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DFTK: A Julian approach for simulating electrons in solids

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Density-functional theory (DFT) is a widespread method for simulating the quantum-chemical behaviour of electrons in matter. It provides a first-principles description of many optical, mechanical and chemical properties at an acceptable computational cost [16, 2, 3]. For a wide range of systems the obtained predictions are accurate and shortcomings of the theory are by now well-understood [2, 3]. The desire to tackle even bigger systems and more involved materials, however, keeps posing novel challenges that require methods to constantly improve. One example are so-called high-throughput screening approaches, which are becoming prominent in recent years. In these techniques one wishes to systematically scan over huge design spaces of compounds in order to identify promising novel materials for targeted follow-up investigation. This has already lead to many success stories [14], such as the discovery of novel earth-abundant semiconductors [11], novel light-absorbing materials [20], electrocatalysts [8], materials for hydrogen storage [13] or for Li-ion batteries [1]. Keeping in mind the large range of physics that needs to be covered in these studies as well as the typical number of calculations (up to the order of millions), a bottleneck in these studies is the reliability and performance of the underlying DFT codes.

To tackle these aspects multidisciplinary collaboration with mathematicians developing more numerically stable algorithms, computer scientists providing high-performance implementations, physicists and chemists designing appropriate models, and application scientists integrating the resulting methods inside a suitable simulation workflow is essential. While to date already a sizeable number of DFT codes exist, e.g. ABINIT [19], Quantum-Espresso [6] or VASP [15] to name only a few, they lack sufficient flexibility inside their low-level computational routines to easily support fundamental research in computer science or mathematics. To test emerging approaches motivated from these subjects in DFT — such as automatic differentiation, multi-precision methods, GPU acceleration, error estimation and numerical analysis — these communities have in the past resorted to developing their own codes. These codes in turn are not performant enough to scale to the level required to test resulting DFT approaches in practical simulations.

To overcome this barrier we have developed the density-functional toolkit (DFTK, `https://dftk.org`), a Julia package for DFT simulations in solid-state systems with the explicit goal to bundle the research efforts of all involved communities, see Figure 1. With an accessible code base (around 6000 lines) and a performance comparable to established DFT packages it can both be employed for mathematical research on reduced models and toy problems, but also for simulations including systems beyond 800 electrons. After less than two years of development our code shows a sizeable feature set: We support 1D / 2D / 3D problems, a multitude of solution algorithms for DFT, hybrid thread / MPI-based parallelism. Problems can be based upon custom analytic potentials,

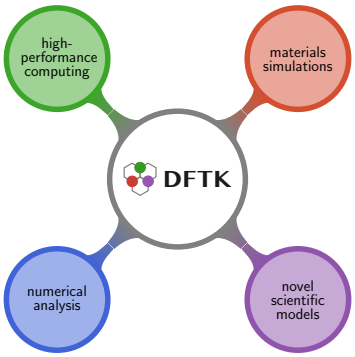

Fig. 1. The multidisciplinary directions of research in density-functional theory for which DFTK provides a joint software platform.

e.g. where results can be mathematically proven, but also state-of-the-art DFT methods such as PBE [18] in combination with Goedecker-type pseudopotentials [7]. Our code is well-integrated in the Julia ecosystem and features interfaces to established Python packages in the materials science community such as the atomistic simulation environment (ASE) [12] or pymatgen [17] for setting up or post-processing simulations. The entrance barrier to get started with DFTK is kept low by designing the code in line with the mathematical and physical structure of the DFT problem.

As a result DFTK is highly suitable to rapidly prototype new physical models or support the mathematical analysis of DFT methods, which is demonstrated in a number of recent papers [4, 5, 9, 10] by us and our collaborators. In particular our recent research employed DFTK (a) to derive *a posteriori* error estimates for simple DFT-like models [10], which will help to construct automatic error balancing strategies in the future, and (b) to develop black-box preconditioning strategies to speed up DFT calculations on large inhomogeneous systems [9]. Both these projects were only possible since DFTK allowed us to tackle reduced models, where one could obtain mathematical or physical insight, and then test the new methods on realistic full-scale applications. We hope that DFTK will be a useful platform for future multidisciplinary developments in density-functional theory. See `https://docs.dftk.org` for documentation and examples to get started with DFTK.

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