Workshops

Workshop II: HPC and Data Science for Scientific Discovery

Part of the Long Program Science at Extreme Scales: Where Big Data Meets Large-Scale Computing

OCTOBER 15 - 19, 2018

OVERVIEW

SPEAKER LIST

LODGING

SCHEDULE

APPLICATION & REGISTRATION

Overview

With the gradual establishment of computational science as the "third pillar of science" over the last few decades, it has been steadily moving from a supporting towards a leading role. HPC applications – usually based on numerically solving sets of ODEs or PDEs – are increasingly expected to supplement a test-based approach, helping to establish a *truly predictive* computational science. With pre-exascale simulations involving and producing ever-increasing amounts of data, also from experiments or observations, there exist various critical open questions at the interface of extreme-scale data handling and HPC, including the following:

Can we devise innovative pathways to overcome the communication bottleneck on large supercomputers by exploiting information efficiency at extreme scales – e.g., by data compression/reconstruction or variable precision computing – as well as by minimizing data motion via algorithmic advances?
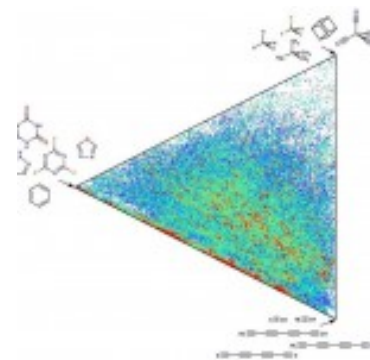
With simulations often producing very large data sets and databases, how can these be efficiently analyzed and visualized? What is the most effective use of machine learning in this context? Can we develop novel techniques for automated scientific discovery from complex scientific data?

How can we move towards a much more integrated analytics of experimental/observational and simulation data, based on methods from modern data science? This may involve, e.g., complex types of uncertainty quantification, inverse problems, and data assimilation.

These (and related) challenges and opportunities affect a wide range of scientific communities, from plasma physics and materials science to medicine and the geosciences, and will be discussed in an interdisciplinary fashion at this workshop.

This workshop focuses on applications that are typically driven by ODEs and PDEs. It complements the third workshop in this long program which focuses on applications that are typically data driven.

This workshop will include a poster session; a request for posters will be sent to registered participants in advance of the workshop.

ORGANIZING COMMITTEE

David Balaban (AMGEN Inc, Research & Development Informatics)

George Biros (University of Texas at Austin)

Claudia Draxl (Humboldt-Universität)

Frank Jenko (Max Planck Institute for Plasma Physics and UCLA, Physics and Astronomy)

Klaus-Robert Müller (Technische Universität Berlin)

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