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PHD PROPOSAL

Title: Reduced models and machine learning for eigenvalue problems arising in electronic structure calculation.
Key-words: Numerical analysis, reduced bases, *a posteriori* analysis, goal-oriented estimates, electronic structure calculation, tight-binding models, density functional theory
Thesis supervision: Geneviève Dusson & Alexei Lozinski (Laboratoire de Mathématiques de Besançon, Université Bourgogne Franche-Comté, France)

The thesis is expected to start between October 2020 and January 2021 and will be carried out at the Laboratoire de Mathématiques de Besançon.

Summary

To simulate molecular systems and compute their physical properties, it is common to use electronic structure models, which predict the behavior of electrons given the nuclei positions. These models require to solve eigenvalue and nonlinear partial differential equations, such as the Hartree–Fock equations, or equations coming from the density functional theory. Such calculations are at the basis of molecular dynamics simulations, where they are repeated for a large number of particle configurations, which requires significant calculation time. There exists simplified models which allow to reduce the computational time, at the expense of a loss in precision, which can be difficult to control.

The objective of this thesis is therefore to develop reduced models allowing to keep track of the quality of the approximations. The thesis will be particularly focused on the case where the equations are solved many times for different parameters. The thesis will be devoted to the numerical analysis of reduced models, to the development of error bounds, as well as the implementation of these models to test their quality.

A first approach will consist in developping a linearization of the non-linear operator using interpolation or learning methods, based for example on [Van der Oord, Dusson, Csányi, Ortner, Machine Learning: Science and Technology, 1 (2020)] and [Dusson, Bachmayr, Csányi, Drautz, Etter, van der Oord, Ortner, arxiv 1911.03550]. A second approach will be to start from linear reduced models such as tight-binding models, and to improve them with the resolution of a few non-linear problems, based for example on the method presented in [Maday , Patera, Penn, Yano, ESAIM: Proceedings and Surveys, 50, 144–168 (2015)]. Finally, we will be interested in the prediction of specific quantities of interest, like the energy of the system, and we will try to estimate the quality of the approximations, both in a context of reduced modelling and learning, in order to guarantee the quality of the approximations and / or the machine learning.

Expected skills

A master's degree in applied mathematics is expected. The successful candidate will have solid experience in numerical methods for partial differential equations. Programming skills (e.g. Julia, Python, C ++) will also be appreciated.

Information regarding the application

Additional information can be requested by email to Geneviève Dusson (`genevieve.dusson@math.cnrs.fr`) and Alexei Lozinski (`alexei.lozinski@math.cnrs.fr`).

Applicants are requested to send an email containing a CV and a cover letter to `genevieve.dusson@math.cnrs.fr` as well as `alexei.lozinski@math.cnrs.fr`.
The deadline to apply is May 27, 2020.