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Could 135,000 Laptops Help Solve the Energy Challenge?

U.S. Energy Secretary Steven Chu has just announced the largest ever awards of the Department's supercomputing time to 57 innovative research projects -- using computer simulations to perform virtual experiments that in most cases would be impossible or impractical in the natural world. Utilizing two world-leading supercomputers with a computational capacity roughly equal to 135,000 quad-core laptops, the research could, for example, help speed the development of more efficient solar cells, improvements in biofuel production, or more effective medications to help slow the progression of Parkinson's disease.

The projects include both academic and commercial research, including partnerships with companies such as GE and Boeing to use sophisticated computer modeling in the development of better wind turbines and jet engines.

Specifically, the Department is awarding time on two of the world's fastest and most powerful supercomputers -- the Cray XT5 ("Jaguar") at Oak Ridge National Laboratory and the IBM Blue Gene/P ("Intrepid") at Argonne National Laboratory. Jaguar's computational capacity is roughly equivalent to 109,000 laptops all working together to solve the same problem. Intrepid is roughly equivalent to 26,000 laptops.

The awards include nearly 1.7 billion processor hours on the Department of Energy's advanced supercomputers -- the largest total ever -- reflecting both the growing sophistication of the field of computer modeling and simulation and the rapid expansion of supercomputing capabilities at DOE National Laboratories in recent years.

Awarded under the Department's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program, many of the new and continuing INCITE projects aim to further renewable energy solutions and understand of the environmental impacts of energy use. The program, open to all scientists, is supported by the Department's Office of Science and managed by the DOE Leadership Computing Facilities at the Department's Argonne and Oak Ridge National Laboratories, which host some of the world's fastest supercomputers.

INCITE program goals include:

- Illuminating the roles of ocean, atmosphere, land, and ice in climate change
- Advancing materials for lithium air batteries, solar cells, and superconductors
- Understanding how turbulence affects the efficiency of aircraft and other transportation systems
- Designing next-generation nuclear reactors and fuels and extending the life of aging reactors
- Developing fusion energy systems
- Improving combustion in fuel-efficient, near-zero-emissions systems
- Exploring carbon sequestration

Projects were selected on a competitive, peer review basis and evaluated for computational readiness. Selected projects were chosen for their potential to advance scientific discoveries, speed technological innovations, and strengthen industrial competitiveness and for their ability to make use of hundreds of thousands of processors to work in concert to do so. More than half of the projects are led by university researchers, with the remainder of the awards going to government and industry scientists and engineers.

Several awards -- from improving battery technology to better understanding Parkinson's Disease -- are profiled below in brief summaries.

Simulating Treatment for Parkinson's Disease

Principal Investigator: Igor Tsigelny, University of California -- San Diego Researchers will use the Intrepid supercomputer to learn more about Parkinson's disease and explore ways to treat it. As the second most common neurological disorder in adults, the personal and economic impacts of Parkinson's disease are enormous. Through computational modeling, the research team will study various mutations of the disease. These findings will provide a test bed for identifying possible healing interventions for treating the disease and could halt the progression of Parkinson's as well as other similar conditions.

Transporting Hazard Explosives Safely

Principal Investigator: Martin Berzins, University of Utah The research team will utilize the Jaguar supercomputer to examine different packing arrangements of commercial explosives in order to prevent a violent blast. The driving force for this research was a 2005 semi-truck accident on U.S. Route 6 in Utah in which 36,000 lbs of explosives used for mining and seismic exploration were ignited and detonated, destroying a highway and railway. Since thousands of pounds of explosives are transported across the U.S. daily, researchers will examine different packing arrangements of devices to ensure the safe transport of materials for public safety.

Understanding the Ultimate Battery Chemistry: Rechargeable Lithium/Air

Principal Investigator: Jack Wells, Oak Ridge National Laboratory Utilizing both the Jaguar and Intrepid supercomputers, the research consortium will study and demonstrate a working prototype of a rechargeable Lithium/Air battery. The Lithium/Air battery can potentially store ten times the energy of a Lithium/Ion battery of the same weight. Realizing this enormous potential is a very challenging scientific problem. If successful, this will enable rechargeable batteries that compete directly with gasoline, making fully electric vehicles practical and widespread.

Hydrogen as Alternative Fuel -- Simulation

Principal Investigator: John Bell, Lawrence Berkeley National Laboratory Hydrogen is a clean fuel that, when consumed, emits only water and oxygen making it a potentially

promising part of our clean energy future. Researchers will use the Jaguar supercomputer to better understand how hydrogen and hydrogen compounds could be used as a practical fuel for producing power and heat.

Simulating Blood Clots in the Brain to Prevent Aneurysms

Principal Investigator: George Karniadakis, Brown University Researchers will use the Intrepid supercomputer to conduct multi-scale simulations for modeling blood flow in human brain blood vessels to better predict and understand the rupture of aneurysms, sickle cell anemia and cerebral malaria.

Simulating Large Regional Earthquakes

Principal Investigator: Thomas H. Jordan, University of Southern California, The research team will utilize the Intrepid supercomputer to analyze earthquake-wave-simulations of large-scenario (Mw7.0+) earthquakes at frequencies above 1Hz on a regional scale. Using a realistic 3-D structural model of Southern California, these simulations will help geoscientists better understand the characteristics of large-magnitude events in this region, including the duration and distribution of strong ground motions at different frequencies to enable structural engineers to develop buildings that can withstand such frequencies.

Modeling Nuclear Reactors for Electrical Power

Principal Investigator: Thomas Evans, Oak Ridge National Laboratory Utilizing the power of the Jaguar supercomputer, the research team will study the power distribution in a boiling water reactor, a type of nuclear reactor used for the generation of electrical power. By using novel computational tools researchers will focus on improving performance of both current and next-generation reactors potentially saving millions of dollars, through increased power efficiency and a reduction in fuel failures.

Full listing of awards available at

http://www.energy.gov/news/documents/2011_INCITE_Fact_Sheets.pdf