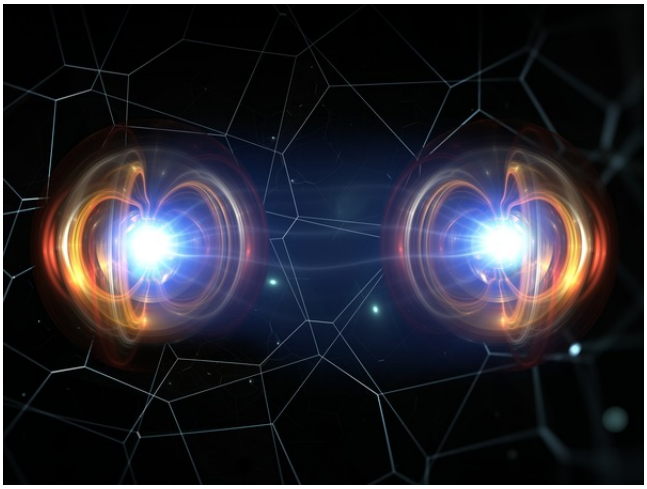
INNOVATION PARTNERSHIPS
UNIVERSITY OF MICHIGAN

DFT-FE v0.6 Software

TECHNOLOGY NUMBER: 2022-007



OVERVIEW

Massively parallel, real-space DFT calculations for large-scale electronic structure analysis

- Outperforms traditional plane-wave DFT codes in scalability and computational efficiency
- Materials science, quantum chemistry, nanotechnology, battery and catalyst research

BACKGROUND

Density Functional Theory (DFT) is a cornerstone computational tool in quantum chemistry and materials science, allowing researchers to study the electronic properties of atoms, molecules, and solids. Historically, DFT implementations have relied heavily on plane-wave basis sets and reciprocal-space methods, such as those embodied in codes like VASP and Quantum ESPRESSO. While efficient for smaller or periodic systems, these conventional methods face significant challenges in scaling to large, complex systems due to memory, communication bottlenecks, and fixed boundary conditions. Additionally, adapting them to highly parallel modern architectures can be difficult. As material systems and research questions become more complex, there is a need for methods that can efficiently handle larger simulations and leverage current high-performance computing resources more effectively, prompting the development of scalable, flexible, and open approaches to DFT calculations.

INNOVATION

Technology ID

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Category

Software
Software & Content
MOSS - Michigan Open Source Support

Inventor

Shiva Rudraraju
Denis Davydov
Shukan Parekh
Krishnendu Ghosh
Phani Motamarri
Vikram Gavini
Sambit Das

Further information

Ashwathi Iyer
ashwathi@umich.edu

View online

DFT-FE introduces a real-space, finite-element-based approach to DFT simulations, enabling unprecedented scalability across thousands of processors and applicability to both periodic and non-periodic boundary conditions. Unlike traditional plane-wave methods, DFT-FE's real-space framework allows for adaptive mesh refinement, reduced memory overhead, and flexible handling of complex geometries. Its open-source LGPL licensing and broad distribution on GitHub further enable collaborative development and accessibility. Technical advances include efficient parallelization, support for both electronic structure and quantum mechanical molecular dynamics, and compatibility with advanced high-performance computing platforms. These improvements make DFT-FE a powerful tool for large-scale simulations in materials science, nanotechnology, battery design, catalysis, and quantum chemistry, opening new opportunities for investigation and innovation in computational research.

ADDITIONAL INFORMATION

PROJECT LINKS:

- DFT-FE Github

DEPARTMENT/LAB:

- Vikram Gavini, Computational Materials Physics Group, Mechanical Engineering

LICENSE:

- GNU LGPL 2.1