Tensor Network Methods in Quantum Dynamics

Quantum Dynamics Network and Wolfgang Pauli Institute Vienna
Organizers: Henrik R. Larsson, Norbert J. Mauser and Fabien Gatti

Location: HS 11 Fak. Math. OMP1, Uni Wien

Talks: 35 minutes + 10 minutes discussion

Tuesday, July 18

Session I, Chair: Fabien Gatti

13:45 – 14:00 Organizers: *Welcome*

14:00 – 14:45 Henrik R. Larsson: *Introduction to MCTDH and Tensor Network States*

14:45 – 15:30 Uwe Manthe: *Developments in the non-hierarchical multi-layer MCTDH approach*

15:30 – 16:00 **break**

16:00 – 16:45 Christian Lubich: *Time integration of tree tensor networks*

16:45 – 17:30 Benedikt Kloss: *Subspace expansions: Schemes to dynamically adapt the approximation rank or bond dimension*

Wednesday, July 19

Session II, Chair: Oriol Vendrell

 9:15 – 10:00 Nina Glaser: *Large-scale anharmonic vibrational calculations with the DMRG algorithm*

10:00 – 10:45 Pierre-Nicholas Roy: *Quantum Critical Molecular assemblies: from matrix product states to path integrals*

10:45 – 11:15 **break**

11:15 – 12:00 Uli Schollwöck: *Dynamics of singlet fission in covalently linked tetracene dimers using tensor network states*

12:00 – 14:00 **lunch**

Session III, Chair: Tucker Carrington

14:00 – 14:45 Irene Burghardt: *Multiconfigurational quantum dynamics with multiplicative neural network potentials*

14:45 – 15:30 Daniel Pelaez: *Towards high-dimensional analytical sum-of-products representations*

15:30 – 16:00 **break**

16:00 – 16:45 Markus Schröder: *Compact representation of operators in sum-of-products form*

16:45 – 17:30 Sudip Sasmal: *Compact sum-of-products form of the molecular electronic Hamiltonian and its application within the MCTDH method*

Thursday, July 20

Session IV, Chair: Eric Fischer

 9:15 – 10:00 Roman Ellerbrock: *Quantum Circuit simulations with Tree Tensor Network States*

10:00 – 10:45 Haobin Wang: *ML-MCTDH simulation in the interaction picture*

10:45 – 11:15 **break**

11:15 – 12:00 Tucker Carrington: *Obviating the need for as many points as basis functions when using collocation with MCTDH to do efficient and accurate quantum dynamics on a general PES*

12:00 – 14:00 **lunch**

Session V, Chair: Henrik R. Larsson

14:00 – 14:45 Micheline Soley: *Tensor Trains and Quantum Computing for Highly Multidimensional Molecular Simulations*

14:45 – 15:30 Örs Legeza: *Simulation of long time and Lindbladian evolution via massively parallel hybrid CPU-GPU based tensor network state algorithms*

15:30 – 16:00 **break**

16:00 – 16:45 Graham Worth: *New Applications Using ML-MCTDH: Gaussian basis sets and Density Matrices*

Workshop Dinner: 19:30

On the "summer stage" near WPI.

Friday, July 21

Session VI, Chair: Graham Worth

9:15 – 10:00 David Mendive-Tapia: *Finding optimal multi-layer trees through graph theory*

10:00 – 10:45 Jiajun Ren: *Tensor Network Methods for Electron-Phonon Problems*

10:45 – 11:15 **break**

11:15 – 12:00 Eric Fischer: *How Chemistry and Physics Meet in Optical Infrared Cavities: Application of the MCTDH Method to Vibrational Strong Coupling Models*

12:00 – 14:00 **lunch**

Session VII, Chair: Norbert Mauser

14:00 – 14:45 Ofir Alon: *How accurate the MCTDHB wavefunction is: Lessons from numerics, analytics, and examples*

14:45 – 15:30 Peter Schmelcher: *Impurities in highly imbalanced ultracold mixtures: Controlled transport and counterflow dynamics*

15:30 – 15:45 Organizers: *Goodbye*