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450 McNamara Alumni Center
200 Oak Street SE
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a. REPORT	b. ABSTRACT	c. THIS PAGE			Peter Olver
UU	UU	UU	UU		19b. TELEPHONE NUMBER 612-625-5591

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as of 09-Jul-2018

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INVESTIGATOR(S):

Name: Peter Olver
Email: olver@umn.edu
Phone Number: 6126255591
Principal: Y

Organization: **University of Minnesota - Minneapolis**
Address: 450 McNamara Alumni Center, Minnepolis, MN 554552070
Country: USA
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Phone: (612) 625-5591
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STEM Degrees: **STEM Participants:**

Major Goals: This grant supported the workshop: Multiscale Theory and Computation, which was held during September 23-25, 2017, at the University of Minnesota, Twin Cities. There were more than 60 participants from the US, Europe, and Asian. There were 23 presentations, and also a dozen of posters.

The workshop focused on future directions and challenges for multiscale modeling, analysis, and computation with applications to materials science, quantum and molecular mechanics, fluid and solid mechanics, chemistry, electronics, and optics. Each of the plenary talks presented the state-of-the-art for a mathematical approach or application area, and follow-up discussions explored opportunities for cross-fertilization of methods across application areas.

The workshop provided a unique venue for both senior and junior, theoretical and computational, multiscale researchers to exchange ideas on the progress of current multiscale research and develop future collaborations. The discussion of a broad spectrum of multiscale areas and the interaction between theory and computation provided a fertile environment for the further development of interdisciplinary research. This was particularly helpful for the younger researchers looking to enter these new and promising areas of multiscale research and application.

Accomplishments: See attached pdf document under Upload

Training Opportunities: The workshop provided a unique venue for both senior and junior, theoretical and computational, multiscale researchers to exchange ideas on the progress of current multiscale research and develop future collaborations. The discussion of a broad spectrum of multiscale areas and the interaction between theory and computation provided a fertile environment for the further development of interdisciplinary research. This was particularly helpful for the younger researchers looking to enter these new and promising areas of multiscale research and application.

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https://math.umn.edu/events/multiscale-theory-and-computation

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Participant Type: PD/PI
Participant: Peter Olver
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Other Collaborators:

Participant Type: Faculty
Participant: Mitchell Luskin
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
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Other Collaborators:

Participant Type: Faculty
Participant: Stanley Osher
Person Months Worked: 1.00 **Funding Support:**
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Other Collaborators:

Participant Type: Faculty
Participant: Irene Fonseca
Person Months Worked: 1.00 **Funding Support:**
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Final Project Report

Workshop on Future Directions in Multiscale Theory and Computation

PI: Peter Olver (University of Minnesota)

ARO W911NF-17-1-0285. Program manager: Joseph Myers

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The workshop

- examined the recent progress in multiscale research on stochastic modeling and analysis, partial differential equations, and scientific computing and numerical analysis with applications in materials science, fluids, imaging science, and quantum and molecular mechanics.
- facilitated the exchange of ideas and stimulated discussions on advancing multiscale research towards understanding fundamental scientific principles of multiscale phenomena, and transforming theories and methods to applications in science and engineering.
- provided opportunities for young researchers, particularly women and minorities, to interact with and gain research experience from senior researchers, to expose them to an environment of exciting interdisciplinary research, and to develop interdisciplinary research collaborations.

Topics covered included:

- Theory and computation of electronic structure
- Coupling quantum mechanical and molecular mechanical descriptions
- Accelerated molecular dynamics simulations and free-energy calculations
- From microstructure to macroscopic behavior of crystalline solids
- Coarse-grained and effective theories for materials and biological systems
- Atomistic-to-continuum coupling in the description of material defects
- Grain boundaries, two-dimensional materials, and thin structures
- Pattern formation in both equilibrium and non-equilibrium materials, chemical, and biological systems
- Stochastic modeling, analysis, and simulations

Titles and Abstracts of Talks

Dio Margetis (Maryland)

The problem of small temperatures in a quantum gas

Recent progress in understanding the fundamentals of a system of interacting particles with Boson statistics at low temperature was reviewed. The description of this system beyond the usual mean-field-type approach was presented. The study of the underlying formalism involving the passage from the microscopic dynamics of mixed states to coupled PDEs at the macroscopic scale offers new opportunities for multiscale mathematical modeling.

Irene Fonseca (CMU)

Epitaxially Strained Elastic Films: Quantum Dots and Dislocations

The formation and assembly patterns of quantum dots plays a central role on the optoelectronic properties of semiconductors. The quasistatic equilibria and regularity of islands (quantum dots) was studied using De Giorgi's minimizing movements and short time existence results for a surface diffusion evolution equation with curvature regularization in the context of epitaxially strained films was presented. Challenges in the development and analysis of variational models for the nucleation of misfit dislocations were presented.

Claude Le Bris (ENPC and Inria, France)

Nonperiodic multiscale problems: some recent mathematical and numerical advances

The modelling and numerical simulation of multiscale materials was presented. The general purpose of the set of approaches developed is to be able to address realistic materials with nonperiodic microstructures, and possibly defects. New lines of research aimed at making multiscale finite element methods more versatile and robust were presented.

David Kinderlehrer (CMU)

Towards A Gradient Flow For Microstructure

A central problem of microstructure is to develop technologies capable of producing an arrangement, or ordering, of the material, in terms of mesoscopic parameters like geometry and crystallography, appropriate for a given application. Is there such an order in the first place? The emergence of the grain boundary character distribution (GBCD), a statistic that details texture evolution, was described and its importance as a material property was presented. Its identification as a gradient flow is tantamount to exhibiting the harvested statistic as the iterates in a mass transport JKO implicit scheme. Consequently, the GBCD was shown to be a solution of a Fokker-Planck Equation. The development exposes the question of how to understand the circumstances under which a harvested empirical statistic is a property of the underlying process.

Stanley Osher (UCLA)

Overcoming the Curse of Dimensionality

It is well known that certain Hamilton-Jacobi partial differential equations (HJ PDE's) play an important role in analyzing control theory and differential games. The cost of standard numerical algorithms for HJ PDE's is exponential in the space dimension and time, with huge memory requirements. Here we propose and test methods for solving a large class of these problems without the use of grids or significant numerical approximation. Osher began with the classical Hopf and Hopf-Lax formulas which enable the solution of state independent problems via variational methods originating in compressive sensing with remarkable results.

The solution can be evaluated in 10-4 to 10-8 seconds per evaluation on a laptop. The method is embarrassingly parallel and has low memory requirements. Recently, with a slightly more complicated, but still embarrassingly parallel method, Osher has extended this in great generality to state dependent HJ equations,, with the help of parallel computers, overcoming the curse of dimensionality for these problems, deriving new Lax and Hopf type formulas in very general situations The term, "curse of dimensionality" was coined by Richard Bellman in 1957 when he did his classic work on dynamic optimization.

Richard James (Minnesota)

Atomistically inspired origami

World population is growing approximately linearly at about 80 million per year. Thus there is necessarily less space per person, and this is particularly acute in cities. Perhaps this is why the scientific community seems to be obsessed with folding things. James presented a mathematical approach to "rigid folding" based on the use of piecewise rigid isometric mappings that have a group structure. The ideas are inspired by the way atomistic structures form naturally. Their characteristic features in molecular science imply highly desirable features for macroscopic structures, particularly 4D structures that deform. He illustrated these by constructing some "objective origami" structures.

Art Voter (LANL)

Increasing the power of accelerated molecular dynamics methods

Many important materials processes take place on time scales that vastly exceed the few microseconds accessible to molecular dynamics simulation. Typically, this long-time dynamical evolution is characterized by a succession of thermally activated infrequent events involving defects in the material. In the accelerated molecular dynamics (AMD) methodology, known characteristics of infrequent-event systems are exploited to make reactive events take place more frequently, in a dynamically correct way. The key feature is that the trajectory itself is allowed to find its own way out of each state, so that no prior assumptions need to be made about the transition states or available reaction paths. These methods have proven powerful for a range of processes, including metallic surface diffusion and growth, radiation damage annealing processes, and nanotube and nanowire dynamics. Voter discussed some recent advances that extend the power and range of applicability of the AMD methods

Christoph Ortner (Warwick)

The Numerical Analysis of Hybrid Models for Crystalline Defects

For many questions of scientific interest, all-atom molecular dynamics simulations are still out of reach, for example when accurate and hence computationally expensive force-fields are used, or in materials modelling where large numbers of atoms are required. A variety of multi-scale / hybrid models has been developed to reduce computational cost.
Ortner reviewed the numerical analysis of these hybrid techniques which was spear-headed by Mitch Luskin and his research group He presented how classical numerical analysis concepts can be applied to (1) identify the various errors committed in the coarse-graining process and (2) how to apply this analysis to optimise practical computational schemes.

Tony Lelievre (ENPC)

Metastability: a journey from stochastic processes to semiclassical analysis

A stochastic process is metastable if it stays for a very long period of time in a region of the phase space (called a metastable region) before going to another metastable region, where it again remains trapped. Such processes naturally appear in many applications, metastability being related to a two time scale mechanism: the small time scale corresponds to the vibration period within the metastable regions and the large time scale is associated with the transitions between metastable states. For example, in molecular dynamics, the metastable regions are typically associated with the atomic conformations of a molecule (or an ensemble of molecules), and one is actually interested in simulating and studying the transitions between these conformations.

Lelievre explained how the exit events from a metastable state can be studied using an eigenvalue problem for a differential operator. This point of view is useful to build very efficient algorithms to simulate metastable stochastic processes (using in particular parallel architectures). It also gives a new

way to prove the Eyring-Kramers laws and to justify the parametrization of an underlying Markov chain (Markov state model), using techniques form semiclassical analysis.

Alexander Shapeev (Skoltech)

Machine learning-based interatomic potentials

Molecular simulations (such as molecular dynamics) is the largest consumer of supercomputing time worldwide. Molecular simulations rely on one of the two models: very accurate and very computationally expensive quantum-mechanical models that resolve the electronic structure, and empirical interatomic models that postulate a simple functional form of interatomic interaction that is fast to compute. Application of ideas of machine learning has recently been put forward as a promising way to get the best out of these two models: accuracy of quantum mechanics and computational efficiency of the interatomic potentials.

Machine learning-based interatomic potentials and active learning algorithms that automatically construct an optimal training dataset of atomistic configurations for such interatomic potentials were presented with applications of these methods in molecular dynamics, crystal structure prediction, alloy discovery and cheminformatics.

Efthimios Kaxiras (Harvard)

Wandering in Flatland: the wonders of 2D materials

Two-dimensional materials, having started as a curiosity with graphene, are becoming ripe for real applications. Kaxiras surveyed some theoretical predictions of how 2D layers of different materials behave when stacked in different arrangements, in terms of their response to external fields and to excitation by light.

Yalchin Efendiev (Texas A&M)

Multiscale Model Reduction for heterogeneous problems

Efendiev gave some general strategies for coarse-grid multiscale model reduction techniques for heterogeneous problems. The proposed methods are designed for problems with high contrast and multiple scales. I will also describe applications to inverse problems.

Thomas Hou (Caltech)

Sparse Operator Compression for Higher Elliptic PDEs with Rough Coefficients and Graph Laplacians

Hou introduced the sparse operator compression to compress a self-adjoint higher order elliptic operator with rough coefficients and various boundary conditions. The operator compression is achieved by using localized basis functions, which are energy minimizing functions on local patches. On a regular mesh with mesh size h, the localized basis functions have supports of diameter O(h log(1/h)), and give optimal compression rate of the solution operator. He showed that by using localized basis functions with supports of diameter O(h log(1/h)), his method achieves the optimal compression rate of the solution operator. From the perspective of the multiscale finite element method to solve elliptic equations, the localized basis functions have the optimal convergence rate O(h^k) for a (2k)th-order

elliptic problem in the energy norm. From the perspective of the Sparse PCA, his results show that a large set of Matern covariance functions can be approximated by a rank-n operator with a localized basis and with the optimal accuracy. Finally, he discussed some recent progress in extending this method to solve graph Laplacians with nearly linear complexity.

Bjorn Engquist (Texas)

Multiscale dynamical systems

Molecular and planetary systems and are example of multiscale ordinary differential equations with highly oscillatory solutions and they pose severe challenges for computer simulations. Distributed computing is a natural tool for large-scale simulations but causality makes it challenging to develop parallel algorithms for dynamical systems. The parareal framework has been successful for dissipative systems. Engquist discussed the more difficult case of Hamiltonian systems by using phase plane maps as coarse solver.

Eric Cances (ENPC)

Computational non-commutative geometry for materials science: The example of multilayer 2D materials

After recalling the standard mathematical formalism used to model disordered systems such as random composite materials (mesoscale disorder), doped semiconductors, alloys, or amorphous materials (atomic-scale disorder), Cances presented a tight-binding model for computing the electrical conductivity of incommensurate multilayer 2D materials. All these models fall into the scope of the mathematical framework, based on non-commutative geometry, introduced by Bellissard to study the physical properties of aperiodic systems. Surprisingly, this rather abstract theoretical framework leads to completely new numerical schemes allowing one to perform simulations out of the scope of usual methods.