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SDSC's Trestles Supercomputer Speeds Clean Energy Research

Harvard-based Project Aims to Create Cheap, Efficient Organic Solar Cells

Energy Project team at Harvard University. From left berto Olivares-Amaya, Suleyman Er, Johannes , and Alán Aspuru-Guzik. Image courtesy of CEP.

A team of Harvard University researchers has been allocated time on the *Trestles* supercomputer at the San Diego Supercomputer Center (SDSC) at the University of California, San Diego to perform computational calculations with the goal of creating the next generation of organic solar cells as an inexpensive and efficient source of energy.

The allocation is a key part of the team's efforts to conduct larger, data-intensive computations related to its Clean Energy Project (CEP), which combines the group's computational chemistry expertise with the large, distributed computing power of IBM's World Community Grid (WCG).

Specifically, the CEP combines theory, computation, experiments, and grid computing by harvesting idle computing time from donors around the world using the WCG to perform *ab initio* computational quantum chemistry calculations on a large number of candidate molecules that could potentially form the next generation of solar cells. The complete CEP database will soon be made publicly available to the scientific community.

Despite the success of the CEP – more than 6 million molecular motifs of potential interest have been characterized and thousands of new molecules are being added to its database every day – the program's research of larger, more complex datasets has been limited because

the majority of WCG compute resources consist of home or office PCs and are on public networks, which create issues such as hardware heterogeneity, data transfer speeds, and tailoring of computing times according to the needs and interests of donors.

Enter SDSC's *Trestles* system, a resource for modest-scale researchers who need to be as computationally productive as possible. Alán Aspuru-Guzik, an associate professor with Harvard University's Department of Chemistry and Chemical Biology and head of the CEP initiative, was allocated more than 1.36 million service units, or core-hours, on *Trestles* through the National Science Foundation's (NSF) Extreme Science and Engineering Discovery Environment, or XSEDE program, to perform these high-volume computations.

"*Trestles* allowed us to perform calculations on larger molecular systems that are difficult to calculate elsewhere," said Aspuru-Guzik. "We were able to perform more complex calculations of systems with more than 300 electrons, which are currently impossible to run on smaller systems. As well as large molecules, the computing power of *Trestles* let us gather most interesting and promising candidate molecules at a higher level of theory, resulting in a much improved molecular characterization of those systems of interest."

"*Trestles* is targeted to users such as Dr. Aspuru-Guzik, who have a large number of long-running, modest core-count jobs," said Richard Moore, SDSC deputy director and head of SDSC's data-enabled scientific computing program. "Our ability to provide flexible scheduling without long wait times enables XSEDE users to increase their research productivity."

The ultimate goal of Aspuru-Guzik's research is to reduce global dependency on fossil fuel-based economies by developing renewable energy-related technologies such as organic photovoltaics to provide inexpensive solar cells, polymers for the membranes used in fuel cells for electricity generation, and how best to assemble the molecules to make those devices.

"Solar cells are environmentally friendly but still very expensive investments," said Aspuru-Guzik. "Highly engineered materials are needed, as well as novel designs for solar cells and fuel cells based on organic molecules, which often require compounds with very specific characteristics to efficiently capture and/or storage energy. To make them cost-competitive and more widely accessible, we need new, inexpensive materials that perform better than existing technologies."

Solar cells built from organic compounds also have the potential of being inexpensive, non-hazardous, lightweight, and semi-transparent. Moreover, they can be easily processed and molded into any desired shape. But synthesizing organic molecules and characterizing them in

a lab has been a difficult and time-consuming task, and only a few examples can be experimentally studied per year.

The data-intensive computational runs on SDSC's *Trestles* are just one part of a larger effort to develop a broad database for the CEP during the next several months. Aspuru-Guzik and his team then plan to analyze the data for high-performance materials that could potentially lead to new energy technologies.

"Our challenge is to find the right class of molecules that absorb a broad spectrum of sunlight, and efficiently convert it into an easily usable form of energy, such as electricity," said Suleyman Er, a postdoctoral research fellow at Harvard University and a member of Aspuru-Guzik's team. "The CEP database provides on-demand access to specific compounds with a wide range of desired properties and electronic structures, but more powerful systems such as *Trestles* will both increase the speed and expand the scope of our research going forward, and our findings will be appreciated in many other fields of organic electronics."

Additional CEP researchers include Sule Atahan-Evrenk, Roberto Olivares-Amaya, and Johannes Hachmann, postdoctoral research fellows at Harvard University, as well as Supriya Shrestha and Leon Liu, graduate students at Harvard. In addition to Harvard University and IBM's WCG, the CEP is supported by the Stanford Global Climate and Energy Project (GCEP), and Molecular Networks GmbH, of Erlangen, Germany.

For a list of current CEP-related publications, please visit http://aspuru.chem.harvard.edu/the-clean-energy-project/.

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