

Workshop III: Large-Scale Certified Numerical Methods in Quantum Mechanics

Monday May 2, 2022

- 8:00–8:55 *Check-In/Light Breakfast (Hosted by IPAM)*
- 8:55–9:00 *Welcome & Opening Remarks: Dean Miguel García-Garibay (Dean of Physical Sciences, UCLA) and Dima Shlyakhtenko (Director, IPAM)*
- 9:00 *SESSION CHAIR: FRANCOIS GYGI (UC DAVIS)*
- 9:00–9:50 **Chao Yang** (Lawrence Berkeley National Laboratory)
Low rank approximation in electron excitation calculations
- 10:00–10:15 *Break*
- 10:15–10:55 **Julien Toulouse** (Sorbonne University, LCT)
Virtual Talk: Basis-set correction based on density-functional theory: Rigorous framework for a one-dimensional model
- 11:15–11:30 *Break*
- 11:30–12:20 **Lin Lin** (University of California, Berkeley (UC Berkeley))
Large scale hybrid DFT functionals: fast algorithms and finite-size effects
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *SESSION CHAIR: LIN LIN*
- 2:30–3:20 **Xin Xing** (University of California, Berkeley (UC Berkeley))
Finite-size error and its correction in energy calculations for periodic systems
- 3:30–3:45 *Break*
- 3:45–4:25 **Yingzhou Li** (Duke University)
Virtual Talk: Fast Algorithms for FCI excited states
- 4:45–5:00 *Lightning Poster Presentations*
- 5:00–6:30 *Poster Session & Reception (Hosted by IPAM)*

Tuesday May 3, 2022

- 8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00 *SESSION CHAIR: CHAO YANG*
- 9:00–9:50 **Francois Gygi** (University of California, Davis (UC Davis))
Generating Reference Data and Controlling Accuracy in DFT and Hybrid DFT Simulations
- 10:00–10:15 *Break*

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- 10:15–10:55 **Emmanuel Giner** (Centre National de la Recherche Scientifique (CNRS))
Virtual Talk:
- 11:15–11:30 *Break*
- 11:30–12:10 **Antoine Levitt** (Institut National de Recherche en Informatique Automatique (INRIA))
Virtual Talk: Numerical methods for scattering and resonance properties in molecules and solids
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *SESSION CHAIR: VIRGINIE EHRLACHER (École Nationale des Ponts-et-Chaussées (ENPC))*
- 2:30–3:20 **Laura Grigori** (Institut National de Recherche en Informatique Automatique (INRIA))
large scale hybrid functional calculations: fast algorithms and finite size effects
- 3:30–4:00 *Break*
- 4:00–4:50 **Amartya Banerjee** (University of California, Los Angeles (UCLA))
Electronic Structure Calculations of Chiral Matter - From First Principles Methods to Machine Learning Techniques

Wednesday May 4, 2022

- 8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00 *SESSION CHAIR: KEVIN STUBBS (UCLA)*
- 9:00–9:50 **Virginie Ehlacher** (École Nationale des Ponts-et-Chaussées (ENPC))
Multi-center decomposition of molecular densities: a mathematical perspective (joint work with Eric Cancès, Benjamin Stamm and Robert Benda)
- 10:00–10:15 *Break*
- 10:15–10:55 **Markus Bachmayr** (Johannes Gutenberg-Universität Mainz)
Virtual Talk: Constraints on Matrix Product States via Block Sparsity
- 11:05–11:20 *Break*
- 11:20–12:00 **David Gontier** (Université de Paris IX (Paris-Dauphine))
Virtual Talk:
- 12:20–2:00 *Lunch (on your own)*
- 2:00 *SESSION CHAIR: CARLOS GARCIA-CERVERA*
- 2:00–2:50 **Muhammad Hassan** (Sorbonne Université)
Towards the development of a posteriori error estimates for the coupled cluster equations
- 3:00–3:15 *Break*

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- 3:15–4:05 **Mi-Song Dupuy** (Sorbonne Université)
Sparse and symmetry-preserving compression of matrix product operators
- 4:15–4:30 *Break*
- 4:30–5:10 **Huajie Chen** (Beijing Normal University)
Virtual Talk: Convergence of the Planewave Approximations for Quantum Incommensurate Systems

Thursday May 5, 2022

- 8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00 *SESSION CHAIR: LAURA GRIGORI (Institut National de Recherche en Informatique Automatique)*
- 9:00–9:40 **Yvon Maday** (Université de Paris VII (Denis Diderot) et Université de Paris VI (Pierre et Marie Curie))
Virtual Talk:
- 9:50–10:00 *Break*
- 10:00–10:40 **Filippo Lipparini** (Università di Pisa)
Virtual Talk: Black-box optimization of self-consistent field wavefunction for closed and open shell molecules
- 10:50–11:00 *Break*
- 11:00–11:40 **Benjamin Stamm** (RWTH Aachen University)
Virtual Talk: Acceleration of quantum mechanical systems by exploiting similarity
- 11:50–12:00 *Break*
- 12:00–12:40 **Julia Contreras-García** (Sorbonne Université)
Virtual Talk: Math-chimie: developing approaches for predicting new superconductors
- 12:50–2:30 *Lunch (on your own)*
- 2:00 *SESSION CHAIR: FABIAN FAULSTICH (University of California, Berkeley)*
- 2:30–3:10 **David Mazziotti** (University of Chicago)
Virtual Talk: Contracted Quantum Eigensolver for the Quantum Simulation of Many-electron Systems
- 3:30–3:45 *Break*
- 3:45–4:25 **Xiaoying Dai** (Chinese Academy of Sciences)
Virtual Talk: Convergent orthogonality preserving approximations of the Kohn-Sham orbitals

Friday May 6, 2022

- 8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00 *SESSION CHAIR: ANDREAS SAVIN (Centre National de la Recherche Scientifique)*
- 9:00–9:40 **Markus Reiher** (ETH Zurich)
Virtual Talk: Uncertainty Quantification of Quantum Chemical Methods
- 10:00–10:15 *Break*
- 10:15–10:55 **Genevieve Dusson** (Université de Franche-Comté (Besançon))
Virtual Talk: Error bounds for properties in planewave electronic structure calculations
- 11:15–11:30 *Break*
- 11:30–12:10 **Stefano Baroni** (International School for Advanced Studies (SISSA/ISAS))
Virtual Talk: Separating flour from bran: how to optimally estimate transport coefficients from short equilibrium molecular-dynamics simulations
- 12:30–2:30 *Lunch (on your own)*

