Workshop II: HPC and Data Science for Scientific Discovery

Monday October 15, 2018

8:00–8:55 *Check-In/Light Breakfast (Hosted by IPAM)*

8:55–9:00 *Welcome and Opening Remarks*

9:00–9:50 **Karen Willcox** (University of Texas at Austin)
Learning low-dimensional models: Nonlinear model reduction via lifting transformations and proper orthogonal decomposition

10:00–10:15 *Break*

10:15–11:05 **Peter Benner** (Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg)
Low-rank tensor methods for simulation, optimization and uncertainty quantification of parametric PDEs

11:15–11:30 *Break*

11:30–12:20 **Alexander Szalay** (John Hopkins University)
Streaming Algorithms for Halo Finders in Cosmology

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Peter Lindstrom** (Lawrence Livermore National Laboratory)
Alternatives to IEEE: NextGen Number Formats for Scientific Computing

3:30–4:00 *Break*

4:00–4:50 **Franck Cappello** (Argonne National Laboratory)
Three Frontiers of Lossy Compression for Scientific Data

5:00–6:30 *Poster Session & Reception (Hosted by IPAM)*

Tuesday October 16, 2018

8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*

9:00–9:50 **Yannis Kevrekidis** (Princeton University)
No equations, no variables, no parameters, no space, no time: Data and the modeling of complex systems

10:00–10:15 *Break*

10:15–11:05 **Begüm Demir** (Technische Universität Berlin)
Accurate and Scalable Processing of Big Data in Earth Observation

11:15–11:30 *Break*

(Tuesday schedule continued on next page)

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11:30–12:20 **Costas Bekas** (IBM Zürich Research Laboratory)
Cognitive Discovery: Pushing the Frontiers of Technical R&D with AI.

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Maria Girone** (CERN)
Computing Challenges at the Large Hadron Collider (LHC)

3:30–4:00 *Break*

4:00–4:50 **Christoph Koch** (Humboldt-Universität)
Retrieving atomic structure from transmission electron microscopy data: a family of inverse problems

Wednesday October 17, 2018

8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*

9:00–9:50 **Frank Jenko** (Max Planck Institute for Plasma Physics and UCLA)
Combining computing and learning for physics

10:00–10:15 *Break*

10:15–11:05 **Dirk Pflüger** (Universität Stuttgart)
Scalability and Fault Tolerance for Exascale Simulations of Hot Fusion Plasmas

11:15–11:30 *Break*

11:30–12:20 **Michael Eldred** (Sandia National Laboratories)
Multilevel-Multifidelity Sampling and Emulation for Forward UQ

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Rachel Ward** (University of Texas at Austin)
Learning Sparse High-Dimensional Governing Equations from Limited Data

3:30–4:00 *Break*

4:00–4:50 **Clayton Webster** (Oak Ridge National Laboratory)
Sparsity-enforced regularizations for optimal learning of high-dimensional systems from random data

Thursday October 18, 2018

8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*

9:00–9:50 **George Biros** (University of Texas at Austin)
Scalable kernel methods

10:00–10:15 *Break*

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10:15–11:05 **Omar Ghattas** (University of Texas at Austin)
Scalable algorithms for optimal experimental design for large-scale Bayesian inverse problems governed by complex models

11:15–11:30 *Break*

11:30–12:20 **Jochen Garcke** (Universität Bonn and Fraunhofer SCAI)
Domain Knowledge in Data Analysis: A Geometrical Method for Low-Dimensional Representations of Simulations

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **James Demmel** (University of California, Berkeley (UC Berkeley))
Communication-Avoiding Algorithms for Linear Algebra, Machine Learning, and Beyond

3:30–4:00 *Break*

4:00–4:50 **Adrian Tate** (Cray EMEA Research Lab)
Memory- and Data-Centric Abstractions for Management and Optimisation of Data Movement

Friday October 19, 2018

8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*

9:00–9:50 **Claudia Draxl** (Humboldt-Universität)
How FAIR are data repositories in materials science?

10:00–10:15 *Break*

10:15–11:05 **Matthias Scheffler** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
When More Data Do Not Provide A Better Description

11:15–11:30 *Break*

11:30–12:20 **Robert Martin** (Air Force Research Laboratory)
Efficient Adaptive Hybrid Kinetic Simulation: Computing the Signal in the Noise

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Victoria Stodden** (University of Illinois at Urbana-Champaign)
Enabling Reproducibility in Computational and Data-enabled Science

3:30–4:00 *Break*

4:00–4:50 **Mauro Maggioni** (Johns Hopkins University)
Learning and Geometry for Stochastic Dynamical Systems in high dimensions