Internship proposal – Master (M1 or M2) – 4 or 5 months

Space–Time Variational Approaches for Non-Adiabatic Dynamics

Keywords: Photochemistry, Non-adiabatic dynamics, Space-Time Variational Principle

Abstract:

Non-adiabatic dynamics, where electronic and nuclear motions are strongly coupled, are central to photochemistry, ultrafast spectroscopy, and molecular electronics. Conical intersections, points where two electronic potential energy surfaces cross, govern ultrafast transitions and quantum interference effects. Accurately simulating wavepacket evolution near in this context is challenging due to rapid oscillations, strong couplings, and coherence requirements. Traditional time-propagation methods often suffer from instability or only guarantee local-in-time accuracy. This raises the question: can a global-in-time, space-time variational formulation provide a more stable and accurate framework for non-adiabatic quantum dynamics?

The recently developed space-time time-dependent variational principle[2] reformulates the Schrödinger evolution as a global least-squares minimization over the entire space–time domain. By optimizing the wavefunction simultaneously in time and space, this approach avoids separate time-stepping, provides rigorous error control, and guarantees global-in-time existence of low-rank approximations. Applied to a 2D two-state CI model, the method allows accurate propagation of nuclear wavepackets, capturing both population transfer and quantum interference effects with improved stability and efficiency.

In the project, the student will define a 2D-2-state conical intersection model in diabatic and adiabatic representations, implement a space-time Galerkin discretization of the time-dependent variational principle using suitable spatial and temporal bases, perform simulations of nuclear wavepacket dynamics through the conical intersection and compare them with standard time-stepping or split-operator approaches, and analyze convergence, stability, and the impact of low-rank approximations. This project will provide practical experience in quantum dynamics, variational methods, and high-dimensional numerical simulations while exploring the advantages of the new approach formulation in a prototypical non-adiabatic system.

Prerequisites: Basic knowledge in Non-adiabatic dynamics. Coding/programming skills. Ability to read and understand scientific papers in English is required. Strong mathematical skills.

Methods: Numerical integration. Grid methods. Constrained optimization.

Estimated dates: 02/2026 – 07/2026

Contacts:
Virginie Ehrlacher, CERMICS , École des Ponts ParisTech, virginie.ehrlacher@enpc.fr,
Mi-Song Dupuy, LJLL, Sorbonne Université, mi-song.dupuy@sorbonne-universite.fr.
Loïc Joubert-Doriol, MSME, Université Gustave Eiffel, loic.joubert-doriol@univ-eiffel.fr,

References:
1 Domcke, Wolfgang, Koppel, & Yarkony, eds. Conical intersections: Electronic Structure, Dynamics & Spectroscopy" Vol. 15. World Scientific, 2004. 2 Dupuy, Ehrlacher, Guillot, arXiv:2405.18094 (2024).