20 Years of Excellence in Computational Science

OLCF

Oak Ridge Leadership Computing Facility

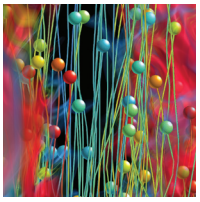
1992–2012

The Center for Accelerated Application Readiness

The Oak Ridge Leadership Computing Facility (OLCF) is working with six world-class applications to demonstrate the promise of hybrid supercomputing and prepare for the arrival this fall of the Titan system. The OLCF's Center for Accelerated Application Readiness (CAAR) has gathered application developers to work with experts from the OLCF, computer maker Cray and GPU manufacturer NVIDIA. Together, they are identifying the most effective strategies for working with Titan in 2013 in particular and hybrid systems in general.

As these teams have discovered, GPUs can revolutionize computational science when they are used as accelerators with CPUs. Below is a brief discussion of the CAAR applications, what they can accomplish without GPUs (today on OLCF's 3.3 petaflop Jaguar system), and what they will be able to accomplish when Titan has enough NVIDIA GPU accelerators to bring it to 20 petaflops.

1. Combustion with S3D



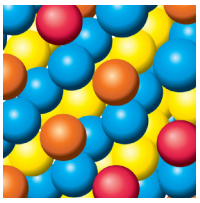
S3D performs direct numerical simulation of fuels burning under highly turbulent conditions.

Without GPUs. S3D will directly simulate compression ignition while resolving features down to 5 microns. These simulations model the burning of syngas, a mix of carbon monoxide and hydrogen that burns more cleanly than coal.

Accelerated to 20 PF. S3D will move beyond simple fuels such as hydrogen, syngas, and hydrocarbon fuels (with up to four carbons). It will tackle far more complex, larger-molecule hydrocarbon fuels such as isooctane (a surrogate for gasoline), commercially important oxygenated alcohols such as ethanol and butanol, and biofuel surrogates (a blend of methyl butanoate, methyl decanoate, and n-heptane.)

Why we care. Three-quarters of the fossil fuel used in the United States goes to cars and trucks, which produce one-quarter of the country's greenhouse gases. Advances in fuel efficiency and alternative-fuel engines benefit national security and the environment.

2. Magnetic systems with WL-LSMS



WL-LSMS analyzes magnetic materials at the nanoscale, allowing researchers to directly and accurately calculate, for example, the temperature above which a material loses its magnetism.

Without GPUs. WL-LSMS can calculate the thermodynamics of magnetic states as a function of temperature.

Accelerated to 20 PF. WL-LSMS will improve calculations of a material's thermodynamics (e.g., the magnetism and its entropy at a given temperature) or calculate the underlying magnetic states (ground states) with greatly reduced margins of error than is currently unavoidable.

Why we care. Magnetism at the atomic scale plays an important role in many industrial materials, including steels and iron-nickel alloys, while lightweight-yet-strong permanent magnets are important components in highly efficient electric motors and generators. Small improvements in the performance of these materials will directly result in more competitive industries and greater energy efficiency.

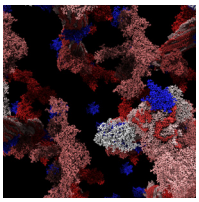
Oak Ridge National Laboratory

U.S. Department of Energy

Office of Science

Contact:
Oak Ridge Leadership Computing Facility
Oak Ridge National Laboratory
P: 865-241-7202
F: 865-241-2850
E: help@olcf.ornl.gov
www.olcf.ornl.gov

3. Biophysical science with LAMMPS



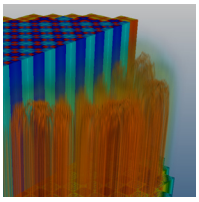
LAMMPS explores bioenergy using molecular dynamics, modeling problems such as membrane fusion, large biomolecular simulations for proteins, and lignocellulose for biofuels.

Without GPUs. For electrically charged systems in which computationally demanding, long-range interactions are treated properly, this system can simulate barely 100,000 atoms.

Accelerated to 20 PF. LAMMPS will be able to overcome size limitations on systems with charged particles, expanding to millions of atoms.

Why we care. This will advance the search for more efficient, economical methods for converting woody plants into biofuel. LAMMPS will advance protein modeling, which in turn opens new opportunities for understanding disease and improving medical treatments such as targeted drug delivery.

4. Nuclear reactors with Denovo



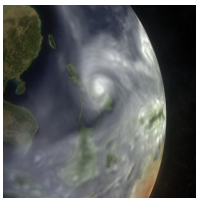
Denovo models and simulates neutron transport for nuclear engineering. It is used in areas such as reactor fuel core analysis, radiation shielding, nuclear forensics, and radiation detection.

Without GPUs. Denovo can simulate a fuel rod through one round of use in a reactor core using 60 hours of wall clock time on the full Jaguar system.

Accelerated to 20 PF. The application will be able to do this simulation using 13 hours of wall clock time.

Why we care. Nuclear power provides abundant, reliable, and emission-free electricity. For it to be effective, though, safety must be guaranteed, and the volume of radioactive waste must be reduced (e.g., by burning the fuel longer in the reactor). Denovo is a powerful tool for ensuring the safe and efficient operation of today's nuclear power plants.

5. Climate change with CAM-SE



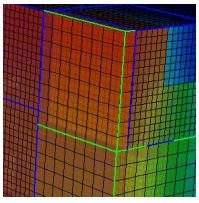
The Community Atmosphere Model–Spectral Element simulates long-term global climate to inform public policy and improve scientific understanding of climate changes.

Without GPUs. The application can simulate our atmosphere on a grid with 14-kilometer cells at a quarter of a simulated year per day of computation.

Accelerated to 20 PF. The application will be able to increase the simulation speed to between one and five years per computing day. The increase in speed is needed to make ultra-high-resolution, full-chemistry simulations feasible over decades and centuries and would allow researchers to quantify uncertainties by running multiple simulations.

Why we care. Improved atmospheric modeling will help climate researchers better understand future air quality as well as the effect of particles suspended in the air. The indirect effects of particles are large sources of uncertainty regarding the climate's response to natural and human effects.

6. Radiation transport and advanced algorithms with NRDF



The Non-Equilibrium Radiation Diffusion application models the journey of noncharged particles. It is also a testbed for advanced computing techniques that enable applications to focus computing power only on critical areas of a simulated system and thereby solve larger problems.

Why we care. NRDF has applications in, for example, astrophysics, nuclear fusion, and atmospheric radiation, while the algorithms being developed should prove valuable in many other areas, such as fluid dynamics, radiation transport, groundwater transport, nuclear reactors, and energy storage.