NEWS RELEASE

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Using the World's Fastest Exascale Computer, ACM Gordon Bell Prize-Winning Team Presents Record-Breaking Algorithm to Advance Understanding of Chemistry and Biology

High Performance Computing Innovation Breaks Million-Electron and 1 EFLOP/s Barrier

Atlanta, GA, November 21, 2024 – ACM, the Association for Computing Machinery, named an eight-member team drawn from Australian and American institutions as the winner of the 2024 ACM Gordon Bell Prize for the project, "Breaking the Million-Electron and 1 EFLOP/s Barriers: Biomolecular-Scale *Ab Initio* Molecular Dynamics Using MP2 Potentials."

The members of the team are Ryan Stocks, Jorge L. Galvez Vallejo, Fiona C.Y. Yu, Calum Snowdon, Elise Palethorpe (all of Australian National University); Jakub Kurzak (Advanced Micro Devices, Inc.); Dmytro Bykov (Oakridge National Laboratory); and Giuseppe M.J. Barca (University of Melbourne).

Molecular dynamics is a computer simulation method that has been developed to better understand the movements of atoms and molecules within a system. Among the different approaches taken are *Ab Intio* (or first principles) calculations, whereby scientists use what is known of the fundamental laws of nature to develop the algorithms they run on computers.

Accurate simulations of the properties of molecules and atoms (as well as how they interact) can lead to a wide range of societal benefits, including developing therapeutic drugs, producing biofuels, recycling plastics, and engineering medical biomaterials.

Although the use of computers for performing molecular dynamics simulations goes back several decades, many traditional approaches have been limited by the accuracy of the force fields (computational models computer scientists develop to describe the forces between atoms and molecules). These limits have undermined the accuracy of the resulting simulations.

While other approaches such as quantum mechanical methods have delivered the desired accuracy, they were not able to scale on powerful supercomputers to model the thousands of atoms within a biosystem.

To address this challenge, the Gordon Bell Prize-winning team developed a new technique combining methods called *molecular fragmentation* and *MP2 perturbation theory*.

Using their algorithmic innovations on a powerful exascale computer, the team was able to achieve a record-breaking performance of simulating more than one million electrons for a computational chemistry application, and to scale their algorithm to an EFlop/s (processing a quintillion calculations per second). The Gordon Bell Prize-winning team's resulting simulation is 1,000 times larger in system-size than the existing state-of-the-art, and was processed 1,000 times faster than any previous model.

The Gordon Bell Prize-winning team performed several Ab Initio Molecular Dynamics (AIMD) time steps on a molecular cluster with over two million electrons utilizing 9,400 nodes on the Frontier exascale supercomputer, significantly larger than any previous AIMD or static energy and/or gradient calculation at a comparable level of accuracy. These calculations achieve 1006.7 PFLOP/s providing a throughput efficiency of 59% of attainable FP64 peak on 99.9% of the machine. In addition, the team demonstrated low time step latency of 3.4 s/timestep on a protein fragment with 1,496 atoms and over 5,500 electrons attaining a simulation throughput of 25,000 time steps per day on 1,024 nodes of Perlmutter.

In their paper, the 2024 ACM Gordon Bell Prize-winning team claims, "This leap forward is not merely incremental; it redefines the boundaries of what is computationally feasible in molecular dynamics, setting a new benchmark for accuracy and efficiency in large-scale simulations. The enhanced scalability and accuracy of our simulation techniques empowers the scientific community to tackle longstanding challenges in both chemistry and biology."

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. As of November 2024, Frontier is ranked as the world's second most powerful supercomputer. The Perlmutter supercomputer is housed at the (US) National Energy Research Scientific Computing Center (NERSC). It is used primarily in applications including climate analysis, quantum information science, clean energy technologies, as well as semiconductors and microelectronics. As of November 2024, it is ranked as the world's 19th 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 (SC24), which is being held November 17 – 22 in Atlanta, Georgia.

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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