

Virginie Erhlacher (mini-course 1): Dynamical low-complexity approximations of high-dimensional evolution equations: specific focus on the Schrödinger equation

Wednesday, June 11, 2025 9:00 AM (1 hour)

The aim of this mini-course is to give an overview of various methods to compute dynamical low-complexity approximations of the solution of high-dimensional evolution Partial Differential Equations (PDEs) with a specific focus on the Schrödinger equation. In this particular case, the solution of the PDE of interest is in general defined on a very high-dimensional space in the case when the number of electrons in the system is large. As a consequence, traditional numerical methods are doomed to failure because of the curse of dimensionality and specific approaches have to be considered. In particular, it is necessary to rely on the use of some subset of functions which can be represented with a low complexity, and find approximations of the exact solution which belong to such a subset at any time. Several different approaches exist to compute such dynamical low-complexity approximations and the aim of the mini-course is to give an introduction to the most popular methods in this context and give some insight about some recent results.

The first part of the course will be devoted to the presentation of the main subsets of low-complexity functions used in the context of the Schrödinger equation such as low-rank tensor formats, polynomial gaussian approximations or neural networks. We will then discuss about the most popular approach used in order to compute dynamical approximations in these subsets, namely the so-called Dirac-Frenkel variational approximation. Lastly, we will discuss about recent results where an alternative variational principle to compute dynamical low-complexity approximations was proposed, relying on a well-conditioned least-square variational formulation of the time-dependent Schrödinger equation was proposed. We will discuss about the pros and cons of this new variational principle in comparison with the famous Dirac-Frenkel variational principle.