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The INQ code: reinventing the electronic-structure code

Electronic structure codes are a fundamental tool for the computational study of matter in the ground and the excited states. They are complex pieces of software that need to be accurate, reliable, and implement a wide array of functionalities and features. On top of that, given the costly nature of first principles simulations, they need to be computationally efficient and take advantage of modern high-performance computing (HPC) platform. Many existing codes have been in development for decades and are very large, some of them have several hundred thousand lines of code. This makes them very difficult to maintain, optimize and adapt to new platforms. This last point is particularly critical as in the last few years we have seen a radical change in the design of HPC systems. Graphical processing units (GPUs) have become the standard computational element in supercomputers and clusters. However, many electronic structure codes cannot use GPUs efficiently, especially when running in parallel. At the same time, new ideas have appeared in software engineering that have revolutionized code development. These new approaches not only involve how to write the code, but also how to design it, develop it collaboratively, debug it, test it, and maintain it. We apply these principles to the electronic structure problem in a new software package called INQ, that is currently in development at Lawrence Livermore National Laboratory.

INQ is a compact code that implements density functional theory (DFT) and time-dependent functional theory (TDDFT). It uses modern code design features and techniques that make the development fast and simple, and ensure the quality of the program. By designing the code around algorithms, rather than against specific implementations and numerical libraries, we provide a concise and modular code that is simple to understand, flexible, and extensible. The core code is accompanied by a large set of tests that check the individual components and the program as a whole. This is ensures that the program always works correctly as it is developed and that it gives reliable results.

INQ is based on the plane wave approach and can simulate both finite and (partially) periodic systems. It implements the standard DFT semi-local functionals as well as hybrid functionals. Hybrids are applied using the adaptively compressed exchange (ACE) approach to make the calculations computationally affordable. Its current focus is the simulations of the excited state of large systems using real-time TDDFT. However, it is a general code that can calculate ground state properties as well. INQ was designed from the scratch to run in parallel on multiple GPUs. In TDDFT simulations on GPU-based supercomputers INQ achieves excellent performance. It can handle hundreds and thousands of atoms, with simulation times of a second or less per time-step, and scale to thousands of GPUs. The code is open source and it is freely accessible at http://gitlab.com/npneq/inq

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