SDSC joins the Intel Parallel Computing Centers program

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The San Diego Supercomputer Center (SDSC) at the University of California, San Diego, is working with semiconductor chipmaker Intel Corporation to further optimize research software to improve the parallelism, efficiency, and scalability of widely used molecular and neurological simulation technologies.

The collaboration is part of the Intel Parallel Computing Centers program, which provides funding to universities, institutions, and research labs to modernize key community codes used across a wide range of disciplines to run on current industry-standard parallel architectures.

Initial research focused on optimization of the PMEMD classical molecular dynamics code, part of the widely used AMBER Molecular Dynamics software, on multi-core Intel® Xeon® processors and "manycore" Intel Xeon Phi processors. This work in the molecular dynamics field is continuing with plans for extension to multi-node Intel Xeon Phi processor-based systems and aggressive optimization.

SDSC researchers are now expanding the Intel relationship to cover additional research areas and software packages. This includes improving the performance of multi-scale Quantum Mechanics / Molecular Mechanics (QM/MM) simulations on manycore architectures, a field that has been largely neglected during earlier software optimization efforts that have focused on purely classical models. QM/MM simulations allow researchers to study chemical reactions

directly, without severe approximations. QM/MM simulations are key to studies in areas such as biocatalysis, where studies to improve the efficiency of bioethanol production is one example.

Efforts will also potentially benefit the field of computational neuroscience with a focus on porting and optimizing the open source NEURON software in collaboration with researchers at Yale University. With President Obama's announcement of the BRAIN initiative in April 2013, many are predicting computational neuroscience will have a scientific impact to rival what computational genomics had during the last decade. The collaboration with Intel places SDSC in a position to have a substantial impact on this field.

"This collaboration gives SDSC researchers the ability to interact directly with Intel engineers, which is extremely valuable when tuning codes for the levels of parallelism that modern processors demand," said SDSC Director Michael Norman. "The AMBER MD software is widely used in fields spanning drug discovery, biocatalysis, and enzyme engineering, and we are grateful to Intel for recognizing the importance of this work across so many domains. Research conducted as part of this project will feedback into the AMBER and NEURON code bases, as well as the molecular dynamics and computational neuroscience research communities at large."

Training and Outreach

The Intel Parallel Computing Center at SDSC will also serve as a conduit for offering courses in parallel programming to researchers and students at UC San Diego, as well as the broader San Diego biotech area.

"SDSC has a proud history of helping to train the scientists of tomorrow, and our work with Intel complements these efforts," said Norman. "All programming going forward will be parallel, so it is crucial that we

educate students on how to do this from the very beginning."

A recent SDSC workshop on Intel Xeon-Phi optimization, for example, was attended by researchers from multiple San Diego based universities as well as a number of local biotech companies.

"SDSC has a strong pedigree of innovation and we're excited to have them join the IPCC program, as well as the opportunity this new IPCC center provides for a long-term, productive collaboration," said Bob Burroughs, director of Technical Computing System Enabling at Intel. "The performance increases we anticipate from SDSC's efforts to modernize these critical codes will have a broad impact on scientific discovery for years to come."

Provided by University of California - San Diego