XSCI

eXtreme Scale Computing Initiative

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Pacific Northwest NATIONAL LABORATORY

eXtreme Scale Computing to Enable Scientific Breakthroughs

The eXtreme Scale Computing Initiative (XSCI), launched by the Pacific Northwest National Laboratory in October 2008, will fund development of next-generation, extreme-scale modeling and simulation capabilities to enable scientific advancements and breakthroughs in new energy technologies, environmental impact, and climate change prediction.

The primary goals of the XSCI initiative are the enhancement and development of scalable methods, algorithms, and software for use in computers magnitudes faster than any available today, and the advancement of existing and emerging codes in application areas where PNNL holds a leadership position to be able to use next-generation massively parallel hardware.

The XSCI is organized into three research and development thrust areas:

Scalable Domain Science Applications, focusing initially on the subsurface sciences and molecular sciences, where PNNL already has substantial modeling and simulation capabilities with codes such as STOMP and NWChem.

Applied Computational Mathematics, focusing on the development, evaluation, and scalable implementation of state-of-the-art solvers and other numerical mathematical methods required by application areas targeted by the XSCI.

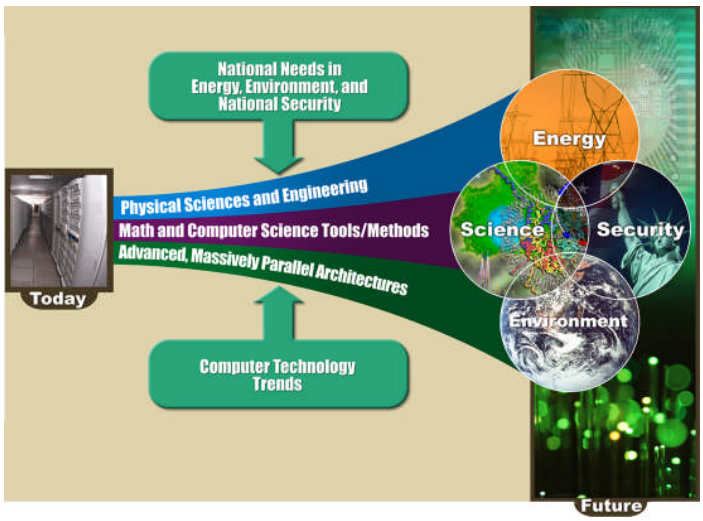
High Performance Computer Science, focusing on development of high performance tools and libraries and validating their effectiveness on massively parallel hardware at PNNL and elsewhere, and on building performance models for extrapolation to peta- and exascale class systems.

An Integrated Approach

The objective and approach of the XSCI is to integrate our computational sciences, computer science, applied mathematics, and scientific data management expertise to enable extreme-scale modeling and simulation to address the major scientific challenges in energy, climate, and the environment. Our focus is on environmental subsurface and molecular sciences as scientific domain areas in which PNNL has a recognized leadership position.

eXtreme Scale Computing Focus Areas

The selection of projects for the XSCI is based on the requirements of existing domain science applications at PNNL with increasing demand for large-scale computational resources. The initial set of projects is focused on developing the computer science and applied mathematics needed to advance the state-of-the-art in subsurface and molecular modeling and simulation. The emphasis is on dramatically improving the scalability of computational kernels in applications, by adopting new software designs and removing scalability bottlenecks. An applied mathematics project is focused on the design of highly scalable solvers, and two computer science projects are performing the verification and evaluation of the effectiveness of these new software designs for emerging



hardware platforms, and development of trace collection and analysis tools to understand performance bottlenecks in applications running at a scale.

Focus Area 1: Scalable Domain Science Applications

Subsurface Modeling

The quantitative prediction through computational modeling and simulation of the movement of fluids and the fate and transport of contaminants in subsurface environments demands an ever increasing availability of high-end computational resources. Developing highly scalable codes for next-generation extreme-scale systems is crucial for addressing a diversity of environmental challenges, including enhanced recovery of hydrocarbons, geologic sequestration of carbon, effective design of subsurface remediation, and accurate assessment of risks associated with subsurface disposal of nuclear wastes. Major advances are needed in our ability to numerically simulate complex hydrologic, geochemical, and microbiological processes of interest, and to accurately characterize spatial and temporal property distributions in the subsurface.

Molecular Modeling

A wide range of molecular processes require highly diversified methodologies to describe systems characterized by different time and spatial scales. The appropriate approach in tackling the majority of these challenges requires incorporating multi-scale multi-physics methods that are built upon basic fundamental solvers. The usability and performance of such combined approaches greatly depends on the scalability and accuracy of the implemented methodologies. This, and the need to enhance modeling and simulation capabilities to physically relevant system sizes and time scales, requires innovative computational techniques designed for next-generation computer architectures.

Focus Area 2: Applied Mathematics

Scalable numerical methods such as equation solvers are the core algorithmic elements that the selected domain applications have in common. Highly scalable implementations of the leading mathematical methods for these specific problem areas require detailed understanding of the problem characteristics, including special and temporal resolution, appropriate handling of nonlinearity, selection and transformation of data structures, providing load balancing as well as other elements necessary to achieve scalability.

Focus Area 3: Computer Science

Tools and Software

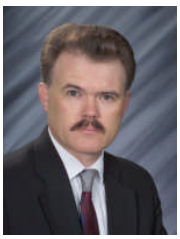
It is critical for developers of scalable implementations of science applications to have reliable performance collection and analysis tools that can be applied to a wide range of application methodologies and computer science algorithms. The initiative is supporting the development of a tool for collection and analysis of communication trace data in parallel programs. It will help diagnose, understand, and remove bottlenecks in applications running on existing hardware, and in some cases predict scalability issues on upcoming massively parallel systems.

Performance on Emerging Architectures

Achieving high performance increasingly depends on a thorough understanding of the underlying computer hardware architectures. It is important to integrate the key features of current and expected future hardware into the design of effective application kernels. A project focused on the specifics of state-of-the-art emerging hardware is investigating merits of using extreme-scale heterogenous computing resources for the XSCI application projects.

Introductions

Dr. Jarek Nieplocha, Initiative Lead, Laboratory Fellow, Ph.D. in Electrical and Computer Engineering, with 20 years of experience in high-performance computing and 10 years in research management.



Dr. T.P. Straatsma, Initiative Lead, Laboratory Fellow, Ph.D. in Mathematics and Natural Sciences, with 25 years of experience in high-performance computational sciences and 10 years in research management.

The XSCI Newsletter is a bi-monthly publication covering research being conducted in PNNL's eXtreme Scale Computing Initiative. For more information, contact the initiative leads or visit our web page http://www.pnl.gov/xsci/.