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NEWS RELEASE

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2020 ACM GORDON BELL PRIZE AWARDED TO TEAM FOR MACHINE LEARNING METHOD THAT ACHIEVES RECORD MOLECULAR DYNAMICS SIMULATION

New Tool Simulates Interactions of 100 Million Atoms

New York, NY, November 19, 2020 – ACM, the Association for Computing Machinery, named a nine-member team, drawn from Chinese and American institutions, recipients of the 2020 ACM Gordon Bell Prize for their project, "Pushing the limit of molecular dynamics with *ab initio* accuracy to 100 million atoms with machine learning."

Winning team members include Weile Jia, University of California, Berkeley; Han Wang, Institute of Applied Physics and Computational Mathematics (Beijing, China); Mohan Chen, Peking University; Denghui Lu, Peking University; Lin Lin, University of California, Berkeley and Lawrence Berkeley National Laboratory; Roberto Car, Princeton University; Weinan E, Princeton University; and Linfeng Zhang, Princeton University.

The famed physicist Richard Feynman once said, "If we were to name the most powerful assumption of all, which leads one on and on to an attempt to understand life, it is that all things are made of atoms, and that everything that living things do can be understood in terms of the jiggling and wiggling of atoms." Molecular dynamics (MD) is a computer simulation method that analyzes how atoms and molecules move and interact during a fixed period of time. MD simulations allow scientists to gain a better sense of how a system (which could include anything from a single cell to a cloud of gas) progresses over time. Practical applications of molecular dynamics include studying large molecules such as proteins for drug development.

Ab initio (meaning in Latin "from the beginning" or "from first principles") Molecular Dynamics (AIMD) is an approach that differs slightly from Standard Molecular Dynamics (SMD) in how interatomic forces are calculated during the simulation. The level of precision that can be gained through AIMD has made it the preferred simulation method of scientists for more than 35 years. At the same time, while AIMD allows for greater accuracy, the approach requires more computation—and has therefore been limited to the study of small-sized systems (systems that have a maximum size of thousands of atoms).

In their Gordon Bell Prize-winning paper, the team introduced Deep Potential Molecular Dynamics (DPMD). DPMD is a new machine learning-based protocol that can simulate a more than 1 nanosecond-long trajectory of over 100 million atoms per day. While other machine learning-based protocols have been introduced for MD simulations in recent years, the authors contend that their protocol achieves the first efficient MD simulation of 100 million atoms with *ab initio* accuracy.

As the Gordon Bell Prize recognizes achievement in high performance computing, finalists must demonstrate that their proposed algorithm can scale (run efficiently) on the world's most powerful supercomputers. The team developed a highly optimized code (GPU Deep MD-Kit), which they successfully ran on the Summit supercomputer. The team's GPU Deep MD-Kit efficiently scaled up to the entire Summit supercomputer, attaining 91 PFLOPS (1 PFLOP = 1 quadrillion floating operation points per second) in double precision (45.5% of the peak) and 162/275 PFLOPS in mixed-single/half precision.

The Summit supercomputer, developed by IBM for the (US) Oak Ridge National Laboratory, was the first supercomputer to reach exaflop speed (1 quintillion operations per second), and was the world's fastest supercomputer from November 2018 to June 2020.

In the abstract of their paper, the Gordon Bell Prize winning team wrote, "The great accomplishment of this work is that it opens the door to simulating unprecedented size and time scales with *ab initio* accuracy. It also poses new challenges to the next-generation supercomputer for a better integration of machine learning and physical modeling."

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 today by ACM President Gabriele Kotsis and Bronis de Supinski, Chair of the 2020 Gordon Bell Prize Award Committee, during the International Conference for High Performance Computing, Networking, Storage and Analysis (SC20), which was held virtually for the first time.

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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