Using the density-functional toolkit (DFTK) to investigate floating-point error and improve SCF convergence in density-functional theory

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Résumé

Progress in density-functional theory is often the outcome of efforts involving physically sound approximate models, performant numerical schemes and optimal use of available computational hardware. In such an interdisciplinary field the lack of flexibility of many state-of-the-art codes poses an obstacle for multiple fields to join forces in one code. To close this gap, we have recently developed the density-functional toolkit, DFTK (https://dftk.org). In less than 3000 lines of Julia code, DFTK is capable of performing basic ground-state DFT simulations at a level of accuracy and performance comparable to well-established packages. At the same time one may conduct calculations using toy Hamiltonians with potentials ranging from a 1D harmonic oscillator to standard GGA functionals.

Two aspects of DFT simulations we currently investigate with DFTK are (a) the influence of floating-point precision and (b) mixing techniques for metal/insulator mixed systems. For the former aspect we exploit that DFTK is completely generic in the floating-point type, which allows to switch to elevated or reduced precision in parts or the complete code at runtime. In combination with interval arithmetic bounds on the floating-point error of a calculation may be computed. Traditionally in plane-wave DFT mixing of SCF iterations is used to improve SCF convergence. For systems with both metallic and insulating regions commonly used approaches are difficult to be made compatible. We investigate the use of the local density of states to construct a mixing scheme, which locally differs in insulating and metallic regions.

Mots-Clés: density, functional theory, plane, wave, self, consistent field, mixed precision, floating, point error

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