Researcher sets record for quantum chemistry calculation

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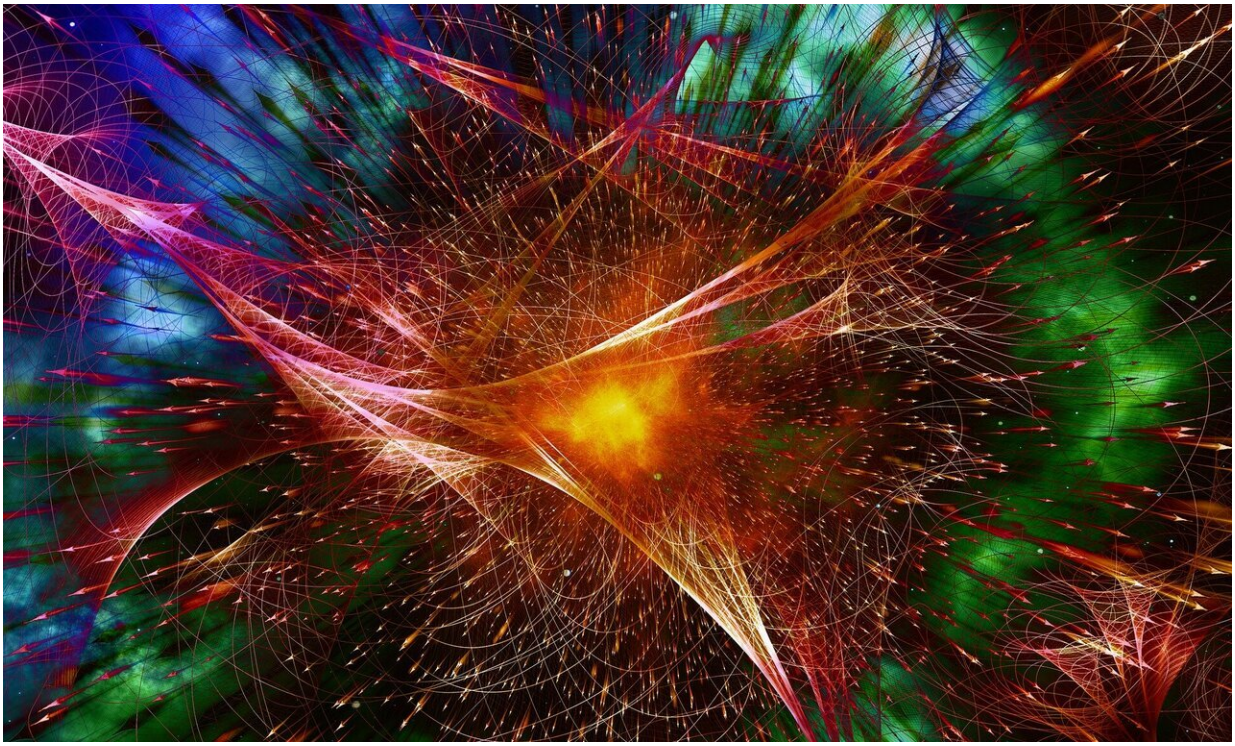

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A researcher from The Australian National University (ANU) has used one of the most powerful supercomputers in the world to predict the quantum mechanical properties of large molecular systems with an accuracy that surpasses all previous experiments.

Calculations of this type have the potential to solve important problems in energy generation, fuel production, water purification, and the manufacturing of medicines, foods, textiles, and consumer goods.

By running his new algorithms on the Summit supercomputer at the Oak Ridge National Lab in the U.S., Dr. Giuseppe Barca has broken the world record for the largest Hartree-Fock calculation ever performed, setting new standards in High-Performance Computing.

The Hartree-Fock method helps determine the electronic structure and the energy of a quantum mechanical molecular system.

The calculation ran for just over half an hour using 26,268 NVIDIA V100 Graphics Processing Units (GPUs) and simulated 20,063 water molecules at a resolution never before possible.

"The new algorithm brings quantum mechanical to the next level in terms of molecular sizes, enabling us to reach scales so large they belong to the domains of biology," Dr. Barca said.

"Such computational predictions open entirely new research horizons in areas where experiments are too expensive or simply impracticable. This result sets the benchmark for comparison for years to come."

Professor Sean Smith, director of the National Computational Infrastructure said the scale of the calculation was "massive."

"GPUs are computationally more powerful and energy-efficient than CPUs, but much more difficult to harness. Using tens of thousands of GPU cores with such efficacy is a computational grand challenge."

The research will be presented at the upcoming Supercomputing 2020 Conference, the preeminent event on the High-Performance Computing

calendar.

More information: Barca et al., Scaling the Hartree-Fock Matrix Build on Summit . *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis* (2020). DOI: 10.5555/3433701.3433808