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AMES LABORATORY TO SHARE IN \$60 MILLION DOE AWARD MONEY
Funds will Help Advance Computational Chemistry to Accelerate Scientific Discovery

AMES, IA – The U.S. Department of Energy’s Ames Laboratory on the Iowa State University campus is one of 30 recipients nationwide to receive a share of \$60 million in DOE award money for computational science projects over the next three to five years. The projects will accelerate such research efforts as designing new materials, developing future energy sources, studying global climate change, improving environmental cleanup methods and understanding physics from the tiniest particles to the massive explosions of supernovae.

The awards are part of the Scientific Discovery Through Advanced Computing-2, or SciDAC-2, program, sponsored by the DOE Office of Science’s Advanced Scientific Computing Research program. SciDAC-2 will unite some of the nation’s top researchers at DOE national labs and U.S. universities to create the software and infrastructure needed to help scientists effectively utilize the next generation of supercomputers.

“We anticipate that they [the SciDAC projects] will develop and improve software for simulating scientific problems and help reduce the time-to-market for new technologies,” said DOE Under Secretary for Science Raymond Orbach.

The Ames Laboratory SciDAC project is a collaborative effort with Iowa State University and the DOE’s Sandia National Laboratory. Mark Gordon, Ames Laboratory program director of Applied Mathematics and Computational Sciences, will work with ISU chemistry professor Theresa Windus and Sandia’s Curtis Janssen to ease access to three of the world’s most important computational chemistry software codes – the General Atomic and Molecular Electronic Structure System, or GAMESS, (Gordon); the Massively Parallel Quantum Chemistry, or MPQC, program, (Janssen); and Northwest Chem, or NWChem, (Windus).

Gordon, who is also an ISU Distinguished Professor of chemistry, said the Ames Laboratory project will receive approximately \$500,000 per year for three years to develop a means by which users of one of the three computational chemistry codes, for example, GAMESS, could also access the functionalities of NWChem and MPQC. “Each code has very different functionalities, so rather than recode all the components from one code to make it work in another code, the idea is to use something called the Common Component Architecture to allow each code to access the functionalities and components of the other two codes,” explained Gordon.

The Common Component Architecture, or CCA, is language-independent and provides a framework for component-oriented software development in high-performance computing. Gordon and his colleagues will use the CCA to develop interfaces among GAMESS, NWChem and MPQC, allowing scientists to employ all three codes when seeking solutions to DOE challenges such as creating efficient combustion systems with reduced emissions of pollutants; new solar photoconversion processes; improved catalysts for clean and efficient production of fuels and chemicals; and better separations and analytical methods for applications in

energy processes, environmental remediation, and waste management.

“Computational chemistry has become a vital element in the chemist’s toolbox,” said Gordon. “It’s now an equal partner with spectroscopy and other experimental analysis tools. Our goal is to develop the kind of flexible, community-based computing architecture that will make this tool accessible to the broadest possible community and applicable to the widest possible set of problems.”

Ames Laboratory is operated for the DOE by ISU. The Lab conducts research into various areas of national concern, including energy resources, high-speed computer design, environmental cleanup and restoration, and the synthesis and study of new materials. More information about Ames Laboratory can be found at www.ameslab.gov.

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Note: For the DOE Headquarters release on the 30 computational science projects awarded SciDAC-2 funding, go to: <http://www.energy.gov/news/4135.htm>.