10 **Marisol Koslowski** (Purdue University)
Sensitivity of mechanical properties to microstructural variability
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:10 **Markos Katsoulakis** (University of Massachusetts Amherst)
UQ Indices, Information Inequalities and applications in chemical kinetics
- 3:30–4:00 *Break*
- 4:00–4:40 **Michal Branicki** (University of Edinburgh)
Path-based measures of transport and expansion rates in stochastic flows

Friday November 17, 2017

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–9:40 **Mark Transtrum** (Brigham Young University)
Parameter uncertainty, model reduction, and effective theories in physics, biology, and beyond
- 10:00–10:15 *Break*
- 10:15–10:55 **Louis Ellam** (Imperial College)
Stochastic Modelling of Urban Structure
- 11:15–11:30 *Break*
- 11:30–12:10 **Fabien Cailliez** (Université d'Orsay)
Statistical approaches to forcefield calibration and prediction uncertainty in molecular simulation
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:10 **Panos Angelikopoulos** (D. E. Shaw Research)
Developing statistically rigorous force fields for molecular dynamics simulations on specialized hardware
- 3:30–4:00 *Break*

