Developing the next generation time-dependent density functional theory code

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Real-time electron dynamics, in particular the real-time version of time-dependent density functional theory (TDDFT), is becoming a widely used tool for simulating materials under non-linear and non-equilibrium conditions.

One of the main computational challenges in real-time electron dynamics is to reach long simulation times in order to resolve the movement of the nuclei and other long time scale phenomena. At the same time, it is necessary to use costly approximations for the electronic interaction, like hybrid functionals, to obtain accurate results.

At the same time, high-performance computing platforms have radically changed over the last decade, now all modern supercomputers are based on graphics processing units (GPUs). GPUs offer huge amounts of computing power, but they require explicitly parallel programming and memory management. This is a challenging scenario for current TDDFT software that was developed for CPU based computers, most of them in the Fortran language.

We are working on a new package for TDDFT simulations that incorporates the experience from implementing TDDFT in previous code, mainly from the Octopus and Qball codes, combined with state of the art programming and tools. This allows to have a code that is simple, flexible, extensible and scalable. The code supports threading, GPU and MPI parallelization from scratch so that it can run efficiently on current and future supercomputing platforms from different vendors.

Our model is to create a simple code that can be called as an engine/library by existing density functional codes, so that many of the existing high level abstract implementation of the physics can be reused.

The code is based on a plane wave discretization, but it is written in an basis-agnostic fashion, so that other representations can be integrated in the future. It has support for hybrid functionals, using techniques to drastically reduce its computational cost, and relativistic effects and spin-orbit interaction.

This code will allow us to understand several non-linear effects in materials, for example second harmonic generation, shift currents in perovskite materials, and nonlinear electrical and thermal conductivity.