INSTITUTE FOR PURE AND APPLIED MATHEMATICS

COMPLEX HIGH-DIMENSIONAL ENERGY LANDSCAPES

September 11 - December 15, 2017 | Los Angeles
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SCIENTIFIC OVERVIEW

Recent advances in computational resources and the development of high-throughput frameworks enable the efficient sampling of complicated multivariate functions. This includes energy and electronic property landscapes of inorganic, organic, biomolecular, and hybrid materials and functional nanostructures. Combined with the recent focus on data science and the materials genome initiative, this leads to a rapidly growing need for numerical methods and a fundamental mathematical understanding of efficient sampling approaches, optimization techniques, hierarchical surrogate models and coarse graining techniques, and methods for uncertainty quantification.

The complexity of these energy and property landscapes originates from their simultaneous dependence on discrete degrees of freedom (e.g. number of atoms and species types) and continuous ones (e.g. position of atoms). The complexity is further exacerbated by the presence of divergences (e.g. when atoms approach one another and at critical transition points) and non-trivial emergent phenomena that are due to collective interactions. Moreover, dynamical behavior governed by complex landscapes involves a rich hierarchy of timescales and is characterized by rare events that often are key to understanding function of the molecular structures under investigation. This complexity provides an ideal test bed for novel mathematical methods that characterize these functions and provide a description as well as optimal numerical methods.

This program will bring together researchers from pure and applied mathematics, computer science, materials science, chemistry, physics, and biomolecular science to advance the understanding of simulation, stochastic sampling and optimization methods for multidimensional energy landscapes and to develop a common language.

WORKSHOP SCHEDULE

- Complex High-Dimensional Energy Landscapes Opening Day: Sept. 11, 2017
- Workshop I: Optimization and Optimal Control for Complex Energy and Property Landscapes: Oct. 2-6, 2017
- Workshop III: Rare Event Sampling of Multidimensional Landscapes: Oct. 30-Nov. 3, 2017
- Workshop IV: Uncertainty Quantification for Stochastic Systems and Applications: Nov. 13-17, 2017
- Culminating Workshop at Lake Arrowhead Conference Center: Dec. 10-15, 2017

PARTICIPATION

This long program will involve senior and junior researchers from several communities relevant to this program. You may apply for financial support to participate in the entire fourteen-week program, or a portion of it. We prefer participants who stay for the entire program. Applications will be accepted through June 11, 2017, but offers may be made up to one year before the start date. We urge you to apply early. Mathematicians and scientists at all levels who are interested in this area of research are encouraged to apply for funding. Supporting the careers of women and minority researchers is an important component of IPAM’s mission, and we welcome their applications.

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