Fast and accurate finite-element based methods for DFT calculations within the projector-augmented wave formalism in the exascale era

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The predictive capability offered by quantum modelling of materials, especially using density functional theory (DFT), has opened up a gateway for gaining crucial insights into materials' behavior, leading to an accurate prediction of mechanical, transport, chemical, electronic, magnetic and optical properties of materials. However, the stringent accuracy requirements required to compute meaningful material properties and the asymptotic cubic-scaling computational complexity of the underlying DFT problem demand enormous computational resources. Thus, these calculations are routinely limited to periodic simulation domains with material systems containing a few hundred atoms. Additionally, these DFT calculations occupy a sizeable fraction of the world's computational resources today but mostly remain in the high throughput calculation mode as the widely used DFT implementations struggle to keep up pace with evolving heterogeneous architectures in today's exascale era. To this end, the talk first introduces the recent advancements in finite-element (FE) based methods for DFT calculations -via- the DFT-FE code, the workhorse behind the ACM Gordon Bell Prize 2023. These methods provide a systematically convergent, computationally efficient and scalable hybrid CPU-GPU framework for large-scale norm-conserving pseudopotential DFT calculations that overcome the aforementioned limitations while accommodating generic boundary conditions. Subsequently, we will discuss our group's very recent efforts to go a step further in developing a fast and scalable approach combining the efficiency of projector-augmented wave (PAW) formalism involving smooth electronic fields with the ability of systematically improvable higher-order FE basis facilitating substantial reduction in degrees of freedom to achieve significant computational gains (~8x-10x) compared to the current DFT-FE calculations for medium to large-scale material systems (5000-50,000 electrons). Moreover, our approach PAW-DFT-FE demonstrates a considerable computational advantage over state-of-the-art plane-wave codes for system sizes greater than 5000 electrons. Notably, our framework represents the first real-space PAW approach capable of competing with plane-wave methods. Furthermore, extensions of the aforementioned PAW-DFT-FE framework to incorporate noncollinear magnetism and spin-orbit coupling effects will also be discussed. Finally, we illustrate the effectiveness of PAW-DFT-FE in enabling large-scale simulations with generic boundary conditions using few case studies.

References

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