Contribution ID: **13** Type: **not specified**

A nonlinear reduced model based on optimal transport for electronic structure calculations

Wednesday, 12 June 2024 11:30 (45 minutes)

Electronic structure calculations are widely used to predict the physical properties of molecules and materials. They require to solve nonlinear partial differential and eigenvalue equations. These equations are generally numerically very demanding, especially since they are parameterized by the positions of the nuclei in the molecule and must be solved a large number of times when these positions vary. This is the case for example when simulating the dynamics of a molecule.
In this talk, I will present a recent work aimed at efficiently calculating approximate solutions of such parameterized PDEs, with the objective of reducing the overall computational time. For this, I will present a non-linear interpolation method between several solutions, based on optimal transport, and using in particular Wasserstein barycenters. I will illustrate this method with simulations carried out on a 1D toy model.

Presenter: DUSSON, Geneviève (CNRS, Université Bourgogne Franche-Comté)