XSCI

eXtreme Scale Computing Initiative

Initiative Leadership

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Upcoming Events

Date: November 10

Event: XSCI Fault Tolerance Brownbag

Location: PNNL Campus

Date: November 12 - 18

Event: Supercomputing 2011

Location: Seattle, Wash.

Date: December 6

Event: Frontiers in Computational Sciences Lecture Series, Professor Barbara Chapman

Location: PNNL Campus

Pacific Northwest
NATIONAL LABORATORY

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Leadership Notes:

The original XSCI projects that ended at the close of FY11 demonstrated impressive technical progress towards the Initiative's goal to deliver the capabilities to design, implement, and deploy highly scalable application software. The Initiative's focus on the continued development of Global Arrays (GA) and Aggregate Remote Memory Copy Interface (ARMCI) as the programming model for exascale computing; and the design of approaches to take optimal advantage of state-of-the-art heterogeneous computer architectures, has allowed our demonstration science applications - Equation of Motion - Coupled Cluster Singles, Doubles and Perturbative Triples (EOM-CCSD(T)), Plane Wave Density Functional Theory – Ab Initio Molecular Dynamics (PWDFT-AIMD), and Subsurface Transport Over Multiple Phases (STOMP) - to achieve scalability to 100,000 cores or more.

In the coming years the Initiative will continue to build on current accomplishments to strengthen PNNL's leadership position in the development of GA as the critical partitioned global address space programming model for exascale computing. Two integration efforts are planned to target a number of applications for the specific computer architectures used in the next generation of supercomputers at the Leadership Computing Facilities at ORNL and ANL. Applications will be selected to promote the adoption of GA by a wider range of users.

In addition to these "integration" projects that highlight computer science capabilities, two new domain-sciences-related projects will be started. In the molecular science domain, a multi-reference coupled cluster (MR- CCSD(T)) approach will be designed as one of the computationally most demanding methodologies in computational chemistry, with the potential to be a true exascale application. In the subsurface science area, the eSTOMP software will be extended to include well models and new meshing capabilities, and to demonstrate the scientific impact by applying it to tackle carbon sequestration problems that cannot be solved by competing codes.

NVIDIA CUDA Research Center

PNNL is now one of 35 new CUDA Research Centers and CUDA Teaching Centers in 14 countries, further advancing the growth of parallel computing across the world. At PNNL, XSCI is using GPU-acceleration of the subsurface transport simulator STOMP to improve public safety by predicting flow of contaminants into underground waterways, and the computational chemistry simulation code NWChem to address key questions about processes such as photosynthesis, protein function, and combustion. The CUDA Research Center program fosters collaboration at institutions that are expanding the frontier of parallel computing. PNNL will receive early access to limited-availability systems, exclusive event invites with key researchers and academics, and a designated NVIDIA technical liaison.

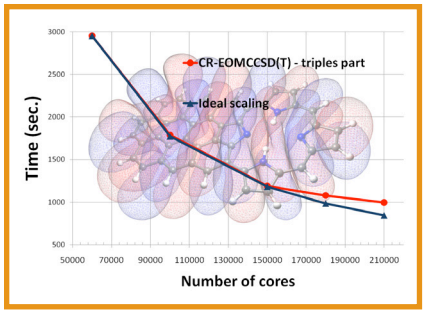
Meet the Team

- » T.P. Straatsma, Molecular Dynamics
- » Abhinav Vishnu, Scalable Fault Tolerance
- » Steven Yabusaki, Subsurface
- » Karol Kowalski, Molecular Modeling
- » Oreste Villa, Architecture Exploration
- » Daniel Chavarria, Performance Optimizations
- » Sriram Krishnamoorthy, Performance Diagnostics
- » Kevin Barker, Power and Performance Modeling
- » Huub Van Dam, Molecular Modeling
- » Bruce Palmer, Functionality & Performance Enhancements

Features of the Quarter: Projects that ended in FY11

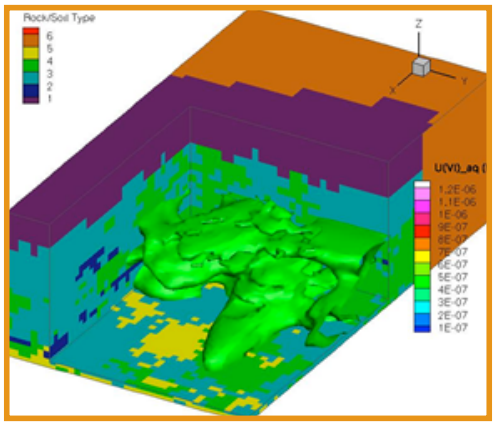
Development of Exascale Algorithms for Molecular Modeling - *PI Karol Kowalski*

The outcomes of this project are computational chemistry algorithms that have been published in scientific literature. The algorithms include scalable, excited-state approaches for exascale molecular simulations; the exascale parallel in-time algorithms (or parareal algorithms) integrated with terascale *ab initio* molecular dynamics and the terascale molecular dynamics programs; and the efficient interface between *ab initio* theories and multiscale; multiphysics simulation modules. With the support from XSCI initiative we published 15 articles in peer-reviewed journals and two book chapters.



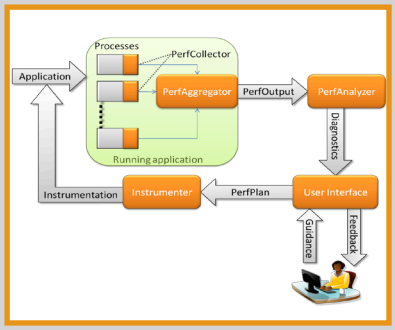
Advanced Scalability for STOMP: Subsurface Simulation and Characterization at Extreme Resolution - *PI Steve Yabusaki*

Successful proposals for time on DOE EMSL Chinook and Oak Ridge Leadership Computing Facility Jaguar led to eSTOMP scaling studies using up to 131,040 processors. eSTOMP was one of four codes selected for the FY11 ASCR Software Metric for Computational Effectiveness to OMB. eSTOMP-CO2 applications included scCO2 injection and entrapment in heterogeneous sandstone formations. Multi-level parallelism using global array processor groups was used for an uncertainty quantification study where the simulation time for 128 realizations of heterogeneous material properties was reduced from weeks to less than one day.



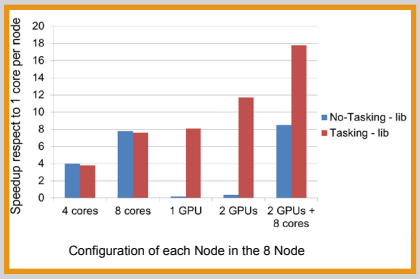
Scalable Performance Diagnostics and Feedback for Massively Parallel Computers - *PI Sriram Krishnamoorthy*

The support for ARMCI in Tuning and Analysis Utilities (TAU) has been strengthened and is now available in the TAU public distribution. The wrappers developed for ARMCI and GA Application Programming Interface (API) is now available for use beyond the initial audience of the project, showing its wider utility. The profiling of NWChem identified the load imbalance cost - due to frequent barriers - in the NWChem CCSD calculation. This motivated the optimization of the iterative coupled cluster methods. The results are part of publications in the Supercomputing 2011 conference proceedings and *Journal of Chemical Theory and Computation*.



Exploring Architectures Suitable for Scientific Applications at Exascale Levels - *PI Oreste Villa*

STOMP is a computer model simulating subsurface flow and transport, specifically designed to provide multidimensional analysis capabilities for modeling subsurface flow and transport phenomena. In this context we have developed a task based library that seamlessly utilizes CPUs and GPUs for the computation of STOMP chemistry reactions. The library uses optimized batching schemes to transfer data In/Out of the GPU memory while overlapping transfers with computation. The overall benefit of this approach gives a speedup of ~18 respects with a single CPU core, by using two GPUs while computing the reactions for 32 species over one million of grid cells.



The XSCI is a quarterly publication covering research being conducted in PNNL's eXtreme Scale Computing Initiative. For more information, contact the initiative leads or visit our web page at *http://xsci.pnnl.gov*.

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Website

http://xsci.pnnl.gov