PhD offer (October 2022-Septembre 2025) at Ecole des Ponts ParisTech and Inria Paris

Model reduction in quantum mechanics

This internship lays in the perspective of the EMC2 multidisciplinary ERC Synergy project on molecular simulation (Sept. 2019-Aug. 2025): `https://erc-emc2.eu`

This project gathers 16 permanent researchers from Ecole des Ponts ParisTech, Inria Paris and Sorbonne University, about 15 PhD students and postdocs, and 12 French and international collaborators.

Molecular simulation has become an instrumental tool in chemistry, condensed matter physics, molecular biology, materials science, and nanosciences. The importance of molecular simulation in today's science was acknowledged by the 1998 and 2013 Nobel prizes in Chemistry. It is also a source of very exciting mathematical and numerical problems.

The fundamental equation in molecular equation is the Schrödinger equation governing the dynamics of the atomic nuclei and electrons composing the molecular system of interest. This model is extremely accurate, but much too complicated to be fully solved numerically. Fortunately, as in many quantum problems, the phenomena of interest take place in a small energy window: this is the case in chemistry (valence electrons are very much affected by chemical reactions, while core electron states are barely modified), as well as in materials science (electronic conductivity in metals is mainly due to the transport of electrons with energy close to the so-called Fermi energy). The purpose of this PhD thesis is to study with full mathematical rigor the reduction process consisting in replacing a reference quantum model with an extended energy range with a reduced model focusing on the energy window of interest. Three systems will be considered: a model one-dimensional quantum system for which most calculations are explicit, a small molecule and a 2D material such as graphene.

Keywords: partial differential equations (PDEs), variational methods, numerical simulation of PDEs, spectral theory of self-adjoint operators,

Requested background: functional analysis and partial differential equations, basics of spectral theory, proficiency in Python, Matlab, or Julia

Location: Ecole des Ponts-ParisTech, 6 & 8 avenue Blaise Pascal, 77455 Marne-la-Vallée, France (access: RER A, Noisy-Champs, 25' from Paris Center)

Net salary: about 1700 euros per month

Contacts: Eric Cancès (eric.cances@enpc.fr) and Antoine Levitt (antoine.levitt@inria.fr)