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The NERSC-8 Cori System

CAMERA: Building New Mathematics for Experimental Science

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ESnet's Network Operating System (ENOS)

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CAMERA: Building New Mathematics for Experimental Science

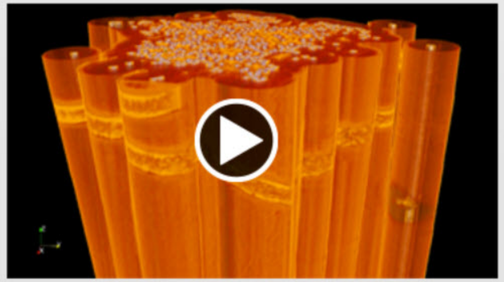
Experimental science is evolving. With the advent of new technology, scientific facilities are collecting data at increasing rates and higher resolution. However, making sense of this data is becoming a major bottleneck. New mathematics and algorithms are needed to extract useful information from these experiments.

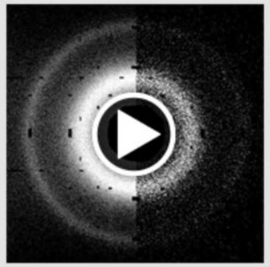
To address these growing needs, the Department of Energy (DOE) invests in the Center for Advanced Mathematics for Energy Research Applications (CAMERA) whose mission is to develop fundamental mathematics and algorithms, delivered as data analysis software that can accelerate scientific discovery.

CAMERA products include new algorithms and software for ptychography (SHARP), grazing incidence shallow angle x-ray scattering (HipGISAXS), reconstruction and analysis of imaged materials (QuantCT and F3D), chemical informatics for analysis of crystalline porous materials (Zeo++), fast methods for electronic structure calculations (PEXSI), nanocrystallography, and fluctuation X-ray scattering.

CAMERA's approach is to assemble teams of applied mathematicians, statisticians, experimental scientists, computational physicists, computer scientists and software engineers. By having a broad range of expertise focused together in one place, the teams are able to reach across traditional boundaries, find a common language, frame experimental data needs in mathematical terms and package mathematical solutions as software usable by the external community.

CAMERA, launched in 2009 as a Laboratory Directed Research and Development program at Lawrence Berkeley National Laboratory. Based on this success, DOE's Office of Advanced Scientific Computing Research and Basic Energy Science jointly invested in CAMERA as a pilot project, and recently awarded it another $10.5 million over three years. This new round of funding will essentially transform CAMERA into a national resource across DOE computational, network and light source facilities.





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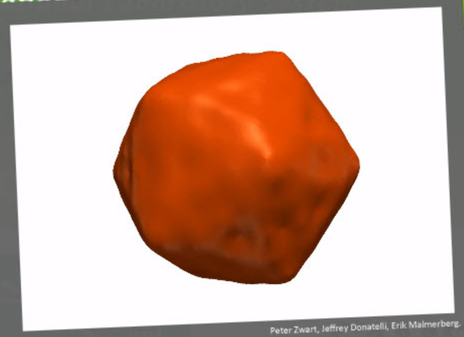


Peter Zwart, Jeffrey Donatelli, Erik Malmerberg.

The structure of the PBCV-1 virus was determined from experimental Fluctuation X-ray Scattering data obtained at the SLAC Linac Coherent Light Source (LCLS), with an algorithm developed by CAMERA researchers. Over 80-thousand diffraction patterns were processed, and resulted in the first structure determination of a virus from experimental Fluctuation X-ray Scattering data of a biological sample. Fluctuation X-ray scattering is a technique currently under development, and will ultimately provide detailed insights in the structure and dynamics of macromolecules in their native environment. The algorithm, called M-TIP, determines the structure from the data, and runs under 5 minutes on a desktop computer. Experimental data was obtained in a multi-institutional collaboration, involving researchers from across the globe.

Donatelli, Zwart & Sethian (2015), PNAS, 112 (33): 10286-10291.

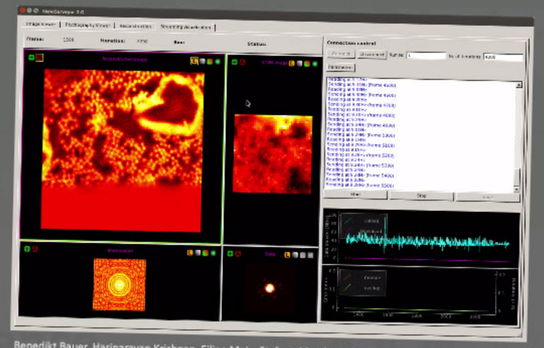
Daniela Ushizima, Dula Parkinson, Talita Perciano, Hari Krishnam, Burlen Loring, Hrishi Bale, Rob Ritchie, Berkeley Lab and UC Berkeley

Applying a combination of pattern recognition techniques, a CAMERA collaboration of computer scientists, materials scientists, and synchrotron researchers developed open-source tools, such as F3D to analyze X-ray microtomography data for extracting deformation measurements.

The video shows a visualization of a ceramic-fiber composite used in jet aircrafts. Researchers captured micro-fractures and matrix cracks in the material under increasing strain with X-ray microtomography at the Department of Energy's Advanced Light Source (ALS). Scientists then used F3D to automatically identify micro-damage. ALS scientists note that the F3D implementation performed 17-times faster than similar tools on a typical image file. The improved efficiency in analysis enables real-time image analysis and reduces turnaround time between experiments from hours to minutes, boosting the number of users who can take advantage of advanced imaging tools at facilities like the ALS.

F3D includes non-linear filters, such as mathematical morphology (MM) operators, bilateral and median filters, implemented in OpenCL to explore GPUs. This image processing toolkit works as a plugin to free software ImageJ/Fiji.

Ushizima, Perciano, Krishnam, Loring, Bale, Parkinson, Sethian (2014), IEEE Big Data: 10286-10291.



Benedikt Bauer, Harinarayan Krishnan, Filipe Maia, Stefano Marchesini, Talita Perciano, James Sethian, David Shapiro, Berkeley Lab, Uppsala University

A CAMERA collaboration of computer scientists, and synchrotron researchers is developing a software infrastructure for real-time streaming and ptychographic reconstruction. Besides overcoming the series of I/O operations and the complexity of the common pipeline used at the beamline, the new pipeline provides real-time feedback while the experimental acquisition is in process.

The video shows a visualization of the user interface provided with the real-time streaming infrastructure. After setting the parameters needed for the acquisition and reconstruction process, the user triggers the streaming pipeline. As data come from the acquisition equipment through the pipeline, the user interface is updated with the result of the ptychographic reconstruction, along with the STXM image (Scanning Transmission X-ray Microscopy), illumination and diffraction patterns. The infrastructure works so that the process is recorded and the user can stop and restart it when necessary, and also save the final reconstruction result for future analysis.

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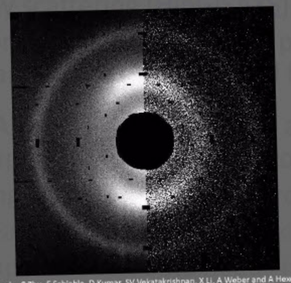
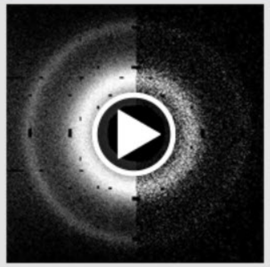


A Sarje, A Kusoglu, C Zhu, E Schlable, D Kumar, SV Vekatakrishnan, X Li, A Weber and A Hexemer

HipRMC is a High-Performance Reverse Monte Carlo (rMC) software that attempts to create the real space images from Small Angles X-ray Scattering (SAXS) data. In principle a SAXS image is the absolute square of the Fourier transform of the electron density of the object being observed under X-rays. Starting with a randomized model, rMC algorithm is used to move the particles, such as the error between the prediction and the data is minimized. This image was designed for a bimodal system with known volume-fractions.

The movie shows SAXS images (on left) of an ionomer, during a tensile test and HipRMC fit (on right). The analysis was done on Oak Ridge Titan using 600 nodes, with each frame taking ~12 minutes.

Funding and Contact Information
FUNDING AGENCY: DOE Office of Science Advanced Scientific Computing Research (ASCR) and Basic Energy Sciences (BES) program
FUNDING ACKNOWLEDGEMENT: Office of Science of the U.S. Department of Energy under contract DE-AC02-06CH11357
CONTACT: James Sethian, jasethian@lbl.gov



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Sept 21 2015: ASCR-BES announce new support for CAMERA for experimental facilities.

CAMERA Applied Math

The Center for Advanced Mathematics for Energy Research Applications (CAMERA) is an integrated, cross-disciplinary center aimed at inventing, developing, and delivering the fundamental new mathematics required to capitalize on experimental investigations at scientific facilities.

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Supported by the US Department of Energy Office of Science
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http://www.camera.lbl.gov/

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Software

F3D

Image Processing and Analysis for High-resolution Volumes

F3D is written in OpenCL, so it achieves platform-portable parallelism on modern multi-core CPUs and many-core GPUs. The interface and mechanisms to access F3D core are written in Java as a plugin for Fiji/ImageJ to deliver several key image-processing algorithms necessary to remove artifacts from micro-tomography data. The algorithms consist of data parallel aware filters that can efficiently utilize resources and can work on out of core datasets and scale efficiently across multiple accelerators. Optimizing for data parallel filters, streaming out of core datasets, and efficient resource and memory and data managements over complex execution sequence of filters greatly expedites any scientific workflow with image processing requirements. F3D preforms several different types of 3D image processing operations, such as non-linear filtering using bilateral filtering and/or median filtering and/or morphological operators (MM). (click here for further information and downloads)

HipGISAXS

High performance GISAXS simulation package

HipGISAXS is a flexible grazing-incidence small-angle X-ray scattering (GISAXS) simulation code in the framework of the distorted wave Born approximation that effectively utilizes the parallel processing power provided by graphics processors and multicore processors. The code, entitled High-Performance GISAXS, computes the GISAXS image for any given superposition of user-defined custom shapes or morphologies in a material and for various grazing-incidence angles and sample orientations. These capabilities permit treatment of a wide range of possible sample structures, including multilayered polymer films and nanoparticles on top of or embedded in a substrate or polymer film layers. In cases where the material displays regions of significant refractive index contrast, an algorithm has been implemented to perform a slicing of the sample and compute the averaged refractive index profile to be used as the reference geometry of the unperturbed system. The parallelized simulation code is well suited for addressing the analysis efforts required by the increasing amounts of GISAXS data being produced by high-speed detectors and ultrafast light sources. (click here for further information and downloads)

PEXSI

Pole EXpansion and Selected Inversion package for electronic structure calculation

http://www.camera.lbl.gov/#!software/ci0g3

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Ptychography: Software: SHARP-CAMERA

* SHARP Documentation, http://sharpcamera.bitbucket.org/
* Workshop Presentations, http://camera.lbl.gov/workshops-and-tutorials/sharp-workshop
* Download Source Code - sharp-release.tar.gz
* CXI Input Format For Ptychography Reconstruction - input_cxi.pdf
* Reference manual:

Dependencies

- An NVIDIA card with compute capability >= 1.2 - CUDA www.nvidia.com/object/cuda_get.html
- Thrust, which is included in recent CUDA versions
- CUSP https://github.com/cusplibrary/cusplibrary
- HDF5 http://www.hdfgroup.org/downloads/index.html
- GSL http://www.gnu.org/software/gsl/
- CMake http://www.cmake.org/cmake/resources/software.html
- Boost http://www.boost.org/users/download/

Building

- Create a directory named build inside of this directory
- Create a link from include/cusp to you local cusp installation
- Create a link from include/thrust to you local thrust installation
- Inside the build directory run "cmake ..".
- Run "make" to build the program

Installing

- Run "make install" to install the program in the system install directory (i.e, /usr/local/bin)
- For custom installations run "cmake -DCMAKE_INSTALL_PREFIX=<INSTALLATION_DIRECTORY> ..".
- Then run "make install" to install the program in custom installation directory

http://www.camera.lbl.gov/#!downloads--ptycho-/wpy3h

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GISAXS: Software and Downloads

HipGISAXS

HipGISAXS is a massively parallel software, which we have developed using C++, augmented with MPI, Nvidia CUDA, OpenMP, and parallel-HDF5 libraries, on large-scale clusters of multi/many-cores and graphics processors. HipGISAXS currently supports Linux based systems, and is able to harness computational power from any general-purpose CPUs including state-of-the-art multicores, as well as Nvidia GPUs and Intel MIC coprocessors. It is able to handle large input data including any custom complex morphology as described in the following, and perform GISAXS simulations at high resolutions.

Software and Documentation:

Supported by the US Department of Energy Office of Science
Advanced Scientific Computing Research (steven.lee@science.doe.gov)
Basic Energy Sciences (Peter.Lee@science.doe.gov)

http://www.camera.lbl.gov/#!downloads--gis-/llzgb

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Software Downloads: Image-Based Experimental Analysis Tools

F3D - Image Processing and Analysis for High-resolution Volumes

F3D is a Fiji plugin, designed for high-resolution 3D image, and written in OpenCL. F3D plugin achieves platform-portable parallelism on modern multi-core CPUs and many-core GPUs. The interface and mechanisms to access F3D accelerated kernes are written in Java to be fully integrated with other tools available within Fiji/ImageJ. F3D delivers several key image-processing algorithms necessary to remove artifacts from micro-tomography data. The algorithms consist of data parallel aware filters that can efficiently utilize resources and can process data out of core and scale efficiently across multiple accelerators. Optimized for data parallel filters, F3D streams data out of core to efficiently manage resources, such as memory, over complex execution sequence of filters. This has greatly expedited several scientific workflows dealing with high-resolution images. F3D preforms two main types of 3D image processing operations: non-linear filtering, such as bilateral and median filtering, and morphological operators (MM) with varying 3D structuring elements.

Download F3D

Quant-CT - Micro-CT Analysis Plugin

Quant-CT allows image enhancement, filtering, segmentation and feature extraction from samples imaged using micro-tomography. A new set of algorithms for Quant-CT uses GPU, and we have obtained 80X speed up of several core filtering algorithms. Check F3D! We have tested our algorithms on data generated at ALS beamline 8.3.2. We are looking forward to testing Quant-CT in data from other beamlines.

Download QuantCT

http://www.camera.lbl.gov/#!downloads--imaging-/ua266

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Zeo++

Zeo++ is a software package for analysis and assembly of crystalline porous materials. Zeo++ can be used to perform geometry-based analysis of structure and topology of the void space inside a material, to alternate or assembly structures as well as to generate structure representations to be used in structure similarity calculations.

Zeo++ calculates the geometrical parameters describing pores. The tool is based on the the fast Voronoi decomposition, which for a given arrangement of atoms in a periodic domain provides a graph representation of the void space. The resulting Voronoi network is analyzed to obtain the diameter of the largest included sphere and the largest free sphere, which are two geometrical parameters that are frequently used to describe pore geometry. Accessibility of nodes in the network is also determined for a given guest molecule and the resulting information is later used to retrieve dimensionality of channel systems as well as in Monte Carlo sampling of accessible surfaces and volumes. Pore size distribution histograms can also be calculated. Zeo++ can also generate a number of structure representations. For example, the Voronoi network can be also used to generate hologram representations of the void space. Alternatively, stochastic ray trace approach can provide another histogram representation of the void space. These structure representations can be used to compare materials, i.e. perform diversity selection of structures from a large set.

Zeo++ offers structure alternation capabilities. For example, it can be used to substitute Si atoms with Al atoms in zeolites on the course of generation of cation-containing zeolite structures. It can also assembly 3D structure models of materials such as metal organic frameworks or covalent organic frameworks from a given set of molecular building blocks. The latter feature can be used to construct databases of predicted material structures.
Zeo++ can be used to either analyze a single structure or perform high-throughput analysis of a large database, and makes use of the fast Voronoi library - Voro++. Current users include the Nanoporous Materials Genome Center, the Materials Project, Bosch, ExxonMobile, SABIC and Samsung.

For details, examples, and complete documentation, please see the official Zeo++ page: www.zeoplusplus.org

Supported by the US Department of Energy Office of Science
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http://www.camera.lbl.gov/#!zeo--dead/gqt53

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PEXSI

The Pole EXpansion and Selected Inversion (PEXSI) method is a fast method for electronic structure calculation based on Kohn-Sham density functional theory. It efficiently evaluates certain selected elements of matrix functions, e.g., the Fermi-Dirac function of the KS Hamiltonian, which yields a density matrix. It can be used as an alternative to diagonalization methods for obtaining the density, energy and forces. The PEXSI library is written in C++, and uses message passing interface (MPI) to parallelize the computation on distributed memory computing systems and achieve scalability on more than 10,000 processors.

The PEXSI library and documentation can be found here http://pexsi.org/

The PEXSI library has recently been integrated into the Siesta for demonstrating efficient and accurate ab initio materials simulation on massively parallel machines, and can regularly handle systems with 10,000 to 100,000 electrons. It has also just recently been added to CP2K.

https://hpcforge.org/plugins/mediawiki/wiki/siesta/index.php/Work-program

http://esl.cecam.org/mediawiki/index.php/PEXSI

http://manual.cp2k.org/trunk/CP2K_INPUT/FORCE_EVAL/DFT/LS_SCF/PEXSI.html

http://www.camera.lbl.gov/#!pexsi-dead/qj1vd

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Laboratory Directed Research and Development (LDRD)

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The Department of Energy's Engine of Discovery

The U.S. Department of Energy (DOE) is charged with a large and complex mission —"to ensure America's security and prosperity by addressing its energy, environmental, and nuclear challenges through transformative science and technology solutions." The DOE executes this mission to a large extent at its seventeen national laboratories, a group of institutions which were created and are supported by the Federal government to perform research and development (R&D) in areas of importance to the DOE and, where appropriate, to other Federal agencies.

RELATED LINKS
- DOE Order 413.2, Laboratory Directed Research and Development
- Annual LDRD Reports to Congress

Today, the national laboratories are performing R&D in support of DOE's goals in catalyzing the transformation of the nation's energy system, securing our leadership in clean energy, maintaining a vibrant scientific and engineering effort, and enhancing nuclear security through defense, nonproliferation, and environmental efforts. In recognition of the importance of the long-term health of these institutions, the U.S. Congress has authorized and encouraged them to devote a relatively small portion of their research effort to creative and innovative work that serves to maintain their vitality in science and technology (S&T) disciplines relevant to DOE and national security missions. Since 1991, this effort has formally been called Laboratory Directed Research and Development (LDRD).

LDRD serves a number of important purposes. It enables high risk R&D at the Department's laboratories in areas of potential value to national R&D programs. Its flexibility allows the laboratories to assemble experts from different fields into teams whose collaboration uncovers synergies and multidisciplinary solutions not otherwise evident without the freedom to reach across traditional technical boundaries. In addition, LDRD serves as a proving ground for advanced R&D concepts that are often subsequently pursued by DOE programs and, at the same time, helps the Government identify more creative approaches to fulfilling future mission needs.

LDRD projects are selected on a competitive basis through rigorous management and peer review processes, thus ensuring the best and most promising ideas are brought to the fore. As a result, LDRD contributes to an environment at the laboratories that encourages and supports creativity and that is poised to respond immediately to DOE mission challenges as they arise. In that way, LDRD helps the laboratories maintain and develop scientific and engineering capabilities in areas of strategic importance to the nation.

Among the most valuable aspects of the LDRD program is its role as an excellent professional development tool. The LDRD program is instrumental in the laboratories' ability to attract promising young scientists and engineers, thus providing the basis for continually refreshing the laboratory research staff, as well as for the education and training of the next generation of scientists. This includes support for both undergraduate and graduate students working on LDRD projects, technical staff retention associated with opportunities to retain and hone scientific skills via LDRD, and a range of university collaborations

http://science.energy.gov/lp/laboratory-directed-research-and-development/

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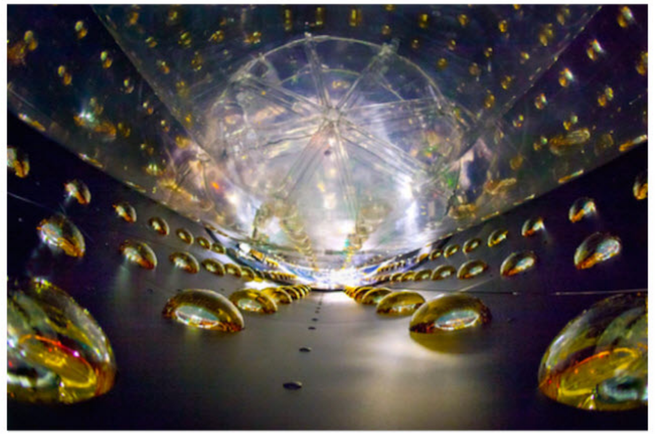

2016 Breakthrough Prize Goes to Five Neutrino Experiments, Three Made Possible by Berkeley Lab

On November 8, Silicon Valley's 2016 Breakthrough Prizes honored five neutrino experiments with $3 million prizes in Fundamental Physics. Three of the five, SNO, KamLAND, and Daya Bay, were made possible by Berkeley Lab scientists and engineers.

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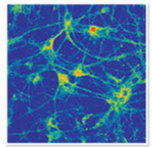

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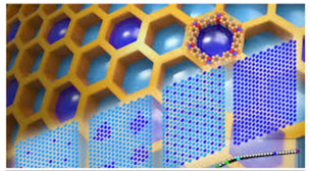

A New Way to Look at MOFs

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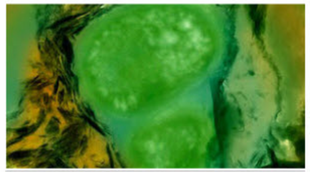

Scientists Call for National Effort to Understand and Harness Earth's Microbes for Health, Energy, Agriculture, and Environment

OCTOBER 2015

FEATURED VIDEO

http://www.lbl.gov/

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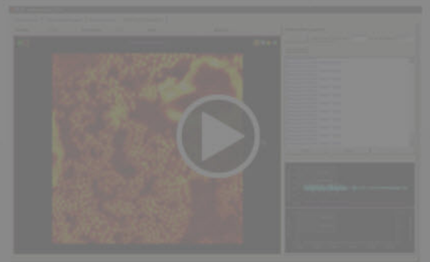

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- Community Resources

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More Information »

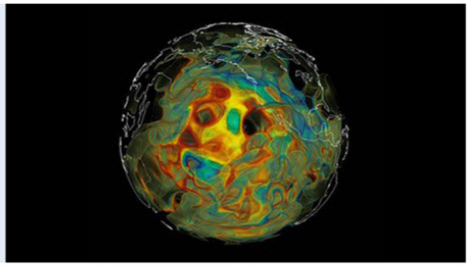
Panel lays out top 10 list of exascale computing hurdles

Exascale computing will require more than processing might

Pictured here: shear-wave perturbations from a seismology simulation code run on the Titan supercomputer

Read More »

1 of 8



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October 13, 2015

CSGF Alumna Sarah Richardson Receives L'Oreal Fellowship

Adding to her growing list of honors, DOE CSGF alumna Sarah Richardson has been named a recipient of a 2015 For Women in Science Fellowship from cosmetics maker L'Oréal USA. The award provides $60,000 for Sarah to advance her research at the Joint BioEnergy Institute at Lawrence Berkeley National Laboratory. Sarah is helping create tools to edit a bacterium's genetic instructions, programming it to produce useful substances like drugs or biofuels. The award also recognizes her outreach to minority and economically disadvantaged youths. She'll receive the award next week in Washington, D.C.

Sarah Richardson

September 15, 2015

Request for Information (RFI) on Science Drivers Requiring Capable Exascale High Performance Computing

This is a multi-agency request for information to identify scientific research topics and applications that need High Performance Computing (HPC) capabilities that extend 100 times beyond today's performance on scientific applications.

June 11, 2015

Additional Information
- Accessing ASCR Supercomputers
- Funding Opportunities
- HPC Facilities Strategic Plan (476KB)

ASCR Quick Links

ASCR Leadership Computing Challenge ALCC

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

SciDAC Scientific Discovery through Advanced Computing

ascr discovery

http://science.energy.gov/ascr/

DOE transforms HPC

BERKELEY LAB

Lawrence Berkeley National Laboratory

CAMERA

Applied Math

Experimental
rates and high
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To address th
Center for Ad
fundamental

CAMERA proc
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CAMERA's ap
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CAMERA, laun
program at La
Office of Adva
invested in CAMERA as a pilot project, and recently awarded it another $10.5 million over three years. This new round of funding will essentially transform CAMERA into a national resource across DOE computational, network and light source facilities.

Basic Energy Sciences (BES)

BES Home
About
Research
Facilities
Science Highlights
Benefits of BES
Funding Opportunities
Basic Energy Sciences Advisory Committee (BESAC)
Community Resources

Science for Energy

Discovery science solves mysteries, sparks innovation, and stimulates future technologies. This principle provides the inspiration for the fundamental energy research and the remarkable collection of major scientific user facilities supported by BES.

Read More »

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E: Email Us

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Summary (1.1MB)

Basic Energy Sciences (BES) supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security. The BES program also plans, constructs, and operates major scientific user facilities to serve researchers from universities, national laboratories, and private institutions. The BES program funds work at more than 160 research institutions through the following three Divisions:

- Materials Sciences and Engineering Division
- Chemical Sciences, Geosciences, and Biosciences Division
- Scientific User Facilities Division

The research disciplines that the BES program supports—condensed matter and materials physics, chemistry, geosciences, and aspects of physical biosciences—are those that discover new materials and design new chemical processes. These disciplines touch virtually every aspect of energy resources, production, conversion, transmission, storage, efficiency, and waste mitigation. BES research provides a knowledge base to help understand, predict, and ultimately control the natural world and serves as an agent of change in achieving the vision of a secure and sustainable energy

What's New
EPSCoR FOA (497KB)
(FAQ) (78KB)
Energy Innovation Hubs
Energy Frontier Research Centers (EFRCs)
Computational Materials Sciences Awards

http://science.energy.gov/BES

BERKELEY LAB

Lawrence Berkeley National Laboratory

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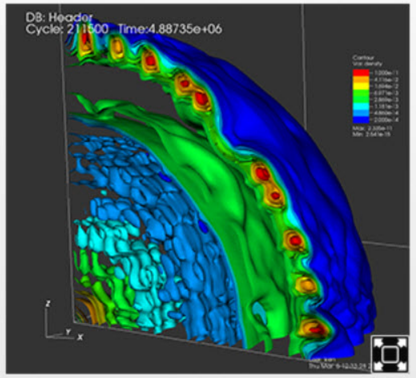
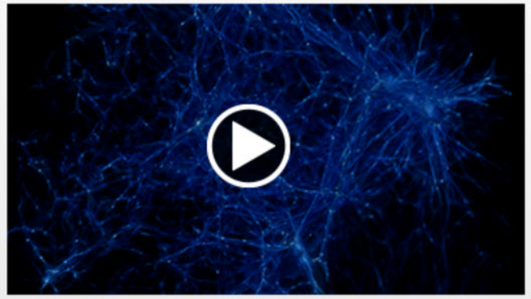
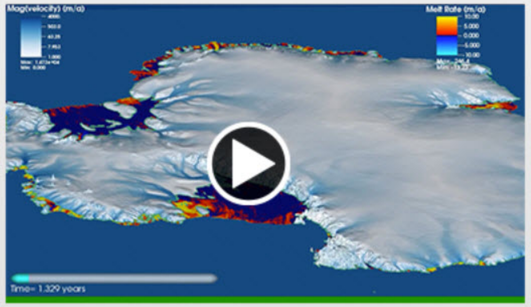
Berkeley Lab Taking Adaptive Mesh Refinement to the Extreme Scale

Berkeley Lab applied mathematicians are recognized internationally for their pioneering work in methods, algorithms and software for modeling and simulating complex scientific and engineering phenomena.







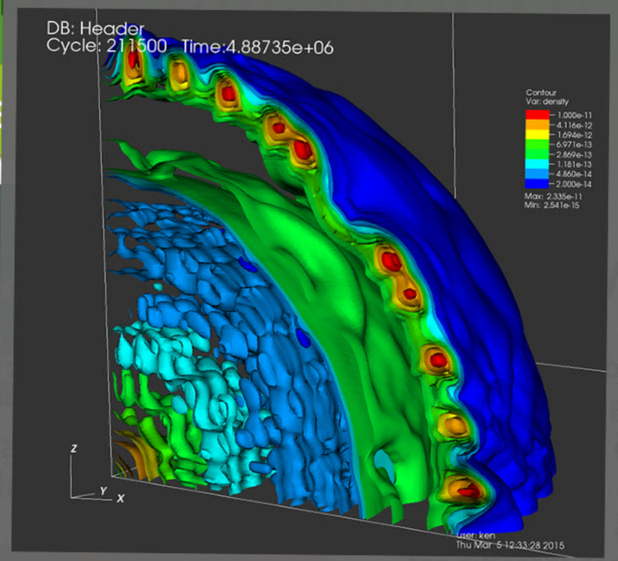
A key research area is adaptive mesh refinement, or AMR, which allows for different resolutions in different regions of the problem, focusing more computing power on the most important parts of the problem. AMR allows scientists to solve bigger, harder problems with higher fidelity and shorter time to solution, while optimizing use of existing computing resources in the process.

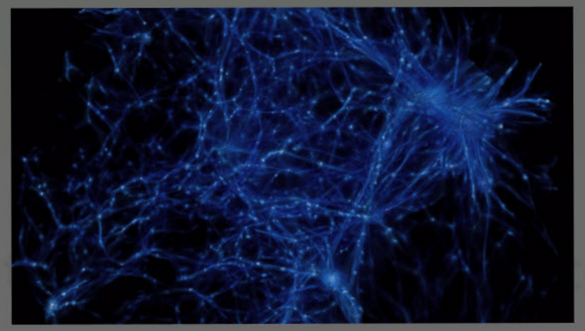
But with exascale computing on the horizon, a new set of challenges must be addressed to ensure that AMR's capabilities can be fully realized on extreme-scale systems.

Because of the wide ranges of applications built on AMR, developing the software so it can operate as effectively and efficiently at exascale is important for DOE's research mission. The areas where Berkeley Lab scientists are applying AMR cover a wide range of scales, from the cosmology of the universe to supernovae, from Earth's climate to subsurface flows, from cleaner combustion to from particle accelerator design.

Advancing AMR to exascale requires both applied math and computer science expertise and Berkeley Lab is committing resources to solve the challenges. Using AMR, scientists use less memory and achieve faster time to solution.

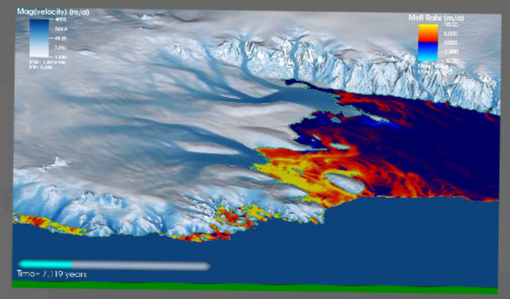
FUNDING & CREDITS





The simulation shows how the universe has evolved from a nearly homogeneous state some 13 billion years ago to the today's universe which is rich in structures that include galaxies; clusters of gravitationally bound galaxies; elongated super-structures called "filaments" that span tens of millions of light-years; and the relatively empty spaces between filaments, called voids. The simulation was performed using the Nyx code -- a gasdynamics and N-body code based on BoxLib framework, and we ran both the simulation and visualization on NERSC's Edison, a Cray XC30 system. Our team uses simulations like this one to model characteristic signature which neutral Hydrogen in the intergalactic medium leaves on the observed spectra of distant quasars.

Both NERSC and the authors are supported by the Office of Science of the U.S.~Department of Energy under Contract No. DE-AC02-05CH11231. Work is in part supported by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Advanced Scientific Computing Research and Office of High Energy Physics.



Understanding Antarctic Ice Sheets
This model of Antarctic ice sheets was generated using BISICLES, a scalable AMR ice-sheet model built upon the Chombo framework developed by the Applied Numerical Algorithms Group at Berkeley Lab. The model shows the ice velocity (darker blue means faster ice flow, so you can see the various ice streams) on the grounded ice. On the floating ice shelves, the subsurface melt rates have been painted, with brighter orange indicating more melting.

Lab Taking Ada

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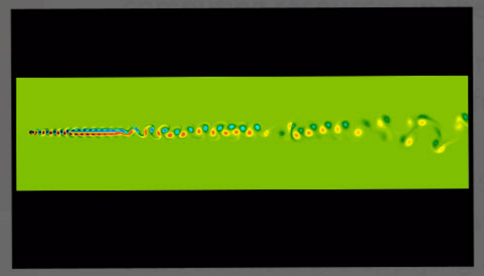
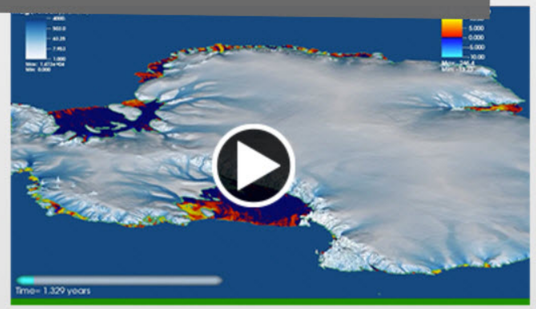


Flow past bluff bodies, in which the flow does not touch the entire surface of the object, has long been studied by fluid dynamicists due to the importance in the aerodynamics industry. The instability that occurs when modeling the 2D flow equations for flow past a cylinder during transition to turbulence is known as the Karman vortex street. This AMR-based model by David Trebotich of Berkeley Lab shows the vortex street at unprecedented scale and resolution, with a wake length of over 200 diameters of the cylinder. These results can be applied to develop new industry standards for the FAA such as take-off and landing patterns in the airline industry.

FUNDING AGENCY: DOE Office of Science Advanced Scientific Computing Research (ASCR) program
FUNDING ACKNOWLEDGEMENT: Office of Science of the U.S. Department of Energy under contract DE-AC02-06CH11357
RESOURCES: Edison and Hopper, National Energy Research Scientific Computing Center; Titan, Oak Ridge National Laboratory
CONTACT: David Trebotich, dptrebotich@lbl.gov; Dan Martin, DFMartin@lbl.gov: Ann Almgren, ASAlmgren@lbl.gov



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ESnet's Science DMZ Architecture Speeding up Science

ESnet

ENERGY SCIENCES NETWORK

Developed by the Department of Energy's Energy Sciences Network (ESnet), the Science DMZ infrastructure architecture is helping researchers at more than 125 universities and national labs make productive use of ever-increasing data flows.

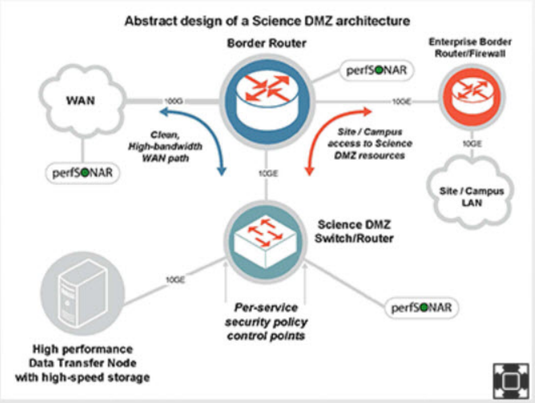
In network security architectures, a DMZ or "demilitarized zone" is a portion specifically dedicated to external-facing services (such as web and email servers). Typically, located at the network perimeter, a Science DMZ is dedicated to external-facing high-performance science services, such as collaborating institutions transferring hundreds of terabytes of data for analysis.

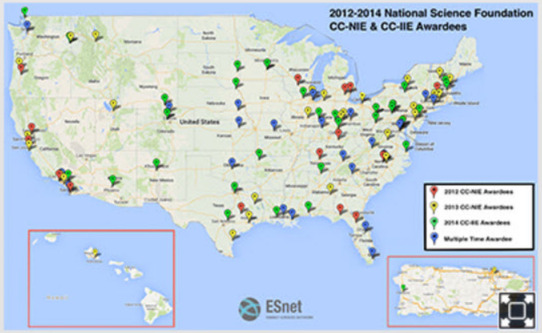
The term "Science DMZ" was first used in 2010 to describe the network configuration linking the Princeton Plasma Physics Laboratory in New Jersey and the National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory in California.

Since then, the concept has been endorsed by the National Science Foundation (NSF), replicated at more than 100 universities and is the basis for the new Pacific Research Platform, a cutting-edge research infrastructure which will link together the Science DMZs of dozens of West Coast research institutions. On July 30, 2015, the NSF announced it would fund a $5 million, five-year award to UC San Diego and UC Berkeley to support the Pacific Research Platform as a science-driven high-capacity data-centric "freeway system" on a large regional scale.

A Science DMZ integrates four key concepts:

- A network architecture explicitly designed for high-performance applications, where the science network is distinct from the general-purpose network
- The use of dedicated systems for data transfer
- Performance measurement and network testing systems that are regularly used to characterize the network and are available for troubleshooting
- Security policies and enforcement mechanisms that are tailored for high performance science environments.





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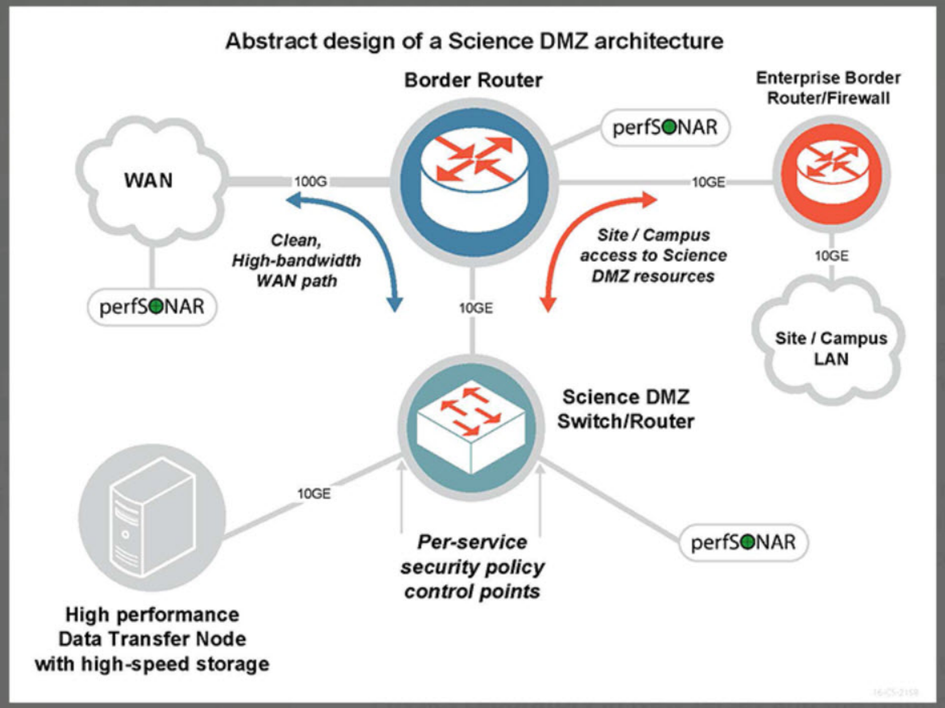
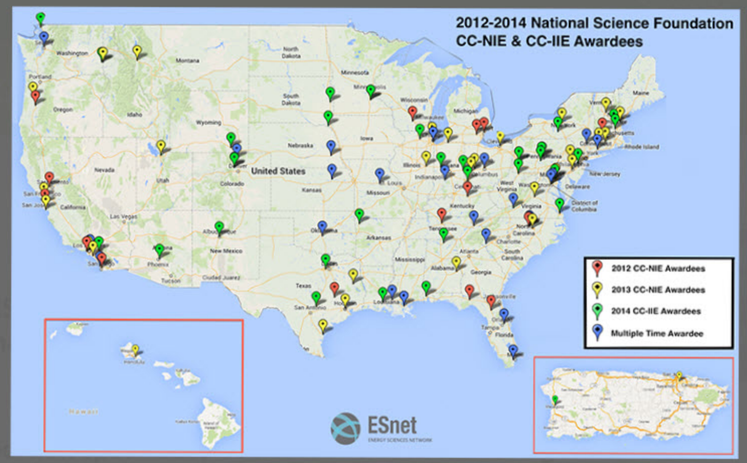


Data comes in from the wide-area network (WAN) into the border router to a designated switch that connects one or more servers that are used to host and run data transfer tools. perfSONAR is a network monitoring and measurement software toolkit that is used to check the throughput and connectivity between institutions.



This map shows the location of universities which have deployed Science DMZs or similar architectures as part of the CC-NIE and CC-IIE programs funded by the National Science Foundation.

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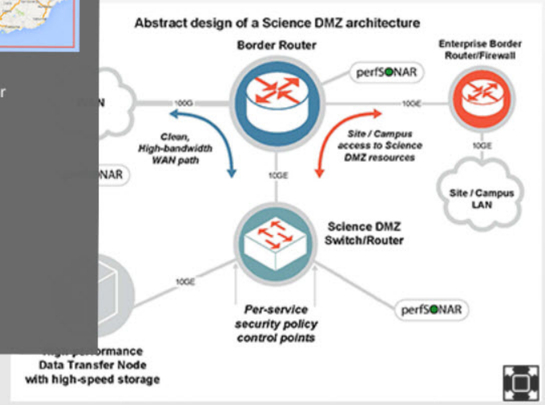
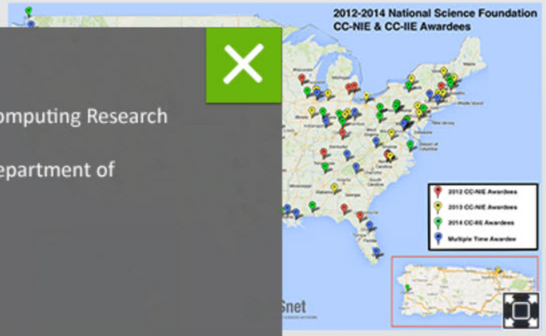
ESnet
ENERGY SCIENCES NETWORK





FUNDING AGENCY: DOE Office of Science Advanced Scientific Computing Research (ASCR) program
FUNDING ACKNOWLEDGEMENT: Office of Science of the U.S. Department of Energy under contract DE-AC02-05CH11231
CONTACT: Science Engagement Team: engage@es.net

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ESnet

ENERGY SCIENCES NETWORK

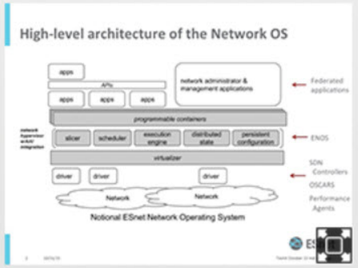
ESnet's Network Operating System (ENOS)

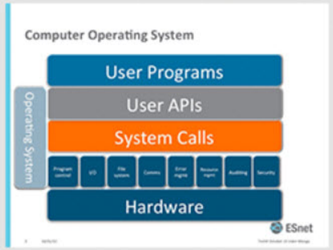
A next-generation operating system for networks

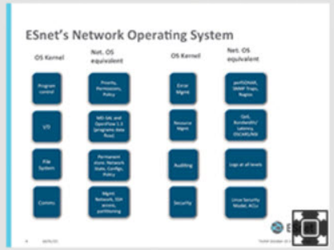
ENOS, the ESnet Network Operating System, is a prototype next-generation architecture for handling data-intensive science workflows. The concept of a "network operating system," a software layer that enables applications to get information about the network and to program it to meet its needs, has been discussed academically for a while but now appears feasible with the wide adoption of the Software-Defined Networking (SDN) paradigm. The SDN paradigm constitutes a network architecture that separates the control plane from the distributed data plane and provides logical centralization of the network control and state. These logical central control plane capabilities can evolve into the operating system through which network policies are implemented across the network and applications can program network behavior.

At a high level, an operating system interacts with hardware using device drivers while providing an environment with sufficient abstractions where multiple applications can run. The current vendor marketplace is focusing on SDN controller platforms that we consider equivalent to the device driver in a generalized OS model. In addition, since this evolution is in the early days there is no industry- or academic-accepted model of a network operating system. ESnet is taking the lead in the Research and Education domain by researching and developing an architectural framework for the NOS and building an experimental version applied towards specific science use-cases.

The ENOS approach will enable ESnet to build better application-engaged scientific networks and provide the interfaces, data and programmability for applications or science virtual organizations to better orchestrate their multi-site complex big data projects and optimize their use of storage, compute and cloud resources. In addition, this software capability will enable ESnet to provide supportable custom services more cost-effectively.







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The National Laboratory System

DOE transforms HPC

ESnet SDN investigations, in a nutshell:

2006

OSCARS, 2006; R&D100 Award 2013 DOE award 2015 → RDMA over Ethernet with OF and NEC, 2011 → Zero Configuration Circuits, 2011 → Network Virtualization "One Switch," Nov. 2012 (2012)

2012

World's first Transport SDN, Dec. 2012 → Software-Defined Exchange @ REANNZ/ ESnet, April 2013 → Multi-domain Circuits with NSI, Oct. 2013 (2013)

2013

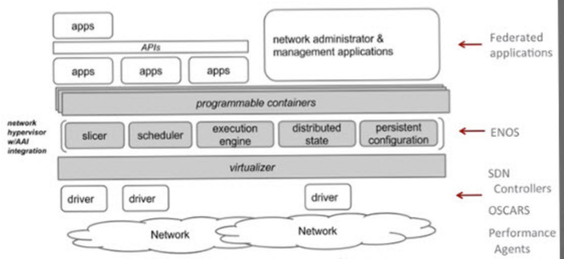
Multilayer Transport SDN Demonstration, Oct .2013 → Scalable BGP "white-box" Router, w/ Corsa, Aug. 2014 → Dynamic L3 and L2, SDN router + NSI, Sept. 2014 (2014)

ESnet

1 10/31/15 TechX October 15 Inder Monga

ESnet has been investigating, developing and deploying SDN-related software and services since 2006.

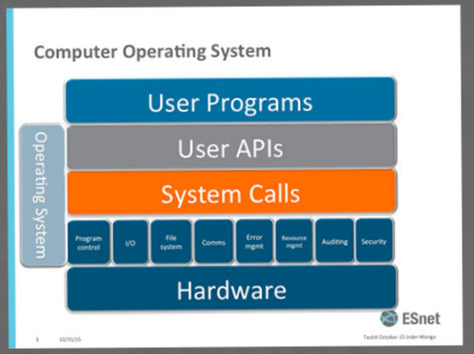
High-level architecture of the Network OS

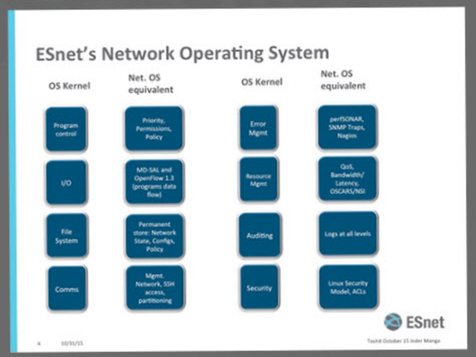


Notional ESnet Network Operating System

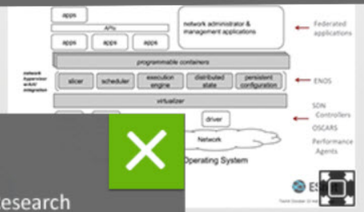
ESnet

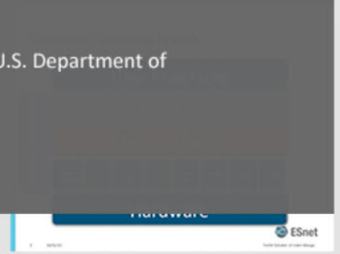
2 10/31/15 TechX October 15 Inder Monga

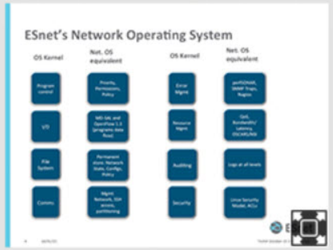




These two images show the differences and similarities between a computer OP and ESnet's network operating system and illustrates the comparable equivalent components.







FUNDING & CREDITS

FUNDING AGENCY: DOE Office of Science Advanced Scientific Computing Research (ASCR) program

FUNDING ACKNOWLEDGEMENT: Office of Science of the U.S. Department of Energy under contract DE-AC02-05CH11231

CONTACT: Inder Monga, ESnet, imonga@es.net

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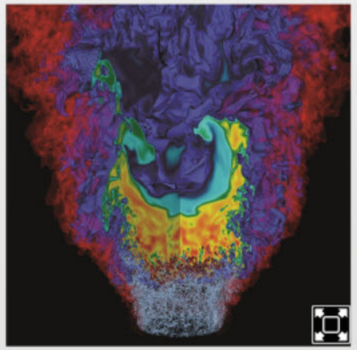
The NERSC-8 Cori System

Cray XC system with over 9,300 Intel Xeon Phi (KNL) nodes

- Delivery in mid 2016
- Self-hosted manycore processor with over 60 cores per node: not an attached accelerator
- On-package high-bandwidth memory (HBM)
- More Info

Data-Intensive Science Support

- 10 Haswell processor cabinets to support data-intensive applications (Cori Phase 1, November 2015)
- NVRAM Burst Buffer to accelerate data-intensive applications
- 28 PB of disk, >700 GB/sec I/O bandwidth
- More Info



Boxlib (simulation pictured on the left) is one of more than 20 applications participating in the NESAP program. More Info

NERSC

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The National Laboratory System

DOE transforms HPC

U.S. DEPARTMENT OF ENERGY

EXPLOR | OLLABORATIVE PROJECTS | BOOTH SCHEDULE | HOME

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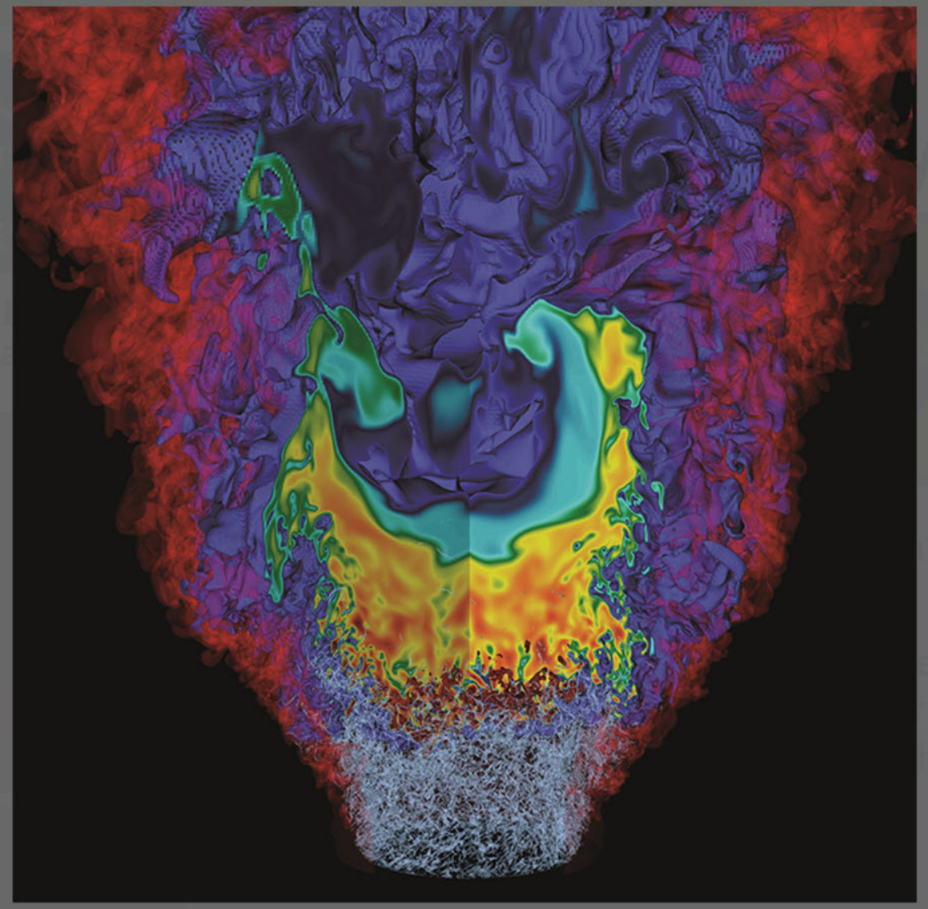

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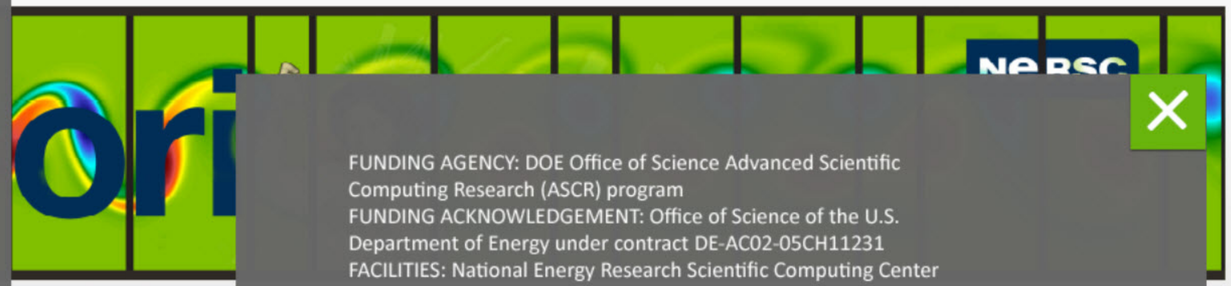

FUNDING AGENCY: DOE Office of Science Advanced Scientific Computing Research (ASCR) program
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FACILITIES: National Energy Research Scientific Computing Center
CONTACT: Richard Gerber, NERSC, ragerber@lbl.gov

el Xeon Phi (KNL) nodes

sor with over 60 cores per node:

memory (HBM)

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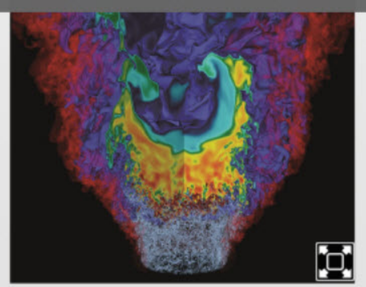

Boxed simulation pictured on the left) is one of more than 20 applications participating in the NESAP program.
More Info

NERSC

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The N

Cray XC

Data-In

- NVRAM Burst Buffer to accelerate data-intensive applications
- 28 PB of disk, >700 GB/sec I/O bandwidth
- More Info

Boxlib (simulation pictured on the left) is one of more than 20 applications participating in the NESAP program.
More Info

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- Accounts & Allocations
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    - Cori Phase I
    - Configuration
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    - Programming
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    - NESAP
    - Burst Buffer
    - NERSC-8 Procurement
    - Programming models
    - File Storage and I/O
  - Edison
  - Hopper
  - PDSF
  - Genepool
  - Testbeds
  - Retired Systems
- Storage & File Systems
- Data & Analytics
- Connecting to NERSC
- Queues and Scheduling
- Job Logs & Statistics
- Application Performance
- Training & Tutorials
- Software
- Policies
- User Surveys
- NERSC Users Group
- User Announcements

CORI

Overview

Cori is NERSC's newest supercomputer system (NERSC-8). It is named after American biochemist Gerty Cori. The Cori system will be delivered in two phases with the first phase online now and the second expected in mid-2016. The Phase-1 system is a Cray XC system based on the Haswell multi-core processor that will include a number of new features that will benefit data-intensive science. The second phase of the Cori system will be installed and merged with Phase 1 in mid-2016. Phase 2 will be based on the second generation of Intel® Xeon Phi™ Product Family, called Knights Landing (KNL) Many Integrated Core (MIC) Architecture.

Updates and Status »

Access to Cori is currently restricted for configuration and testing. General user access coming soon. Known Issues For those who do have access, the below issues are known and being worked on. We expect they will be resolved before general access is granted. MyNERSC doesn't have cori information (queue display, completed jobs etc.) salloc: if just returns you to login node prompt then try deleting cmomXX entrys from .ssh/known_hosts. Also host-based authentication is not setup yet so you... Read More »

Cori Phase I »

The Cori Phase 1 (also known as the "Cori Data Partition") system utilizes Intel Haswell processors and provides approximately the same sustained application performance as the Hopper system. Cori Phase 1 has a number of new features to support data intensive science. Read More »

Configuration »

Details concerning Cori's hardware and software. Read More »

Getting Started »

Before you can use or access Cori, you must have an active NERSC account and valid password. If you don't, see Accounts and Allocations. Cori should be used in the following way: Log in to a "login" node, bring your files and data over, compile your code, and create a batch submission script. Then submit that script so that your application runs on the Cori "compute" nodes. Pay attention to the various file systems available and the choices in programming environments, and make sure you use... Read More »

Programming »

Find information on how to compile your application, use MPI and OpenMP optimally, achieve effective vectorization, and use

http://www.nersc.gov/users/computational-systems/cori/

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The N

Cray XC

Data-In

- NVRAM Burst Buffer to accelerate data-intensive applications
- 28 PB of disk, >700 GB/sec I/O bandwidth
- More Info

Boxlib (simulation pictured on the left) is one of more than 20 applications participating in the NESAP program.
More Info

EARLY USERS TO TEST NEW BURST BUFFER ON CORI

Designed to Accelerate I/O Performance

OCTOBER 5, 2015 | Tags: Burst Buffer, Cori

NERSC has selected a number of HPC research projects to participate in the center's new Burst Buffer Early User Program, where they will be able to test and run their codes using the new Burst Buffer feature on the center's newest supercomputer, Cori.

Cori Phase 1, recently installed in the new Computational Research and Theory building at Berkeley Lab, is a Cray XC system based on the Haswell multi-core processor. It includes a number of new features designed to support data-intensive science, including the Burst Buffer. Based on the Cray DataWarp I/O accelerator, the Burst Buffer is designed to enhance I/O performance and features a layer of non-volatile storage that sits between a processors' memory and the parallel file system.

"Burst Buffers have the potential to transform science on supercomputers: removing I/O bottlenecks, enabling new workflows and bringing together data analysis and simulations," said Wahid Bhimji, a data architect at NERSC who is co-leading the Cori Early User Programs. "However, this is a brand new technology, offering a new way of working and bringing challenges from software to scheduling. So it is really important and exciting to be able to shape the use of this technology in collaboration with these important science projects."

NERSC's Burst Buffer Early User Program is one of several programs NERSC has rolled out this year to help users get up and running on Cori as soon as possible and tune the system to meet science needs. Proposals were solicited beginning in early August; selection criteria included scientific merit, computational challenges and broad use of Burst Buffer data features, such as I/O improvements, checkpointing, workflow improvements, data staging and visualization. The selected projects reflect the range of the six program offices in the DOE Office of Science and the breadth of scientific computing NERSC supports.

"We're very happy with the response to the Burst Buffer Early User Program call," said Deborah Bard, a data architect at NERSC who is also co-leading the Cori Early User Programs. "In fact, we decided to support more applications than we'd originally anticipated." Some applications already had Laboratory Directed Research and Development funding at Berkeley Lab and existing support from NERSC staff. Others will be given earlier access to the Burst Buffer to enable their projects, though without dedicated NERSC support.

Here is a complete list of the NERSC Burst Buffer early use cases:

NERSC-supported: New Efforts

- Nyx/BoxLib cosmology simulations, Ann Almgren, Berkeley Lab (HEP)
- Phoenix: 3D atmosphere simulator for supernovae, Eddie Baron, University of Oklahoma (HEP)
- Chombo-Crunch + Visit for carbon sequestration, David Trebotich, Berkeley Lab (BES)
- Sigma/UniFam/Sipros bioinformatics codes, Chongle Pan, Oak Ridge National Laboratory (BER)
- XGC1 for plasma simulation, Scott Klasky, Oak Ridge National Laboratory (FES)
- PSANA for LCLS, Amadeo Perazzo, SLAC (BES/BER)

http://www.nersc.gov/news-publications/nersc-news/nersc-center-news/2015/early-users-to-test-new-burst-buffer-on-cori/

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BoxLib

BoxLib: Download

To get a copy of the latest version of the **BoxLib** repository using git, please visit our Downloads page.

BoxLib: Users' Guide

The **BoxLib User's Guide** is available in the **BoxLib** git repository in BoxLib/Docs/ (type 'make'). This document contains step-by-step instructions for running simulations in parallel with multiple levels of refinement, with accompanying tutorial applications in BoxLib/Tutorials/.

BoxLib: Tutorials

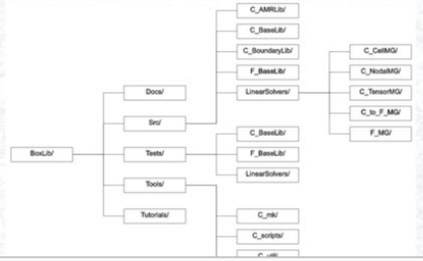
We have created tutorials in the **BoxLib** release that give examples of how to use the extensive functionality that is available. Some of the tutorials available in the download describe:

- How to run a simulation using hybrid MPI/OpenMP
- How to customize boundary condition routines
- How to define a fixed multilevel grid structure
- How to run with adaptive mesh refinement
- How to use BoxLib linear solvers to solve a general Helmholtz operator

BoxLib: Summary of Key Features

BoxLib is the block-structured AMR framework that is the basis for many of CCSE's codes.

- Support for block-structured AMR with optional subcycling in time
- Support for cell-centered, face-centered and node-centered data
- Support for hyperbolic, parabolic and elliptic solves on hierarchical grid structure
- C++ and Fortran90 versions
- Supports hybrid programming model with MPI and OpenMP
- Basis of mature applications in combustion, astrophysics, cosmology, and porous media



https://ccse.lbl.gov/BoxLib/index.html

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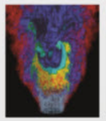
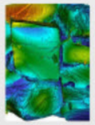
In the first year of NESAP, NERSC hired 6 postdocs to work with code teams, held 4 Dungeon Sessions with 9 codes, completed significant work with Cray and Intel staff on dozens of applications, held multiple user training sessions and hosted the annual Intel Xeon Phi User Group Meeting focused on application performance.

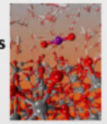
NESAP Projects



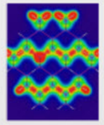
Boxlib AMR Framework
PI: A. Almgren, Berkeley Lab



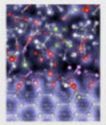
ChomboCrunch Subsurface Flows
PI: David Trebotich, Berkeley Lab



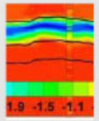
NWChem Computational Chemistry
PI: Eric Bylaska, PNNL



PARSEC Excited State Materials
PI: James Chelikowsky, U of Texas



Quantum Espresso Chemistry & Materials
PI: Paul Kent, ORNL



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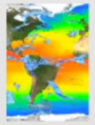

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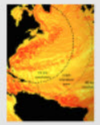

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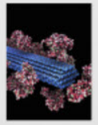

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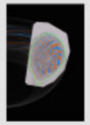

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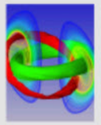

M3D Fusion MHD
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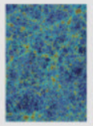

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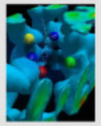

MILC Lattice QCD
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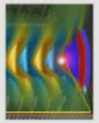

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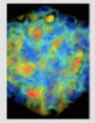

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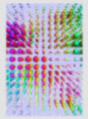

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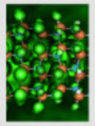

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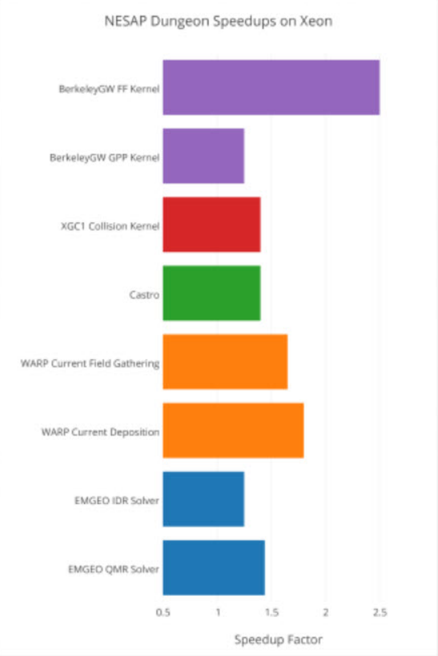
NERSC

Dungeon Sessions Boost Application Kernel Performance



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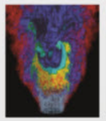
FUNDING AGENCY: DOE Office of Science Advanced Scientific Computing Research (ASCR) program
FUNDING ACKNOWLEDGEMENT: Office of Science of the U.S. Department of Energy under contract DE-AC02-05CH11231
FACILITIES: National Energy Research Scientific Computing Center
CONTACT: Richard Gerber, NERSC, ragerber@lbl.gov

NESAP Projects



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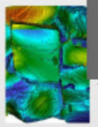

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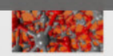

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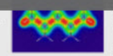

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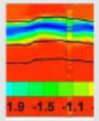

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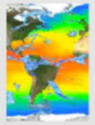

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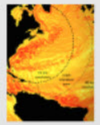

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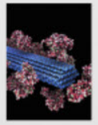

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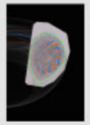

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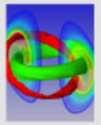

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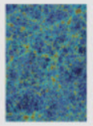

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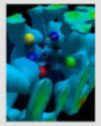

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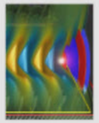

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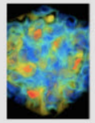

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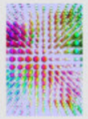

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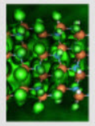

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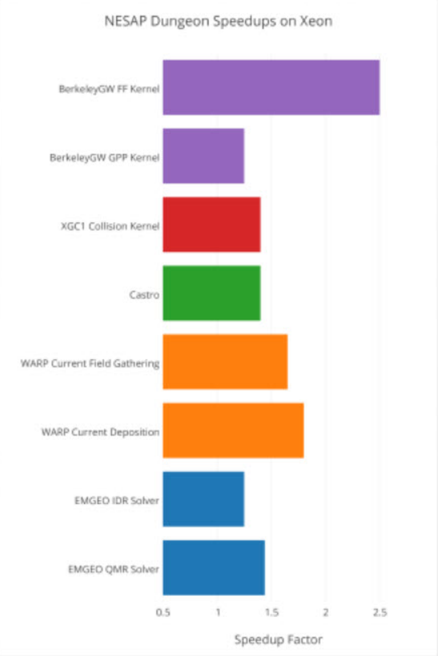

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    - File Storage and I/O
  - Edison
  - Hopper
  - PDSF
  - Genepool
  - Testbeds
  - Retired Systems
- Storage & File Systems
- Data & Analytics
- Connecting to NERSC
- Queues and Scheduling
- Job Logs & Statistics
- Application Performance
- Training & Tutorials
- Software
- Policies
- User Surveys

NESAP

NERSC has launched the NERSC Exascale Science Applications Program, a collaborative effort in which NERSC will partner with code teams and library and tools developers to prepare for the NERSC-8 Cori manycore architecture.

NESAP represents an important opportunity for researchers to prepare application codes for the new architecture and to help advance the missions of the Department of Energy's Office of Science. The NESAP partnership will allow 20 projects to collaborate with NERSC, Cray, and Intel by providing access to early hardware, special training and preparation sessions with Intel and Cray staff. Eight of those 20 will also have an opportunity for a postdoctoral researcher to investigate computational science issues associated with energy-efficient manycore systems. In addition, about 24 more projects as well as library and tools developers will participate in NESAP via NERSC training sessions and early access to prototype and production hardware.

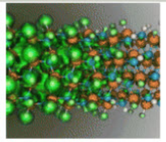
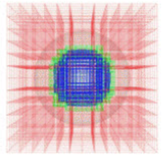
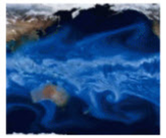
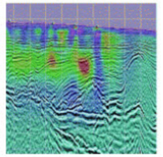
The 20 selected projects were chosen based on computational and scientific reviews by NERSC and other DOE staff. NESAP began during Fall 2014 and will remain active as the Cori system is delivered to NERSC in mid-2016. During this period, twenty of the project teams, guided by NERSC, Cray, and Intel, will undertake intensive efforts to adapt software to take advantage of Cori's Knights Landing manycore architecture and to use the resultant codes to produce pathbreaking science on an architecture that may represent an approach to exascale systems.

Resources available to NESAP Code Teams

- A partner from NERSC's Application Readiness team who will assist with code profiling and optimization
- Access to Cray and Intel resources to help with code optimization
- Up to 1M MPP hours in 2014 and 2M MPP hours in 2015 for code testing, optimization, scaling and debugging on Edison
- Early access to prototype Knights Landing processor hardware (expected in late 2015)
- Early access and significant hours on the full Cori system (expected delivery mid-2016)
- Opportunity for a Post-doctoral researcher to be placed within your application team (NERSC will fund 8 Post-doctoral researchers and place each one within one of the 20 NESAP teams meaning that approximately 40% of NESAP applications teams will include a NERSC sponsored Post-doc)

NESAP Projects »

Projects selected for NESAP span all science areas served by NERSC.

https://www.nersc.gov/users/computational-systems/cori/nesap/