



Association for  
Computing Machinery

*Advancing Computing as a Science & Profession*

## NEWS RELEASE

**Contacts:** Jim Ormond  
212-626-0505  
[ormond@acm.org](mailto:ormond@acm.org)

### **First ACM Gordon Bell Special Prize for High Performance Computing-Based COVID-19 Research Awarded**

**New York, NY, November 19, 2020** – The 2020 [ACM Gordon Bell Special Prize for High Performance Computing-Based COVID-19 Research](#) was presented to a 12-member team for their project “AI-Driven Multiscale Simulations Illuminate Mechanisms of SARS-CoV-2 Spike Dynamics.” The Prize is being awarded in 2020 and 2021 to recognize outstanding research achievement toward the understanding of the COVID-19 pandemic through the use of high performance computing (HPC).

In their paper, the winning team develops a generalizable AI-driven workflow that leverages heterogeneous HPC resources to explore the time-dependent dynamics of molecular systems. They use this workflow to investigate the mechanisms of infectivity of the SARS-CoV-2 spike protein, the main infection machinery of the virus.

Their workflow enables more efficient investigation of spike dynamics in a variety of complex environments, including within a complete SARS-CoV-2 viral envelope simulation that contains 305 million atoms and shows strong scaling on Oakridge National Laboratory’s Summit supercomputer using nanoscale molecular dynamics (NAMD) software.

The team presents several novel scientific discoveries, including the elucidation of the spike’s full glycan shield, the role of spike glycans in modulating the infectivity of the virus, and the characterization of the flexible interactions between the spike and the human ACE2 receptor. They also demonstrate how AI can accelerate conformational sampling across different systems and pave the way for the future application of such methods to additional studies in SARS-CoV-2 and other molecular systems.

The winning team was recognized today at [The International Conference for High Performance Computing, Networking, Storage, and Analysis \(SC20\)](#), which was held this year as a virtual event. The prize-winning paper will also be published in *The International Journal of High Performance Computing Applications (IJHPCA)*.

A cash prize in the amount of \$10,000 accompanies the award, which was conceived and funded by Gordon Bell, a pioneer in high performance computing and researcher emeritus at Microsoft Research.

Winning team members include Rommie Amaro, University of California, San Diego; Arvind Ramanathan, Argonne National Laboratory; Tom Gibbs, NVIDIA; John Stone, University of Illinois at Urbana-Champaign; Jim Phillips, University of Illinois at Urbana-Champaign; Lillian Chong, University of Pittsburgh; Lorenzo Casalino, University of California, San Diego; Abigail Dommer, University of California, San Diego; David Hardy, University of Illinois at Urbana-Champaign; Julio Maia, University of Illinois at Urbana-Champaign; Thorsten Kurth, NVIDIA; and Shantenu Jha, Rutgers University.

### **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.

# # #