NEWS RELEASE

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2023 ACM Gordon Bell Prize Awarded to International Team for Materials Simulations Which Achieve Quantum Accuracy at Scale

Performance of 659.7 PFLOPS Reached on Frontier, the World's First and Fastest Exascale Supercomputer

Denver, CO, November 16, 2023 – ACM, the Association for Computing Machinery, named an eight-member team drawn from American and Indian institutions as the winner of the 2023 ACM Gordon Bell Prize for the project, "Large-Scale Materials Modeling at Quantum Accuracy: *Ab Initio* Simulations of Quasicrystals and Interacting Extended Defects in Metallic Alloys."

The members of the team are: Sambit Das (University of Michigan), Bikash Kanungo (University of Michigan), Vishal Subramanian, (University of Michigan), Gourab Panigrahi (Indian Institute of Science, Bangalore), Phani Motamarri (Indian Institute of Science, Bangalore), David Rogers (Oakridge National Laboratory), Paul M. Zimmerman (University of Michigan), and Vikram Gavini (University of Michigan).

Molecular dynamics is a process by which computer simulations are used to better understand the movements of atoms and molecules within a system. *Ab initio* (Latin for "from the beginning") is a branch of molecular dynamics that has been shown to be an especially effective technique when applied to important problems in physics and chemistry—including efforts to better understand microscopic mechanisms, gain new insights in materials science, and prove out experimental data.

Despite the successes of *ab initio* approaches in a wide range of computer simulations, the team notes that efforts to employ quantum mechanical *ab initio* methods to predict materials' properties has not been able to achieve quantum accuracy and scale on the powerful supercomputers needed to perform these simulations. In their abstract to their Gordon Bell Prize-winning project the authors write, "*Ab initio* electronic-structure has remained dichotomous between achievable accuracy and length-scale. Quantum Many-Body (QMB) methods realize quantum accuracy but fail to scale."

To address this challenge, the Gordon Bell Prize-winning team developed a framework that combines the accuracy provided by QMB methods with the efficiency of Density-Functional Theory (DFT) to access larger length scales at quantum accuracy—a goal that existing approaches have not been able to achieve.

In the prize-winning paper, the team lays out the three interconnected modules that comprise their new method:

- invDFT: a methodological advance in inverse DFT linking Quantum Many-Body (QMB) methods to DFT.
- MLXC: a machine-learned density functional trained with invDFT data, commensurate with quantum accuracy.
- DFT-FE-MLXC: an adaptive higher-order spectral finite-element (FE) based DFT implementation that integrates MLXC with efficient solver strategies and HPC innovations in FE-specific dense linear algebra, mixed-precision algorithms, and asynchronous compute-communication.

The 2023 ACM Gordon Bell Prize-winning team writes, "We demonstrate a paradigm shift in DFT that not only provides an accuracy commensurate with QMB methods in ground-state energies, but also attains an unprecedented performance of 659.7 PFLOPS (43.1% peak FP64 performance) on 619,124 electrons using 8,000 GPU nodes of Frontier supercomputer."

The Frontier supercomputer, located at the Oak Ridge National Laboratory in Oak Ridge, Tennessee, is the world's first and fastest exascale supercomputer. It can perform a quintillion (a billion billion) operations per second. When Frontier came online in 2022, it was 2.5 times faster than the world's second most powerful supercomputer.

The ACM Gordon Bell Prize tracks the progress of parallel computing and rewards innovation in applying high-performance computing to challenges in science, engineering, and large-scale data analytics. The award was presented during the International Conference for High-Performance Computing, Networking, Storage and Analysis (SC23), which was held in Denver, Colorado.

About ACM

ACM, the Association for Computing Machinery is the world's largest educational and scientific computing society, uniting computing educators, researchers, and professionals to inspire dialogue, share resources and address the field's challenges. ACM strengthens the computing profession's collective voice through strong leadership, promotion of the highest standards, and recognition of technical excellence. ACM supports the professional growth of its members by providing opportunities for life-long learning, career development, and professional networking.

About the ACM Gordon Bell Prize

The ACM Gordon Bell Prize is awarded each year to recognize outstanding achievement in high-performance computing. The purpose of this recognition is to track the progress over time of parallel computing, with particular emphasis on rewarding innovation in applying high-performance computing to applications in science. The prize is awarded for peak performance as well as special achievements in scalability and time-to-solution on important science and engineering problems and low price/performance. Financial support for the $10,000 awards is provided by Gordon Bell, a pioneer in high-performance and parallel computing.

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