

POST-DOCTORAL POSITION: AUTOMATIC DIFFERENTIATION FOR ELECTRONIC STRUCTURE CALCULATION

We invite applications for a postdoctoral position (one year with possibility of renewal, available from November 2021) on the use of automatic differentiation in electronic structure methods, and more specifically for the modeling and simulation of 2D materials.

Electronic structure methods in general and approaches based on density functional theory (DFT) are established and used on a routine basis to investigate the properties of molecules and materials. Given a system of interest, DFT software computes the energy, electronic density and various quantities of interest. Since many chemical and physical properties essentially describe the change of the energy in a system with respect to external perturbations, the efficient computation of derivatives is of the utmost importance: derivatives provide access to fundamental quantities such as the forces on atoms, elasticities, response to external pressure or directly measurable spectra describing electronic or phononic excitations. A general formalism has been developed for that purpose, but requires manual implementation for every pair of input and output properties, an extremely costly endeavor in human time. Furthermore, it is not directly possible to compute high-dimensional gradients efficiently.

In recent years, automatic differentiation (AD) has become a critical component of machine learning pipelines: training a machine learning model often amounts to computing the gradient of a loss function with respect to the model parameters. Accordingly, several frameworks have been developed to compute gradients efficiently and automatically. However, they often introduce significant rigidity into the code structure and have various limitations.

In our group, we have recently developed the DFTK code (<http://dftk.org>) to be a simple yet efficient DFT code written in Julia. With its relatively small codebase, DFTK is tractable, which allows the code to be readily adapted to AD tools. Nevertheless DFTK shows a performance comparable to established (much bigger and more complex) DFT packages. We have already used some AD tools with DFTK, in particular to simplify the coding of forces and stresses. We would like to generalize this approach to more general properties, and in particular to reverse-mode automatic differentiation, which allows for the cheap computation of high-dimensional gradients. This requires both the development of a new formalism and its implementation in DFTK.

New science that could potentially be unlocked by this fundamental development includes

- The training of machine learning models in tandem with traditional DFT methods (the exchange-correlation functional as a neural network)
- The optimization of any output parameter (the flatness of the band structure of two-dimensional materials, the distance between the phonon spectrum and a target one...) with respect to any input (positions of atoms, local potential, exchange-correlation functional...)
- The exploration of the sensitivity and uncertainty of DFT results
- ...

The post-doctoral researcher will have the opportunity to shape these emerging research directions based on his/her interests.

Candidate. Due to the extreme interdisciplinary nature of the position, we will consider applicants with a PhD in a variety of disciplines (applied mathematics, physics, chemistry, computer science). Fundamental are a deep understanding and familiarity with differential calculus and the practical tools of scientific computing, as well as a willingness to learn new things. Experience in numerical methods, machine learning, automatic differentiation, the Julia programming language, molecular simulation, electronic structure or materials science is appreciated but not required. Knowledge of French is not required.

Keywords: Automatic differentiation, DFT, perturbation methods, nonlinear partial differential equations, nonlinear systems, numerical analysis, condensed-matter physics, quantum chemistry

Collaborations: the post-doctoral researcher will be based at CERMICS, the applied mathematics department of Ecole des Ponts ParisTech, and collaborate there with Eric Cancès and Antoine Levitt. He/she will be a member of Matherials (<https://team.inria.fr/matherials/>), a joint research team of Ecole des Ponts ParisTech and Inria Paris, and be part of the multidisciplinary Paris ecosystem around molecular simulation, the EMC2 ERC Synergy project. He/she will also work with Michael Herbst (RWTH Aachen), including bilateral visits.

Location: Ecole des Ponts ParisTech, 6 & 8 avenue Blaise Pascal, 77455 Marne-la-Vallée, France (access: RER A, Noisy-Champs, 25' from Paris center). Remote work will be considered on a case-by-case basis, depending on the evolution of the health situation and Covid protocols.

Salary: depending on experience

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