Lab collaborates to prepare photovoltaic materials research for exascale

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A new guide outlines the correct procedures for measuring solar cell efficiency. Image credit: Wikimedia Commons CC BY 3.0

Photovoltaic solar cells are a promising alternative to fossil fuels, but they need to be a lot more efficient before they can go into widespread use. Scientists have pushed current supercomputing power to the limit looking for that improved efficiency, but the arrival of exascale computing within the next few years will allow them to take this quest to the next level.

Toward this end, researchers from Berkeley Lab's Computational Research Division (CRD) and the National Energy Research Scientific Computing Center (NERSC) are collaborating with Carnegie Mellon and a number of other academic institutions to prepare to use the nation's first exascale computer next year to continue the search for new, more efficient photovoltaic solar cell materials. The project will combine analytical simulation with machine learning and data mining to discover new materials.

The collaboration is using software developed by Berkeley Lab scientists to predict excitation properties in potential photovoltaic solar cell materials. The software, BerkeleyGW, is a materials science simulation package that can predict the excited-state properties of materials, which is how a material responds to a stimulant such as a photon coming into it. BerkeleyGW is considered one of the most accurate quantum mechanical simulations for data acquisition.

"While the GW computational approach implemented in BerkeleyGW is highly accurate, it was often considered expensive in terms of computer time required to run the code," says Jack Deslippe, a NERSC group lead and a principal developer of the BerkeleyGW code. "For this collaboration, our team has optimized BerkeleyGW so that it is not only an accurate predictive tool but also scales to peak performance on modern architectures, which allows researchers to analyze up to several thousands of atoms—something that was previously impossible."

Solar cells convert photons from the sun into electricity by absorbing photons and generating a current of electrons. Usually one photon is converted into one electron. The Carnegie Mellon collaboration is looking for materials that can undergo singlet fission, a process by which one photo-generated singlet exciton photon is converted into two triplet excitons, increasing the current being released. The goal of the research is to find the rare materials that can undergo single fission to improve solar cell efficiency.

Attempting to find these types of materials experimentally is an impossible task—researchers liken it to finding a needle in a haystack. "But we can simulate these material properties, use computation to perform screening of the possibilities and pick what we think are the best candidates, then send them to the lab for testing," says Mauro Del Ben, a CRD research scientist who has been working on the BerkeleyGW code. "Since we are looking for excited states in these materials, we need a level of accuracy that goes beyond what's currently available, and that's where BerkeleyGW comes in."

The computational cost is still steep, but improving code performance can help lessen the load. By optimizing parallelization and exploiting accelerators such as GPUs, BerkeleyGW can tackle in just a few nodes computations that previously took thousands of nodes. The research is currently being done on the Theta supercomputer at Argonne National Laboratory, Cori at NERSC, and Summit at Oak Ridge National Laboratory, at present the most powerful supercomputer in the world.

The first exascale supercomputer is scheduled to arrive at Argonne National Laboratory in 2021. The Carnegie Mellon team is aiming to optimize workflows so their research will be ready to run on the new exascale system.

If the project is successful, it could be used as a template for any kind of machine learning, data-driven discovery of new materials in different fields, setting a standard for what can be used in the future for more applications, says Del Ben.

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