XSCI

eXtreme Scale Computing Initiative

Initiative Leadership

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Upcoming Events

Date: January 24th @ 1pm

Event: Frontiers in Computational & Information Sciences Lecture Series

Professor Jack Dongarra on "Architecture-Aware Algorithms and Software for Scalable Performance and Resilience on Heterogeneous Architectures"

Location: EMSL Auditorium

Pacific Northwest
NATIONAL LABORATORY

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Leadership Notes

With the XSCI now entering its third year, our research teams are working hard to achieve the milestones on the original projects. Recently, the molecular- science-focused project achieved scalability of the coupled cluster capability beyond 100,000 cores on the Oak Ridge Leadership Computing Facility (OLCF) machine Jaguar. This work was selected for an invited presentation at the International Conference of Computational Methods in Science and Engineering 2010, during a symposium in honor of Josef Paldus and Jiří Čižek, the developers of the original coupled cluster methodology.

The subsurface modeling and simulation code eSTOMP has been selected as one of the application codes for the FY11 ASCR Joule software metric for computational effectiveness. The goal of the ASCR Joule effort is to-within one year-improve the computational science capabilities as defined by the average percentage increase in computational effectiveness. An allocation of computer time and dedicated support from OLCF is available to achieve this goal.

A new activity this year will be a series of brown-bag events where the project teams will present, and, demonstrate their main project accomplishments. The series will start with a presentation by Karol Kowalski in early February on the scalability of the coupled cluster methodology for excited states. Attending these brown-bag meetings is an excellent opportunity to get to know more about the technical objectives and accomplishment of the XSCI research focus areas. For more information or a schedule of upcoming brown-bags, please contact T.P. Straatsma at tps@pnl.gov.

Karol Kowalski

New Projects

» Development of Parallel Multi-Reference Coupled Cluster Capabilities led by **Huub Van Dam**

Meet the Team

T.P. Straatsma, Molecular Dynamics
Abhinav Vishnu, Scalable Fault Tolerance
Steven Yabusaki, Subsurface
Manoj Krishnan, Data Decomposition
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

Feature of the Quarter

Exploring Architectures Suitable for Scientific Applications at Extreme Scale

Next-generation computer architectures have the potential to be part of future exascale-capable supercomputers. Among them, Graphic Processing Units (GPUs) are gaining attention due to their low cost and high-performance-per-watt ratio. Despite that, the gap between the programmability of conventional architectures (CPUs) and GPUs is still large, making the design of complex scientific applications a hard problem that requires heavy modification to the existing implementations. This project is targeting PNNL applications, focusing on performance, programmability, and productivity, primarily on GPU-based clusters.

Motivation: Changing trends in processor design

Power density is the most significant issue toward exascale. Exascale will be possible only if processor power consumption will dramatically decrease. Mainstream architectures are already changing toward this direction.

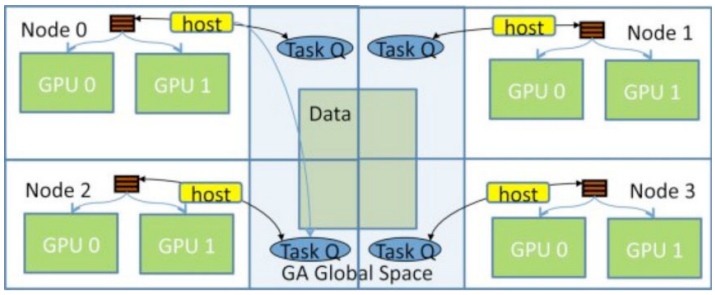
Main Achievements

- Development of an automatic load balancing scheme using task queues in Global Arrays (GA)
- Acceleration of Streamed Tensor Contraction Expressions for NWChem by 10X
- Auto-generation and Auto-tuning of GPU code for Tensor Contraction Engine in NWChem
- Acceleration of DNA analysis applications
- Development of CUDA STOMP via Automatic Code Generation

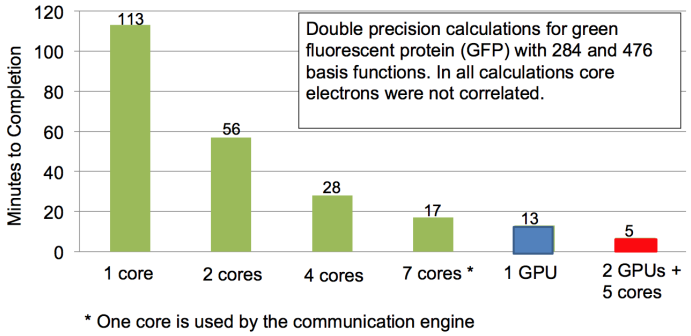
Task-based execution on clusters of GPUs

The automatic load-balancing scheme provides support for automatic balancing applications, such as molecular dynamics, sparse and solvers by using tasks on GA. Tasks can be executed by components that have different hardware capabilities with no impact on the load balancing. It exploits locality by prioritizing tasks with affinity. It also enables forms of fault resiliency by task re-execution on GA "shadow" arrays.

Task based execution on clusters of GPUs



NWChem Coupled Cluster on clusters of GPUs



Results for 60 nodes run (120 Tesla C1070 GPUs)

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.pnl.gov*.

Operational Team

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Website

http://xsci.pnl.gov

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