Workshop IV: Monte Carlo and Machine Learning Approaches in Quantum Mechanics

Monday May 23, 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: David Ceperley*

9:00–9:50 **Brenda Rubenstein** (Brown University)
Extending the Reach of Quantum Monte Carlo Methods via Machine Learning

10:00–10:15 *Break*

10:15–10:55 **Jonathan Weare** (New York University)
A fast Jacobi iteration with repeated random sparsification

11:05–11:30 *Break*

11:30–12:20 **Bryan Clark** (University of Illinois at Urbana-Champaign)
Virtual Talk: Variational Wavefunctions using Machine Learning Architectures for Fermions and Gauge Theories.

12:30–2:30 *Lunch (on your own)*

2:30 *SESSION CHAIR: Kieron Burke*

2:30–3:20 **Eran Rabani** (University of California, Berkeley (UC Berkeley))
Stochastic Density Functional Theory

3:30–3:45 *Break*

3:45–4:35 **Shiwei Zhang** (Flatiron Institute)
Auxiliary-field methods for quantum materials

4:45–5:10 *Lightning Poster Session*

5:10–6:45 *Poster Session & Reception (Hosted by IPAM)*

Tuesday May 24, 2022

8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*

9:00 *SESSION CHAIR: Marivi Fernandez Serrra*

9:00–9:50 **Giuseppe Carleo** (École Polytechnique Fédérale de Lausanne (EPFL))
Virtual Talk: “Fermionic neural-network quantum states”.

10:00–10:15 *Break*

(Tuesday schedule continued on next page)

(Tuesday schedule continued from previous page)

10:15–10:55 **Claudia Filippi** (Universiteit Twente)
Virtual Talk: Targeting excited states with quantum Monte Carlo

11:05–11:30 *Break*

11:30–12:20 **Leslie Vogt-Maranto** (New York University)
Molecular Electron Densities via Machine Learning

12:30–2:30 *Lunch (on your own)*

2:30 *SESSION CHAIR: Jonathan Weare*

2:30–3:20 **Raymond Clay** (Sandia National Laboratories)
Opportunities for Machine Learning in Equation of State and Transport Modeling at Extreme Conditions

3:30–4:00 *Break*

4:00–4:50 **Sandeep Sharma** (University of Colorado Boulder)
Auxiliary field quantum Monte Carlo (AFQMC) with multi Slater wavefunctions

Wednesday May 25, 2022

8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*

9:00 *SESSION CHAIR: Aurora Pribram-Jones*

9:00–9:50 **Juan Carrasquilla** (Vector Institute)
Variational Neural Annealing

10:00–10:15 *Break*

10:15–11:05 **Andrea Tirelli** (International School for Advanced Studies (SISSA/ISAS))
Virtual Talk: TBA

11:15–11:30 *Break*

11:30–12:20 **Anouar Benali** (Argonne National Laboratory)
Virtual Talk: Using multideterminant many-body methods to describe ground state and excited state properties of strongly correlated materials

12:30–2:30 *Lunch (on your own)*

2:30 *SESSION CHAIR: Lucas Wagner*

2:30–3:20 **Robert Webber** (California Institute of Technology)
Approximating matrix eigenvalues by subspace iteration with repeated random sparsification

3:30–4:00 *Break*

4:00–4:50 **Jan Hermann** (Freie Universität Berlin)
Neural-network wave functions for quantum chemistry

Thursday May 26, 2022

8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*

9:00 *SESSION CHAIR: Mark Tuckerman*

9:00–9:50 **William Foulkes** (Imperial College London)
Approximating Many-Electron Wave Functions using Neural Networks

10:00–10:15 *Break*

10:15–11:05 **Kieron Burke** (University of California, Irvine (UCI))
'Conditional probability density functional theory'

11:15–11:30 *Break*

11:30–12:20 **David Ceperley** (University of Illinois at Urbana-Champaign)
Quantum Monte Carlo and Machine Learning Simulations of Dense Hydrogen

12:30–2:00 *Lunch (on your own)*

2:00 *SESSION CHAIR: Shiwei Zhang*

2:00–2:50 **Marivi Fernandez-Serra** (SUNY Stony Brook)
Machine learning approaches to improve the exchange and correlation functional in density functional theory.

3:00–3:15 *Break*

3:15–4:05 **Lucas Wagner** (University of Illinois at Urbana-Champaign)
Obtaining compact representations of excited states from QMC, and using those excited states as data for low-energy models

4:15–4:30 *Break*

4:30–5:20 **Mark Tuckerman** (New York University)
An exact formulation of quantum time correlation functions in terms of an open-chain path integral distribution

Friday May 27, 2022

8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*

9:00 *SESSION CHAIR: TBD*

9:00–9:50 **Julia Westermayr** (University of Warwick)
Physically inspired machine learning for excited states

10:00–10:15 *Break*

10:15–11:05 **Michael Scherbela** (University of Vienna)
Chasing the ground-state: High accuracy wavefunctions using deep-learning-based variational Monte Carlo

11:15–11:30 *Break*

(Friday schedule continued on next page)

(Friday schedule continued from previous page)

11:30–12:20 **Ilyes Batatia** (University of Cambridge)
Unified understanding of E(3)-Equivariant Interatomic Potentials : Theory and Applications