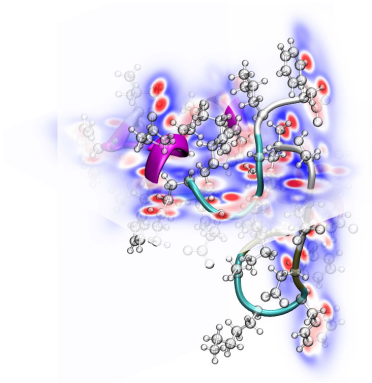
institute for pure & applied mathematics

Workshop I: Multiscale Approaches in Quantum Mechanics

MARCH 28 - April 1, 2022



Scientific Overview

This workshop will set the stage and define research directions for the rest of the program. The idea is to achieve a healthy mix between researchers developing quantum theories and methods on different spatial and temporal scales (from field theory to continuum), providing a forum to discuss the advances in multiscale modeling in quantum mechanics and pave the way to stronger coupling between existing methods and completely novel quantum approaches. The main question is: how to integrate existing quantum methods at different levels of accuracy and efficiency, reduce their weaknesses, improve their applicability, explore limiting behaviors, and enable quantum calculations on much larger scales? For example, electronic orbitals obtained from density-functional theory calculations are being increasingly used in many-body Green's function theories, explicitly correlated methods, quantum impurity models, quantum embedding theories, and quantum computation of electronic structure. Such synergies provide a way to approach the exact solution of the Schroedinger equation, in addition to significantly accelerating the cost of explicit many-body calculations. On a much larger spatial scale, multiscale coupling of approximate many body Hamiltonians with Maxwell's equations allows unifying microscopic and continuum treatments of van der Waals and Casimir interactions, eventually making it possible to push the boundaries of such calculations to macroscopic systems.

Long Program Schedule

This workshop is part of the long program on "Quantum Mechanics with Mathematics and Statistics"

- Opening Day : March 7, 2022
- Advancing Quantum Mechanics with Mathematics and Statistics Tutorials : March 8-11, 2022
- **Workshop I: Multiscale Approaches in Quantum Mechanics : March 28 -April 1, 2022**
- Workshop II: Model Reduction in Quantum Mechanics : April 11-15, 2022
- Workshop III: Large-Scale Certified Numerical Methods in Quantum Mechanics : May 2-6, 2022
- Workshop IV: Monte Carlo and Machine Learning Approaches in Quantum Mechanics : May 23-27, 2022
- Culminating Workshop at Lake Arrowhead : June 5-10, 2022

Participation

Additional information about this workshop including links to register and to apply for funding, can be found on the webpage listed below. Encouraging the careers of women and minority mathematicians and scientists is an important component of IPAM's mission, and we welcome their applications.

Organizers

Eric Cances (École Nationale des Ponts-et-Chaussées), **Maria J. Esteban** (CNRS and Université Paris-Dauphine), **Giulia Galli** (Univ. of Chicago), **Lin Lin** (UC Berkeley), **Alejandro Rodriguez** (Princeton), and **Alexandre Tkatchenko** (Univ. of Luxembourg).

Speakers

George Booth (King's College London), Roberto Car (Princeton University), Gero Friesecke (Technische Universität München), Laura Gagliardi (University of Chicago), Giulia Galli (University of Chicago), Matteo Gori (University of Luxembourg), Timothy Gould (Griffith University), Marco Govoni (University of Chicago), Lin Lin (UC Berkeley), Michael Lindsey (Courant Institute of Mathematical Sciences), Jianfeng Lu (Duke University), Mitchell Luskin (University of Minnesota, Twin Cities), Andrew Millis (Flatiron Institute), Prineha Narang (Harvard University), Christoph Ortner (University of British Columbia), Alejandro Rodriguez (Princeton University), Angel Rubio (Max Planck Institute for the Structure and Dynamics of Matter), Reinhold Schneider (Technische Universität Berlin), Martin Stoehr (University of Luxembourg), Alexandre Tkatchenko (University of Luxembourg), Hakan Tureci (Princeton University), Michael Weinstein (Columbia University), Leonardo Zepeda-Nunez (University of Wisconsin-Madison), and Dominika Zgid (University of Michigan).

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For more information, visit the program web page:

www.ipam.ucla.edu/QMMWS1