Getting Started at the OLCF

20 Years of Excellence in Computational Science

OLCF

Oak Ridge Leadership Computing Facility

1992–2012

Presented by:

Jack C. Wells

Director of Science

Oak Ridge Leadership Computing Facility (OLCF)

National Center for Computational Sciences (NCCS)

OLCF New User Training

October 8, 2012

Oak Ridge

U.S. DEPARTMENT OF ENERGY

Oak Ridge National Laboratory

MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

ORNL's mission

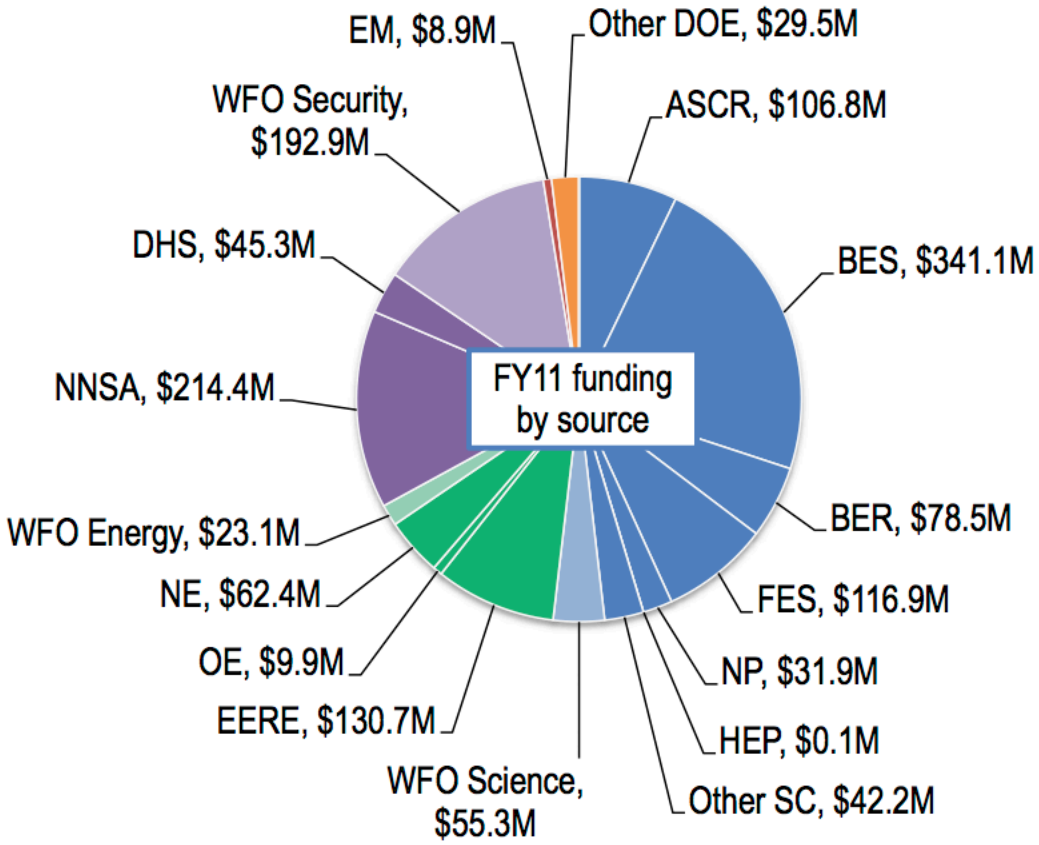
Deliver scientific discoveries and technical breakthroughs that will accelerate the development and deployment of solutions in clean energy and global security, and in doing so create economic opportunity for the nation

Funding and human capital

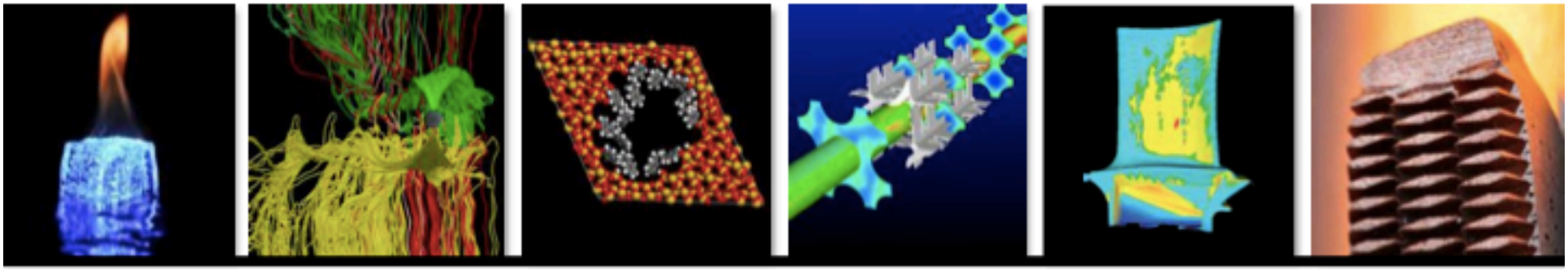
Operating cost, FY11	
Total DOE/NNSA	$1,164M
Non-DOE (excluding DHS)	$227M
DHS	$45M
Total (excluding ARRA)	**$1,436M**

Human capital	
FTE employees	4,533
Joint faculty	122
Postdoctoral researchers	370
Undergrad/grad students	1,383
Facility users	3,116
Visiting scientists	2,283

- 1/3 of staff <5 years
- >1/2 of staff <10 years



Science strategy for the future: Major initiatives

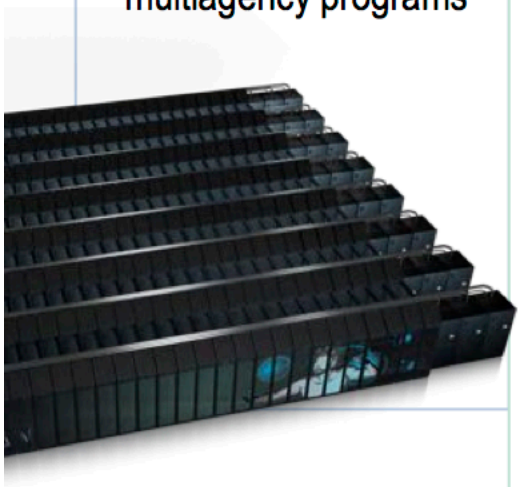


Deliver forefront science using neutrons	Scale computing, data infra-structure, and analytics for science	Develop and demonstrate advanced materials for energy applications	Advance the scientific basis for breakthrough nuclear technologies and systems	Deliver solutions to pressing energy challenges	Provide science and technology for global security challenges

Scale computing, data infrastructure, and analytics for science

Vision

- World's most capable complex for computational science: Infrastructure, staff, multiagency programs

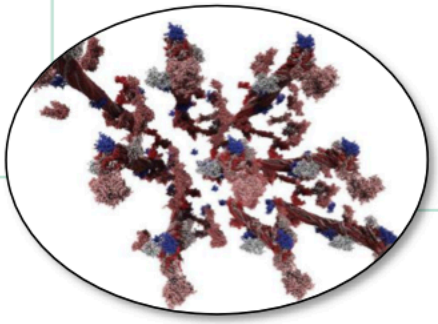


Strategy

- Provide the nation's most capable computational site for advancing to the exascale and beyond
- Leverage DOE-NSA partnership to lead development of exascale computing and data
- Attract top talent; deliver outstanding user program; educate and train next generation of researchers

Leadership areas

- Delivering leading-edge computational science for DOE missions
- Deploying and operating computational resources required to tackle national challenges in science, energy, and security
- Scaling applications to the exascale

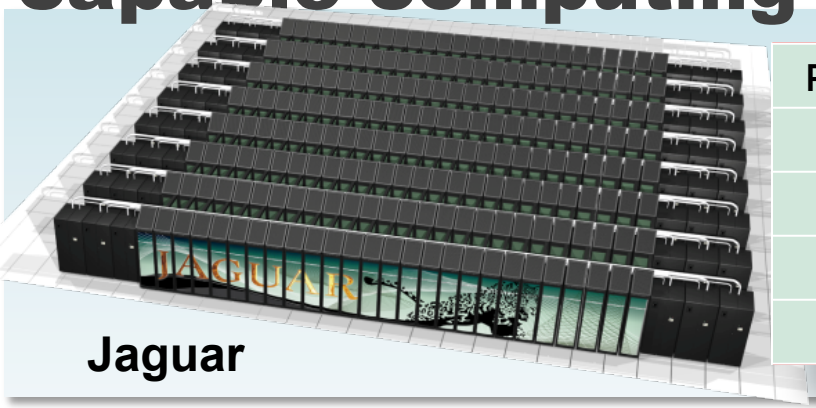


Recent achievements

- First phase of Jaguar upgrade complete; delivering early science on TitanDev
- Industry collaborations addressing complex, competitively important problems
  - Continuing: United Technologies, Ramgen, Global Foundries, GE
  - New: Ford, GM, Caterpillar, P&G
- Exceeded all user facility metrics

Today, we are among the world's most capable computing facilities

June 2012

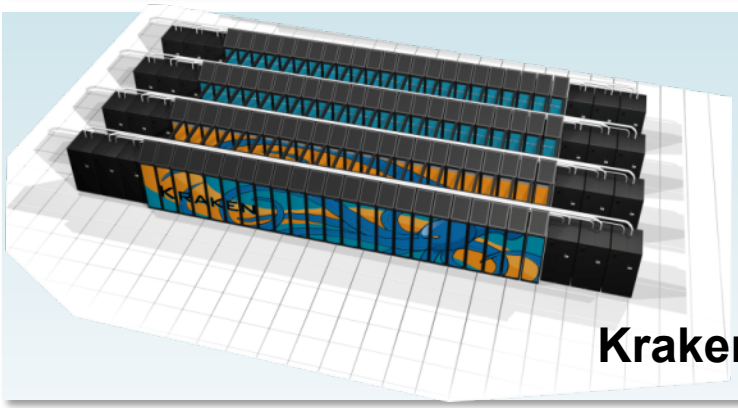


Jaguar

Peak performance	2.63 PF/s
Memory	600 TB
Disk bandwidth	> 240 GB/s
Square feet	5,000
Power	7 MW

TOP500® SUPERCOMPUTER SITES #6

Dept. of Energy's Office of Science

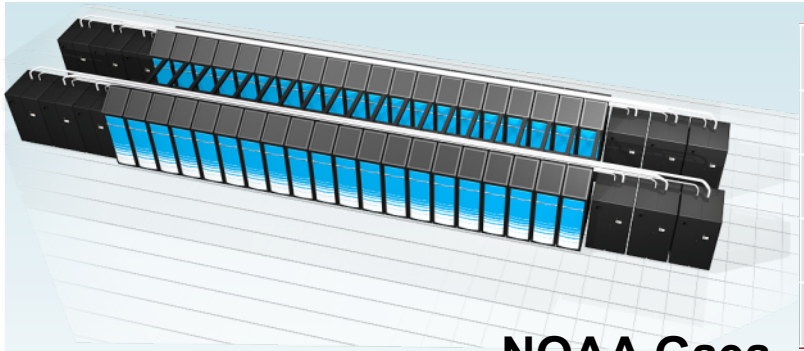


Kraken

Peak performance	1.2 PF/s
Memory	147 TB
Disk bandwidth	> 50 GB/s
Square feet	2,300
Power	3 MW

TOP500® SUPERCOMPUTER SITES #21

National Science Foundation



NOAA Gaea

Peak Performance	0.7 PF/s
Memory	248 TB
Disk Bandwidth	104 GB/s
Square feet	1,600
Power	1.0 MW

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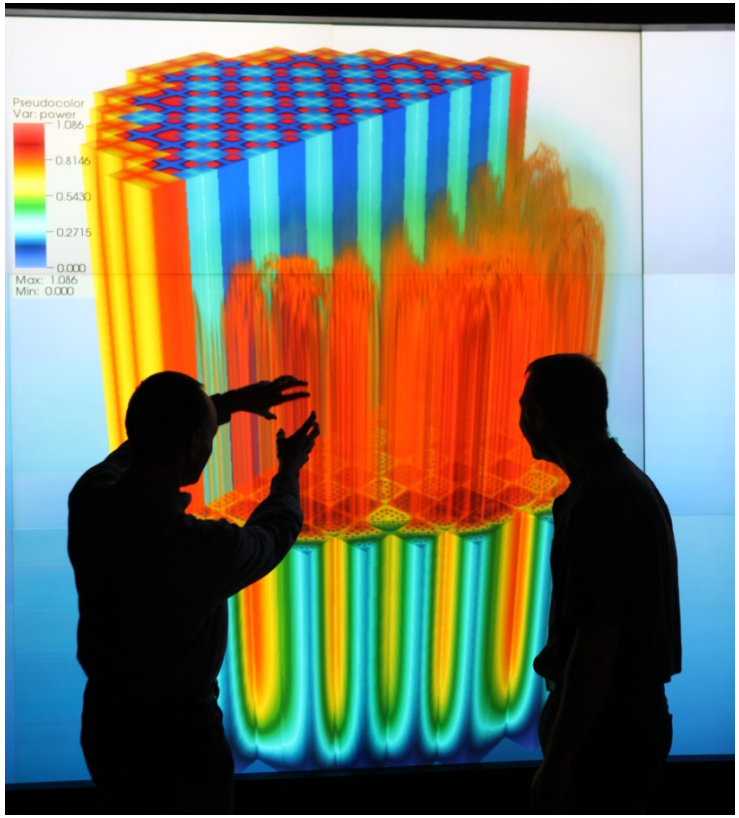
National Oceanic and Atmospheric Administration

OAK RIDGE National Laboratory

Oak Ridge Leadership Computing Facility Mission

The OLCF is a DOE Office of Science National User Facility whose mission is to enable breakthrough science by:

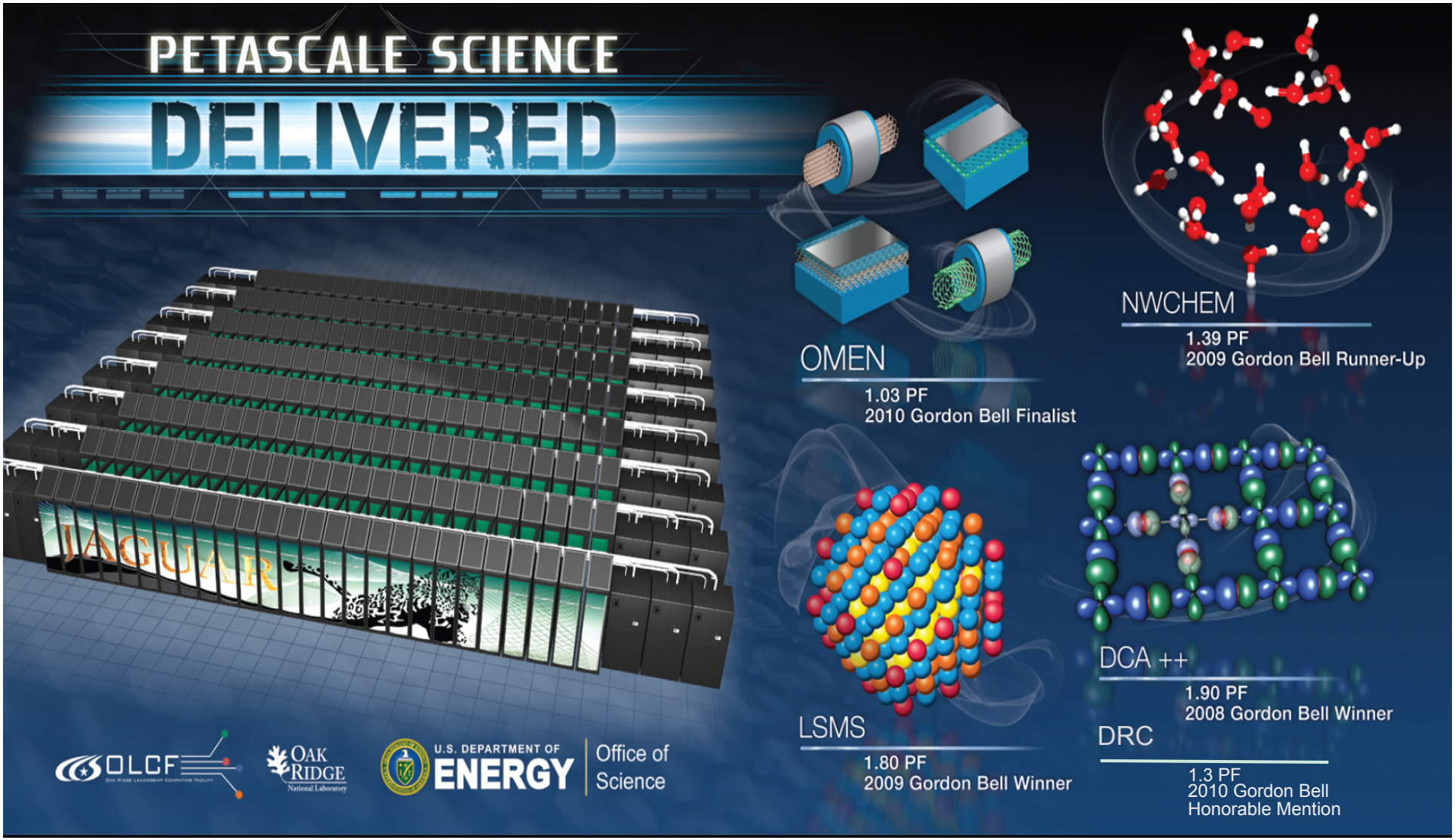
- Fielding the most powerful capability computers for scientific research,
- Building the required infrastructure to facilitate user access to these computers,
- Selecting a few time-sensitive problems of national importance that can take advantage of these systems,
- And partnering with these teams to deliver breakthrough science.



Scaling of Codes on 224,256 core Jaguar

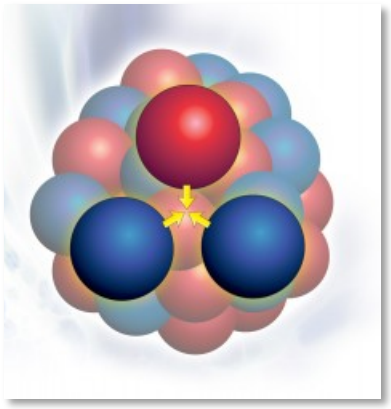
Science Area	Code	Contact	Institution	Cores	Total Performance	Notes
CFD	MoBo	Rahimian	Georgia Tech	200,000	700 TF	2010 Gordon Bell Winner
Seismology	AWP-ODC	Cui	SDSC	223,074	220 TF	2010 Gordon Bell Finalist
Materials	DRC	Kozhevnikov	ETH Zurich	186,624	1.3 PF	2010 Gordon Bell Honorable Mention
Geoscience	P4est	Burstedde	UT-Austin	224,000		2010 Gordon Bell Finalist
Materials	DCA++	Schulthess	ETH & ORNL	213,120	1.9 PF*	2008 Gordon Bell Winner
Materials	WL-LSMS	Eisenbach	ORNL	223,232	1.8 PF	2009 Gordon Bell Winner
Chemistry	NWChem	Apra	ORNL PNNL	224,196	1.4 PF	2009 Gordon Bell Finalist
Nano Materials	OMEN	Klimeck	Purdue	221,400	1.28 PF	2011 Gordon Bell Finalist
Seismology	SPECFEM3D	Carrington	SCEC	149,784	165 TF	2008 Gordon Bell Finalist
Weather	WRF	Michalakes	NREL	150,000	50 TF	
Combustion	S3D	Chen	Sandia	144,000	83 TF	
Fusion	GTC	Chang	PPPL	102,000	20 billion Particles / sec	
Materials	LS3DF	Lin-Wang Wang	Berkeley	147,456	442 TF	2008 Gordon Bell Winner
Chemistry	MADNESS	Harrison	ORNL UTenn	140,000	550+ TF	

The research and activities described in this presentation were performed using the resources of the Oak Ridge Leadership Computing Facility at Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC0500OR22725.

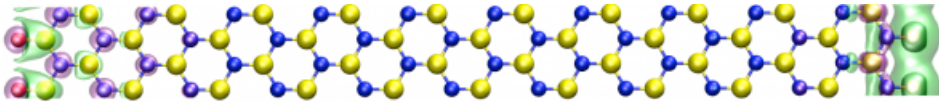


Breakthrough Science at Every Scale

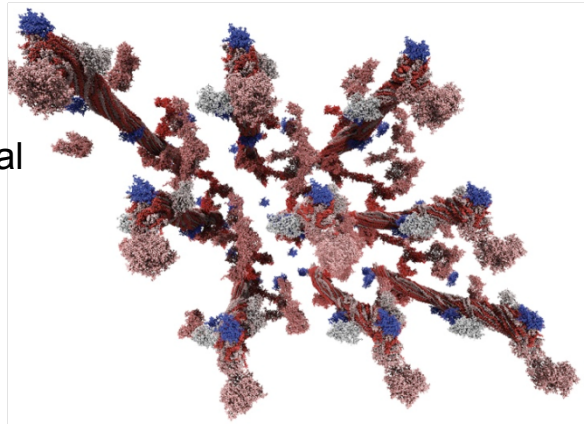
Nuclear Physics
Vary et al., discover that nuclear structure and lifetimes using first-principles nuclear theory requires accounting for the complex nuclear interactions known as the three-body force

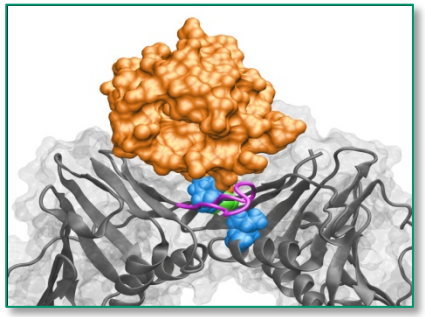


New Materials
Lopez-Bezanilla et al., discover that boron-nitride monolayers are an ideal dielectric substrate for future nanoelectronic devices constructed with graphene as the active layer

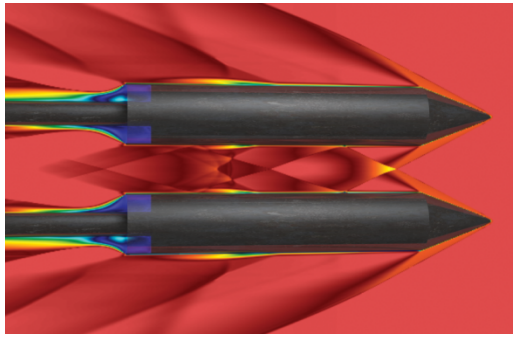


Biofuels
Smith et al., reveal the surface structure of lignin clumps down to 1 angstrom



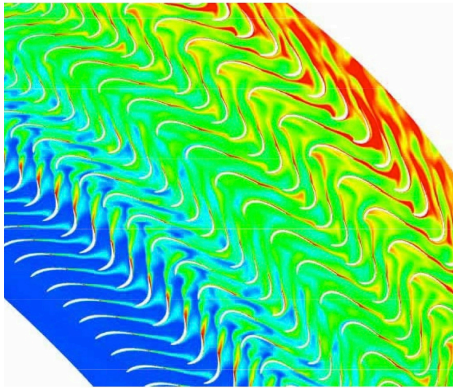


Biochemistry
Ivanov et al., illuminate how how DNA replication continues past a damaged site so a lesion can be repaired later



Design Innovation
Ramgen Power Systems accelerates their design of shock wave turbo compressors for carbon capture and sequestration

Turbo Machinery Efficiency
General Electric, for the first time, simulated unsteady flow in turbo machinery, opening new opportunities for design innovation and efficiency improvements.



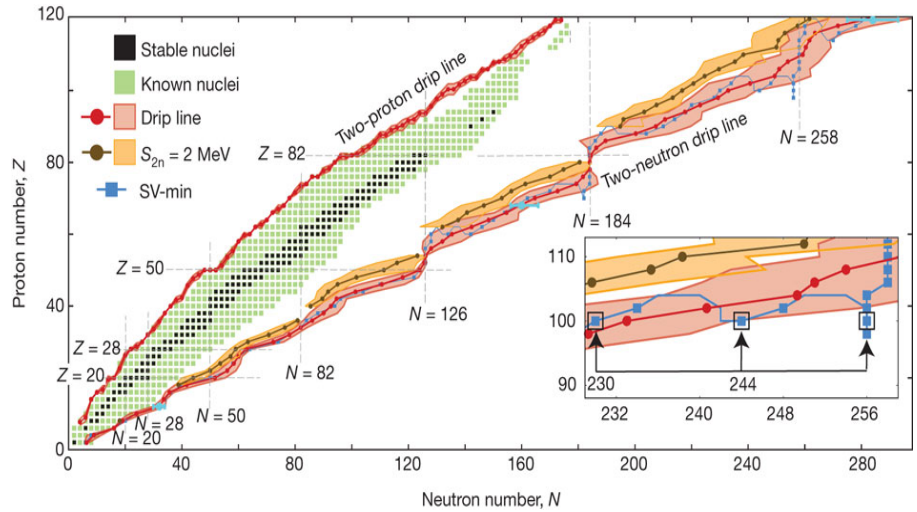
Nuclear Physics

The Limits of the Nuclear Landscape

Project PI: James Vary, Iowa State University
Allocation Program: INCITE

Science Objectives and Impact

- Identify how many protons and neutrons can be bound within a nucleus.
- Identify the nuclear drip lines that denote the end of nuclear binding.
- Project represents at step toward "designer nuclei," with uses ranging from potential cancer treatments to a better understanding of superconductivity.



There are 767 even–even isotopes known experimentally, both stable (black squares) and radioactive (green squares). Mean drip lines and their uncertainties (red) were obtained by averaging the results of different models.

Application Performance

- Code (co-authored by OLCF staff member Hai Ah Nam) used density functional theory to solve the nuclear structure, which involved a large algebraic non-linear eigenvalue problem.
- Each set of nuclei took about two hours to calculate on 224,256-processor Jaguar system.
- Each run considered about 250,000 possible nuclear configurations.

Results (Erier, et al., Nature 2012)

- Calculations identified about 7,000 possible combinations of protons and neutrons allowed in bound nuclei with up to 120 protons.
- Several leading models of nuclear interaction shown to be largely in agreement.
- Accurate calculation of the number of bound nuclei in nature.

Publication:
J. Erier, et al. 2012. "The Limits of the Nuclear Landscape." *Nature* **486**, 509-512. doi:10.1038/nature11188

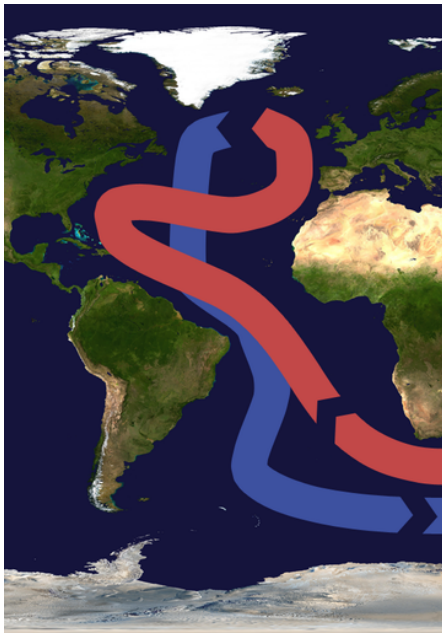
Climate Science

Carbon Dioxide Drove Planetary Warming During Last Deglaciation

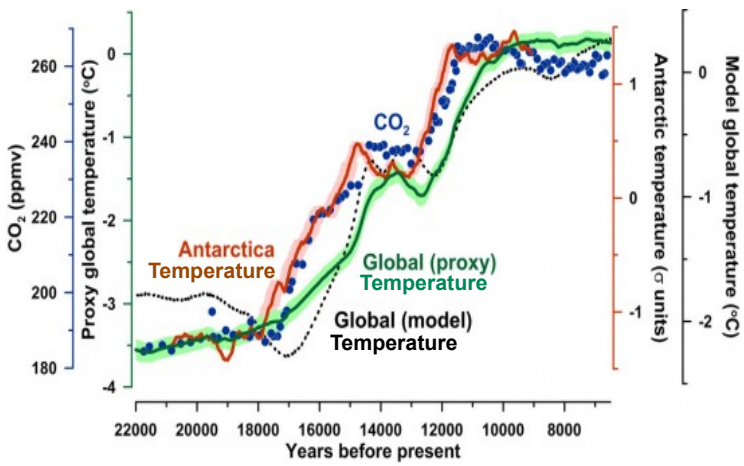
Science Objectives and Impact

- Covariance of CO2 and Temperature in Antarctic ice cores has created a mystery about CO2 role in last deglaciation
- Objective is to solve this mystery by explaining the global temperature record during the last deglaciation
  - Produce a more comprehensive global temperature dataset
  - Simulate earth system energy transport mechanisms

INCITE Project
Warren Washington, PI
300 TB data set generated and processed



Atlantic Meridional Overturning Circulation: plays an important role in inter-hemispheric energy transport; upper ocean circulation in red, deep ocean circulation in blue



Global paleoclimate reconstruction of temperature and CO_2 and the Jaguar supercomputer simulation at Oak Ridge National Laboratory which suggest that CO_2 drove global warming at the end of the last ice age. Image credit: Jeremy Shakun

Results (Shakun et al., Nature 2012)

- Innovative reconstruction of global temperature record
  - Explained lag in global surface temperature response to CO2
- Transient global Earth System Model simulation
  - 15,000 year simulation reproduces reconstructed global temperature response to CO2
  - Illustrates how variations in the Atlantic Meridional Overturning Circulation caused a "seesawing" of heat between hemispheres
  - Explains misleading lag of CO2 behind Antarctic temperature records and points to CO2 role in driving global climate change over glacial cycles

Computational Fluid Dynamics
"Smart Truck Optimization"

PI Mike Henderson,

Science Objectives and Impact

- Apply advanced computational techniques from aerospace industry to improve fuel efficiency of Class 8 Long Haul Trucks
- New California Air Resources Board (CARB) requires 5% fuel efficiency increase on all Class 8 trucks; national drive to reduce emissions.
- Determine design of add-on parts to substantially reduce drag
- If all 1.3 million trucks operated with a passenger car's drag:
  - ✓Save 1.5 billion gallons of diesel annually
  - ✓Reduce 16.4 million tons CO_2 annually
  - ✓Save $5 billion in fuel costs annually

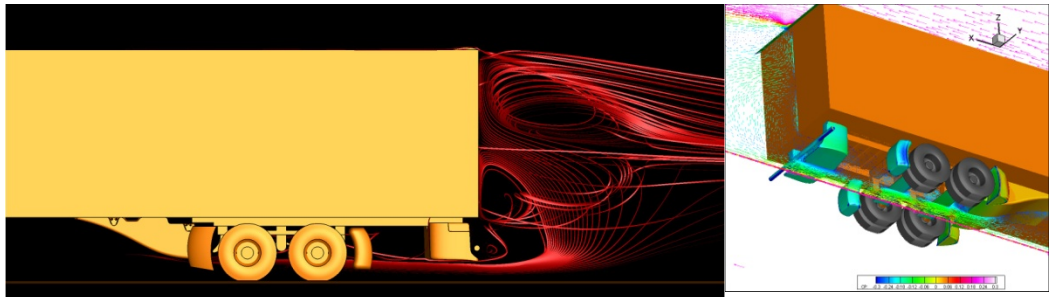
Science Results

Unprecedented detail and accuracy of a Class 8 Tractor-Trailer aerodynamic simulation.

UT-6 Trailer UnderTray System reduces Tractor/ Trailer drag by 12%.

- Minimizes drag associated with trailer underside components
- Compresses and accelerates incoming air flow and injecting high energy air into trailer wake
- Pulls high energy, attached air flow from the top of the trailer down into trailer wake

Application Performance



- CFD results using NASA'a FUN3D within 1% of physical test results
- Access to Jaguar reduced single run times from 15 hours to less than 2 hours
- Stage set to do full Navier-Stokes-based optimization of large trucks

Competitiveness Impact

For BMI:

- Time from conception to manufacture reduced 50% (from 3 years t0 1.5 years)
- Early-to- market advantage will result in earlier and greater revenue recognition

For BMI's customers

- Demonstrated fuel mileage improvements of 7% to 12% available 2011. Exceeds California CARB requirements.

Turbo Machinery Efficiency

Removing Steady-Flow Assumptions Helps Improve Efficiency and Reduce Noise

Project PI: Holmes, GE
Allocation Program: Discretionary

Science Objectives and Impact

- Design efficient turbo machinery generating less noise
  - 1% reduction in fuel consumption can save $20B
- What is the "steady-flow" assumption hiding?

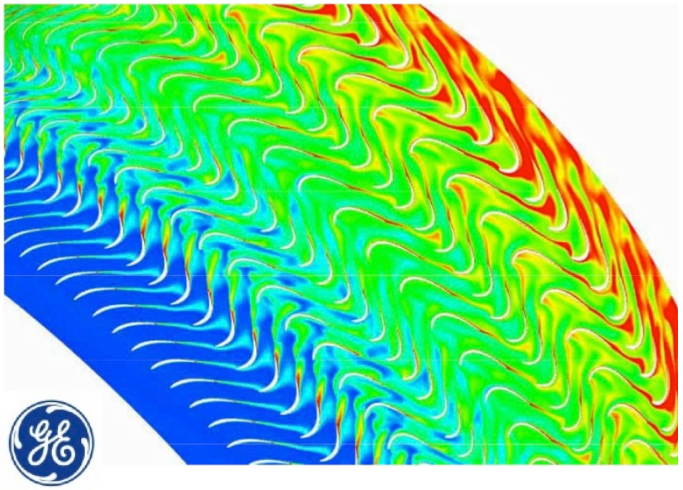


Image on right:
Computational Fluid Dynamics results depicting entropy for unsteady flow through turbine with fan blades removed.

Holmes, et al., SciDAC (2011)

Application Performance

- Scaled GE's TACOMA CFD code from ~1K cores to 8K cores
- TACOMA has good weak scaling

OLCF contributions:

- Recruit GE to OLCF, and guide them in porting TACOMA.

Results

- GE ran their largest ever CFD simulation on Jaguar
- Unsteady flow and efficiency losses localize at end walls
- On the basis of the success of these calculations, GE Global Research has purchased a Cray XE6

"Our two million hours on 8K processors of Jaguar has allowed us to see phenomena we have never seen before."
-- Graham Holmes, GE Global Research

OLCF allocation programs
Selecting applications of national importance

	60% INCITE		30% ALCC		10% Director's Discretionary	
Mission	High-risk, high-payoff science that requires LCF-scale resources		High-risk, high-payoff science aligned with DOE mission		Strategic LCF goals	
Call	1x/year – (Closes June)		1x/year – (Closes February)		Rolling	
Duration	1-3 years, yearly renewal		1 year		3m,6m,1 year	
Typical Size	30 - 40 projects	20M - 100M core-hours/ yr.	5 - 10 projects	1M – 75M core-hours/yr.	100s of projects	10K – 1M core-hours
Review Process	Scientific Peer-Review	Computational Readiness	Scientific Peer-Review	Computational Readiness	Strategic impact and feasibility	
Managed by	INCITE management committee (ALCF & OLCF)		DOE Office of Science		OLCF management	

INCITE: Innovative and Novel Computational Impact on Theory and Experiment

INCITE promotes transformational advances in science and technology through large allocations of computer time, supporting resources, and data storage at the Argonne and Oak Ridge Leadership Computing Facilities (LCFs) for computationally intensive, large-scale research projects.

INCITE awards history

Hours requested vs allocated: *~2.3X per year* *~3.3X per year*

	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013
Hours allocated	4.9M	6.5M	18.2M	95M	268M	889M	1.6B	1.7B	1.7B	***5B***
Projects	3	3	15	45	55	66	69	57	60	*TBD*

NERSC: 3 projects and 4.9M hours awarded

ALCF, OLCF, PNNL join INCITE

INCITE management by ALCF and OLCF; PNNL and NERSC transition out at end of 2009*

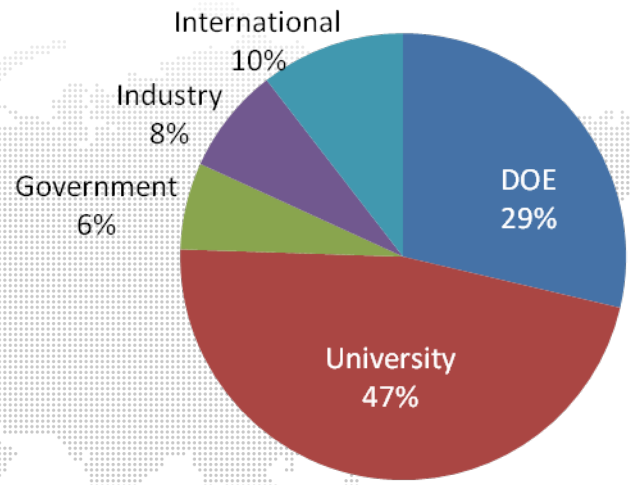
ALCF and OLCF: Mira and Titan

20X growth in number of projects

… but 1000X growth in hours

2013 INCITE Call for Proposals

- Request for Information helped attract new projects
- Call closed June 27th, 2012
- Total requests **~15 billion core-hours**, 3x more than the 5 billion core-hours requested last year
- Number of proposals submitted increased **nearly 20%**
- Awards of ~5 billion core-hours to be announced in November for CY 2013
- Average award to exceed 50 million core-hours



Number of 2013 INCITE Submittals by PI Affiliation

Reaching out to Researchers

Nearly 50% of the non-renewal proposals are by new PIs.

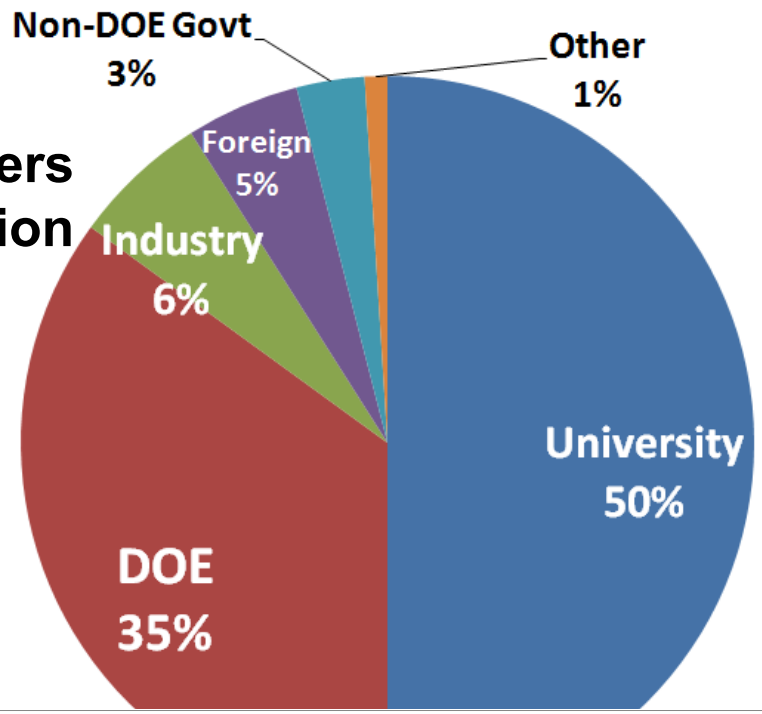
Contact information

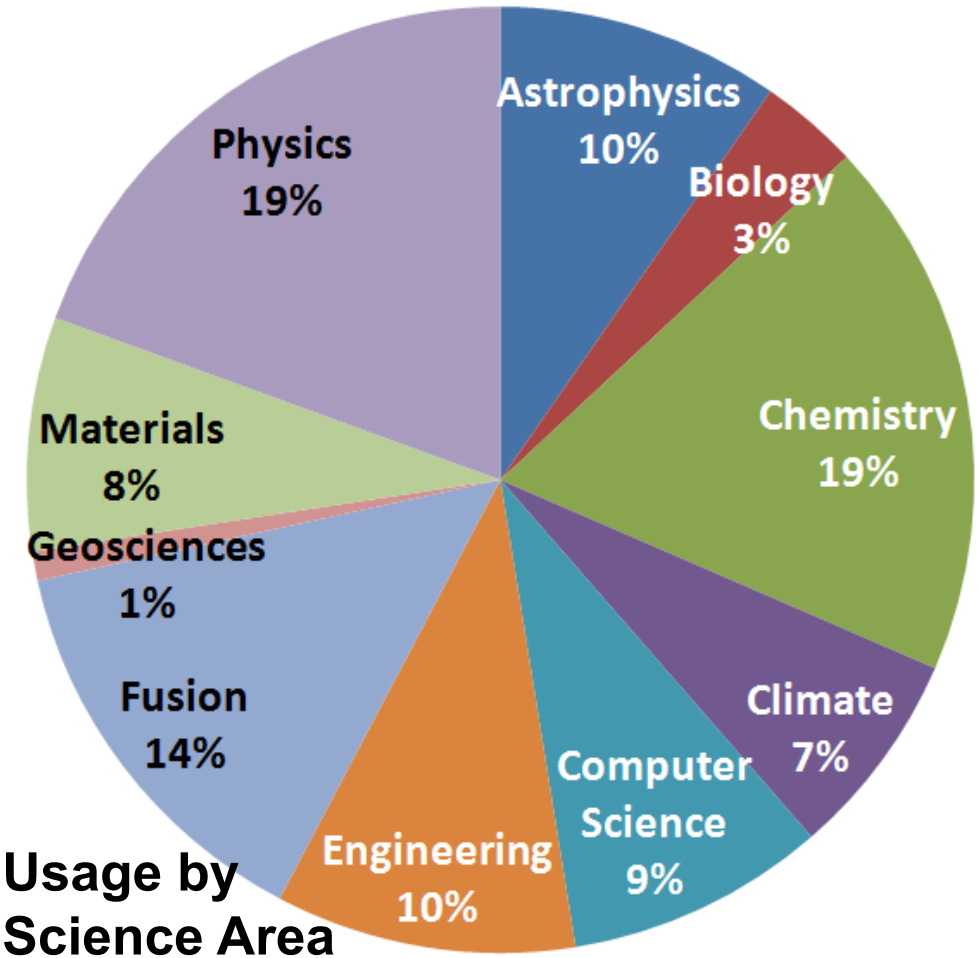
Julia C. White, INCITE Manager
whitejc@DOEleadershipcomputing.org

OLCF User Demographics

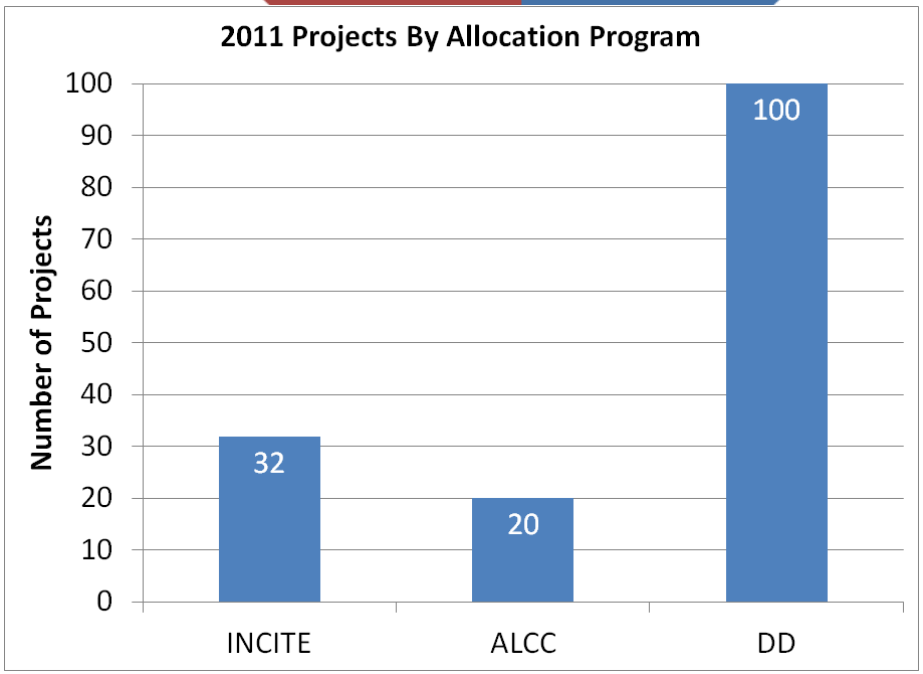
- Number of Users: 857

Percentage of Users by Affiliation





Usage by Science Area



Leadership Metric and Scheduling Policy

As a DOE Leadership Computing Facility, the OLCF has a mandate to be used for large, *leadership-class* (aka *capability*) jobs.

To that end, the OLCF implements queue policies that enable large jobs to run in a timely fashion.

- Basic queue priority is set by the time a job has been waiting relative to other jobs in the queue.
- However, we use several factors to modify the *apparent* time a job has been waiting. These factors include:
  - The job's processor core request size.
  - The queue to which the job is submitted.
  - The 8-week history of usage for the project associated with the job.
  - The 8-week history of usage for the user associated with the job.

Leadership Usage Metric:

35% of the CPU time used on the system will be accumulated by jobs using 20% or more of the available processors (60,000 cores)

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OLCF Scheduling Policy

Bin	Min Cores	Max Cores	Max Walltime (Hours)	Aging Boost (Days)
1	180,000	- - - - -	24	15
2	60,000	179,999	24	5
3	5,008	59,999	12	0
4	2,004	5,007	6	0
5	1	2,003	2	0

Bin 2 is the leadership mark.

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OLCF Allocation Overuse Policy

Projects that overrun their allocation are still allowed to run on LCF systems, although at a reduced priority.

- For projects that have used between 100% and 125% of their allocations, the following rules apply:
  - Jobs have their priority reduced by 30 days.
- For projects that have used greater than 125% of their allocation, the following rules apply:
  - Jobs have their priority reduced by 365 days.

To view the entire scheduling policy please see:
http://www.olcf.ornl.gov/kb_articles/scheduling-policy-olcf/

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OLCF Pull Back Policy for INCITE Projects

On May 1 of the current INCITE calendar year:

- if usage is less than 15% remove up to 15% of the unused balance
- if usage is less than 10% remove up to 30% of the unused balance

On September 1 of the current INCITE calendar year:

- if usage is less than 50% remove up to 33% of the unused balance
- if usage is less than 33% remove up to 50% of the unused balance
- if usage is less than 10% remove up to 75% of the unused balance

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OLCF Quarterly Reports

Principal Investigators of current OLCF projects must submit quarterly progress reports. The quarterly reports are essential as the OLCF must track and report the use of the center's resources.

The OLCF (and DOE Leadership Computing Facilities in general) imposes the following penalties for late submission:

- One Month Late:
  - Job submissions against offending project will be suspended.
- Three Months Late:
  - Login privileges will be suspended for all OLCF resources for all users associated with offending project.

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OLCF Storage Policy

Users are provided with several storage areas, each of which serve different purposes and have different quotas, backup policies, and retention times.

Area	Nickname	Type	Quota	Backups	Purge	Rentention
User Home	-	NFS	5 GB	Yes	Not purged	1 month after project deactivation
User Work	“Spider”	Lustre	None	**No**	Files > 14 days are subject to deletion	Not retained
User Archive	“HPSS”	HPSS	2 TB or 2,000 Files	Yes	Not purged	3 months after project deactivation
Project Home	-	NFS	50GB	Yes	Not purged	1 month after project deactivation
Project Work	“Spider”	Lustre	1 TB	**No**	Not purged	Not retained
Project Archive	“HPSS”	HPSS	45TB (or 4,500 files)	Yes	Not purged	3 months after project deactivation

OLCF Publications

	2011
Number of 2011 publications reported to OLCF or identified by OLCF	670
Number of refereed publications reportable within OA guidance	300

Selected High-Impact

- 1 *Science*
- 25 *Phys. Rev. Lett*
- 4 *Geophy. Rev. Lett*
- 3 *NanoLetters*

OLCF Acknowledgement:

This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

Procedure implemented for collecting publications:

- Collect publications from users' quarterly reports
- Manual search to identify non-reported publications

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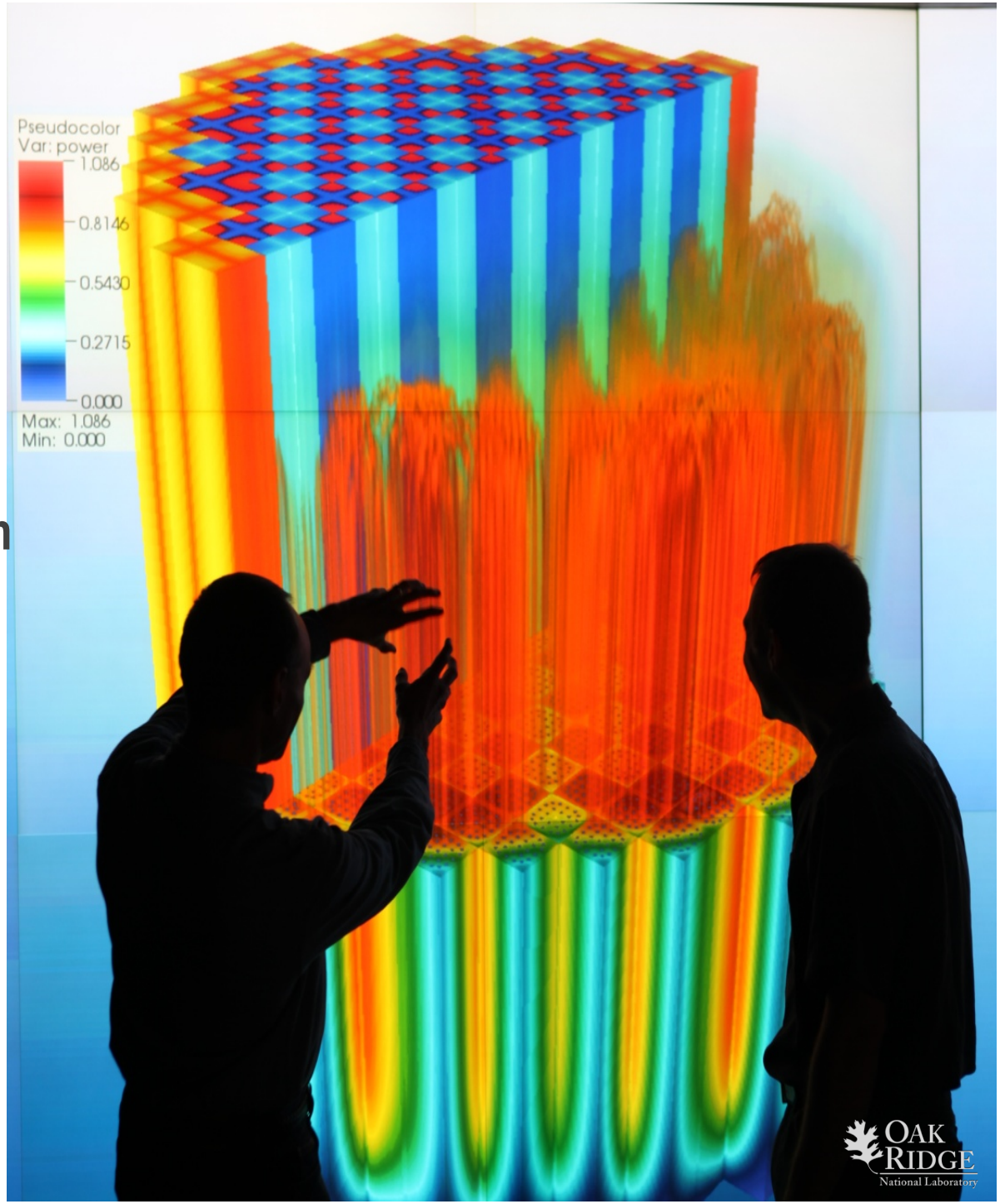
What is Titan?

- The next phase of the Leadership Computing Facility program at ORNL
- An upgrade of Jaguar from 2.3 Petaflops today to between 10 and 20 PF by the end of 2012 with operations in 2013
- Built with Cray's newest XK6 compute blades



Cray XK6 Compute Node

XK6 Compute Node Characteristics
AMD Opteron 6200 Interlagos 16 core processor @ 2.2GHz
Tesla M2090 @ 665 GF with 6GB GDDR5 memory
Host Memory 32GB 1600 MHz DDR3
Gemini High Speed Interconnect
Upgradeable to NVIDIA's next generation KEPLER processor in 2012
Four compute nodes per XK6 blade. 24 blades per rack

Titan breakthrough performance

Jaguar specs (2011)	
Compute nodes	18,688
Login & I/O nodes	512
Memory per node	24 GB
# of Opteron cores	224,256
# of NVIDIA K20 “Kepler” processors (2013)	NA
Total system memory	450 TB
Total system peak performance	2.3 petaflops

Titan specs (2013)	
Compute nodes	18,688
Login & I/O nodes	512
Memory per node	32 GB + 6 GB
# of Opteron cores	299,008
# of NVIDIA K20 “Kepler” processors (2013)	Over 15,000
Total system memory	710 TB
Total system peak performance	20+ petaflops

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Hybrid Programming Model

- On Jaguar today with 299,008 cores, we are seeing the limits of a single level of MPI scaling for most applications
- To take advantage of the vastly larger parallelism in Titan, users need to use hierarchical parallelism in their codes
  - Distributed memory: MPI, SHMEM, PGAS
  - Node Local: OpenMP, Pthreads, local MPI communicators
  - Within threads: Vector constructs on GPU, libraries, CPU SIMD
- ***These are the same types of constructs needed on all multi-PFLOPS computers to scale to the full size of the systems!***

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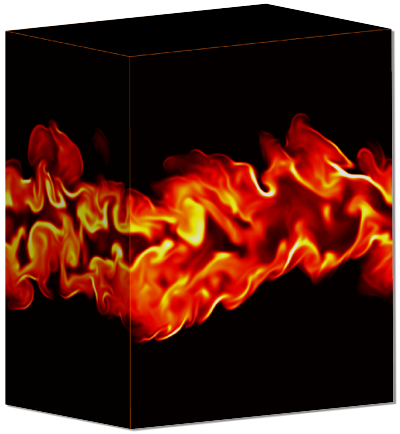
Titan: Early Applications & Stretch Goals

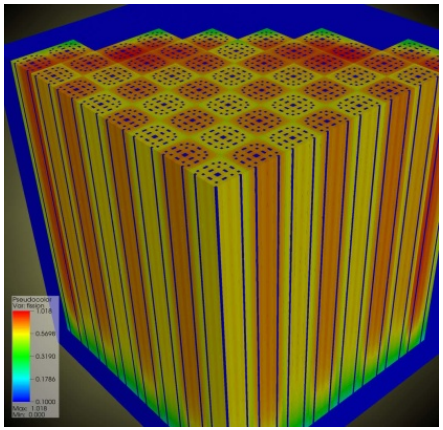
S3D: Turbulent Combustion

Directly solves Navier-Stokes equations. Stretch goals is to move beyond simple fuels to realistic transportation fuels, e.g., iso-octane or biofuels



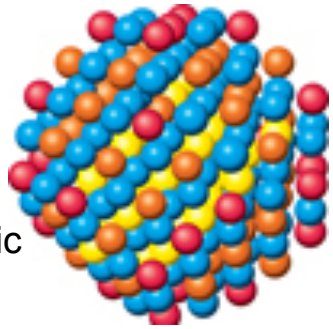
DENOVO: Neutron Transport in Reactor Core

DENOVO is a component of the DOE CASL Hub, necessary to achieve CASL challenge problems



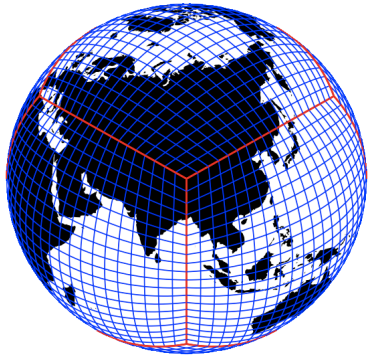
WL-LSMS: Statistical Mechanics of Magnetic Materials

Calculate the free energy for magnet materials. Applications to magnetic recording, magnetic processing of structural materials



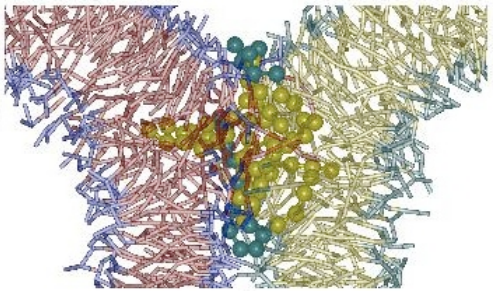
CAM-SE: Community Atmosphere Model – Spectral Elements

CAM simulation using Mozart tropospheric chemistry with 106 constituents at 14 km horizontal grid resolution



LAMMPS: Biological Membrane Fusion

Coarse-grain MD simulation of biological membrane fusion in 5 wall clock days.



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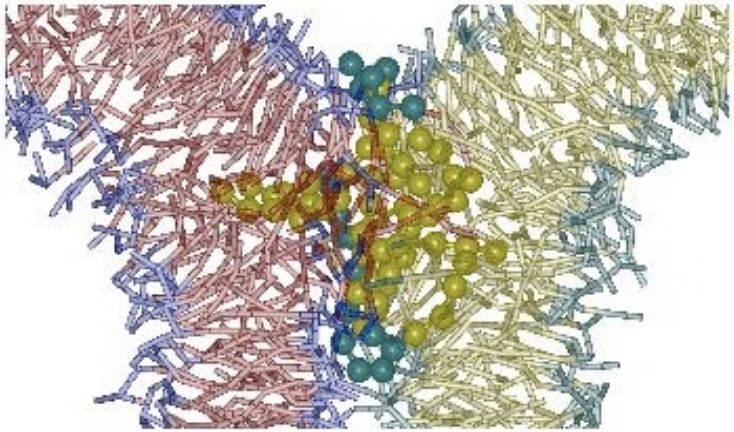
LAMMPS

Large-scale, massively parallel molecular dynamics

Code Description

- Classical N-body problem of atomistic modeling
- Force fields available for chemical, biological, and materials applications
- Long-range electrostatics evaluated using a "particle-particle, particle-mesh" (PPPM) solver.
- 3D FFT in particle-mesh solver limits scaling



Insights into the molecular mechanism of membrane fusion from simulation. Stevens et al., *PRL* **91** (2003)

Porting Strategy

- For PPPM solver, replace 3-D FFT with grid-based algorithms that reduce inter-process communication
- Parallelism through domain decomposition of particle-mesh grid
- Accelerated code builds with OpenCL or CUDA

Early Performance Results on XK6:

- XK6 outperforms XE6 by 3.2x

Science Target (20PF Titan)

- Simulate biological membrane fusion in coarse-grained MD within 5 wall clock days

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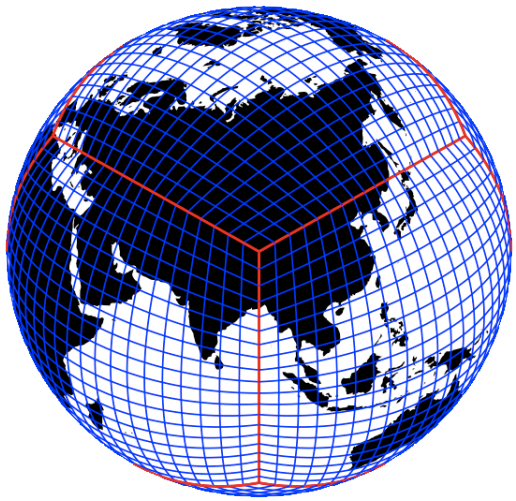
CAM-SE

Community Atmosphere Model – Spectral Elements

Code Description

- Employs equal-angle, cubed-sphere grid and terrain-following coordinate system.
- Scaled to 172,800 cores on XT5
- Exactly conserves dry mass without the need for *ad hoc* fixes.
- Original baseline code achieves parallelism through domain decomposition using one MPI task per element



Cubed-sphere grid of CAM spectral element model. Each cube panel is divided into elements.

http://www-personal.umich.edu/~paullric/A_CubedSphere.png

Porting Strategy

- Using realistic "Mozart" chemical tracer network, tracer transport (i.e., advection) dominates the run time.
- Use hybrid MPI/OpenMP parallelism
- Intensive kernels are coded in CUDA Fortran
- Migration in future to OpenACC

Early Performance Results on XK6:

- Refactored code was 1.7x faster on Cray XT5
- XK6 outperforms XE6 by 1.5x

Science Target (20PF Titan)

- CAM simulation using Mozart tropospheric chemistry with 106 constituents at 14 km horizontal grid resolution

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How Effective are GPUs on Scalable Applications?

OLCF-3 Early Science Codes -- Performance Measurements on TitanDev

Application	XK6 vs. XE6 Performance Ratio Titan Dev : Monte Rosa
S3D Turbulent combustion	**1.4**
Denovo 3D neutron transport for nuclear reactors	**3.3**
LAMMPS Molecular dynamics	**3.2**
WL-LSMS Statistical mechanics of magnetic materials	**1.6**
CAM-SE Community atmosphere model	**1.5**

Cray XK6: Fermi GPU plus AMD 16-core Opteron CPU
XE6: 2X AMD 16-core Opteron CPUs

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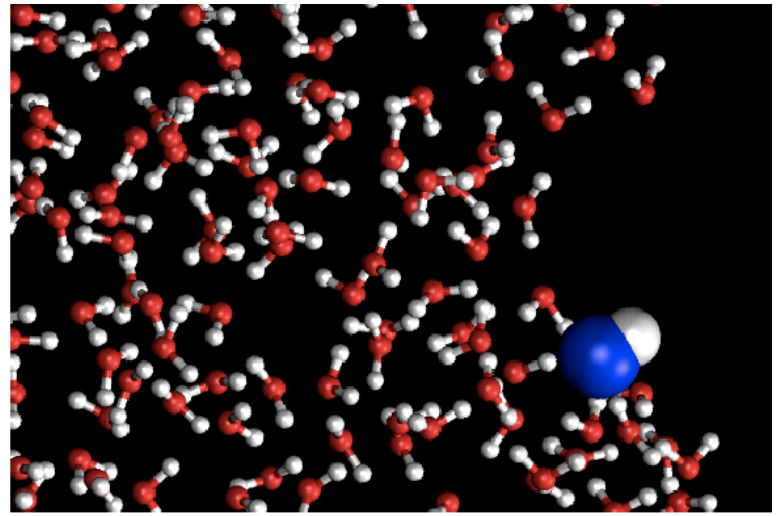
Performance of additional community codes

CP2K: Molecular Simulation

J. Hütter, J. VandeVondele, Zürich

Explore electronic and chemical phenomena in complex systems and materials. Compute the free-energy profiles of individual chemical reactions using ensemble methods to statistically explore the important configurations that give rise to novel phenomena,

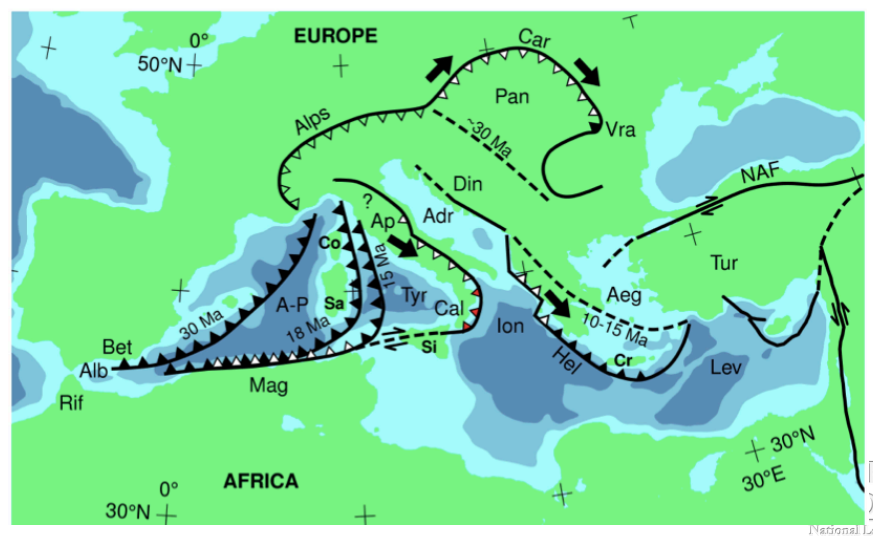


SPECFEM-3D Seismic Imaging

O. Schenk, Lugano

Seismic imaging uses waves generated by earthquakes to reveal the structure of the solid Earth. SPECFED-3D can be used to solve both the forward problem and the inverse problem. Inverse problems require of O(10^8) core-hours.

Mediterranean-Calabria Paleotectonics

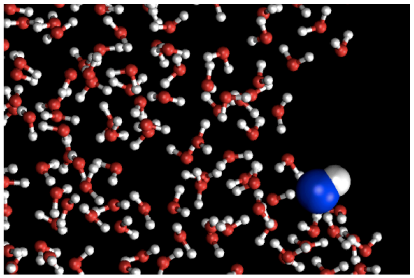


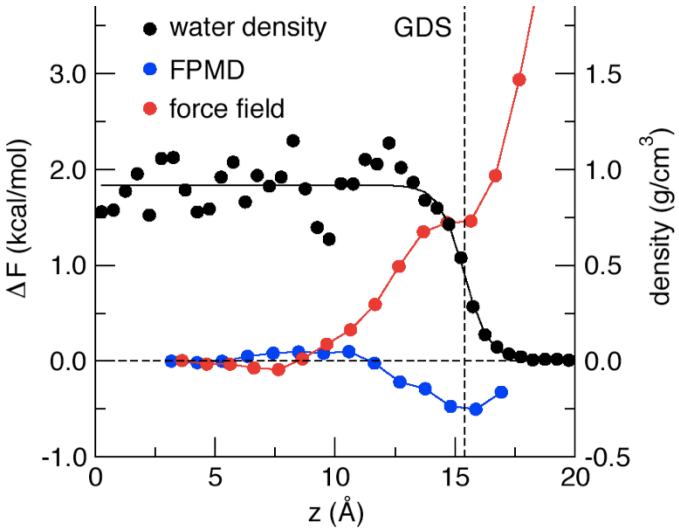
CP2K

"Swiss-army knife for molecular science"

Code Description

- Open source, global user base
  - J. Hutter, J. VandeVondele
- Density-functional theory:
  - Linear-scaling SCF
  - GGA, HFX, & MP2
- Hybrid QM/MM calculations
- Dense & sparse linear algebra
- Regular grid: multigrid and FFT





Is the surface of liquid water is acidic or basic? Mundy et al. show that the hydroxide anion is slightly stabilized at the interface – **Mundy, et al., *Chem. Phys. Letts.* 481, 2 (2009)**

Porting Strategy

(J. VandeVondle, ETH)

- Port sparse linear algebra library
- Matrix multiply kernels are coded in CUDA
- MPI performance is crucial
- Early days, results will improve

Early Performance Results on XK6:

Peter Messmer (NVIDIA)

- XK6 outperforms XE6 by 1.5x

Science Target (20PF Titan)

Chris Mundy (PNNL)

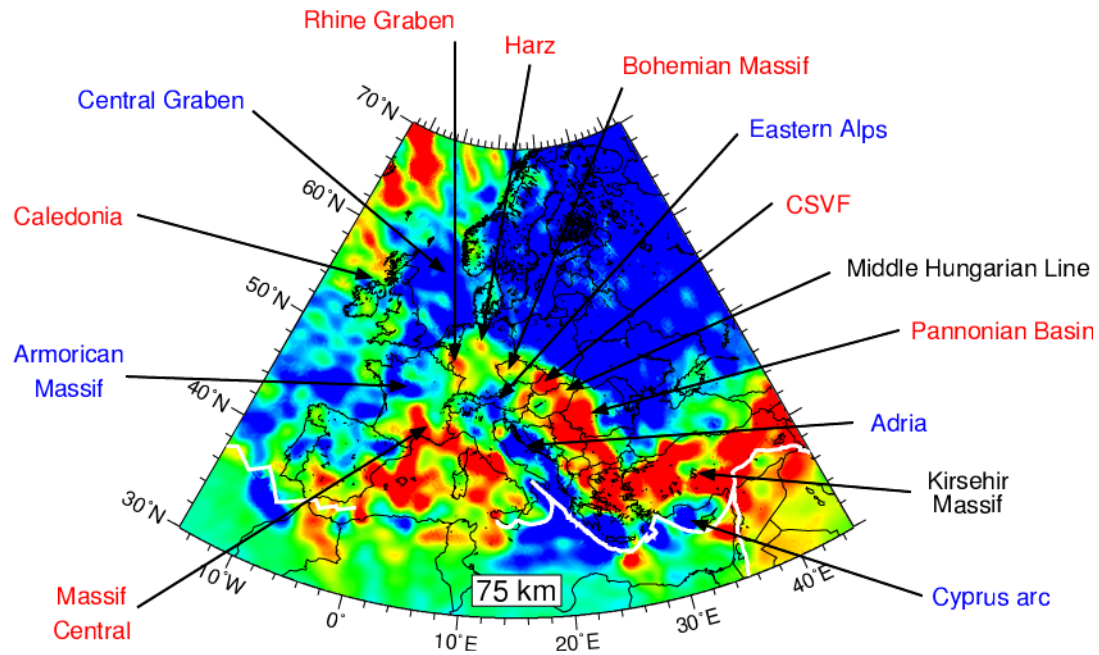
- Ion adsorption at interfaces, for fuel cells, chemical catalysis, biological pumps, atmospheric science

SPECFEM-3D

Seismic imaging

Code Description

- Open source, global user base
- Spectral element wave propagation
- Unstructured grids
- Explicit time propagation
- Full-space waveform inversion
- MPI parallel, excellent scaling
- GB Prize (SC03, SC08 - finalist)



Porting Strategy

(Olaf Schenk - Lugano)

- Force calculation is the heaviest kernel
- Stencil kernels are memory bound, data locality is crucial
- CUDA accelerated

Early Performance Results on XK6:

Peter Messmer (NVIDIA)

- XK6 outperforms XE6 by 2.5x

Science Target (20PF Titan)

Jeroen Tromp (Princeton)

- Adjoint tomography of the entire planet -- requires analysis of 5,000 earthquakes worldwide, using an estimated 739 million core-hours (on Cray XT5)

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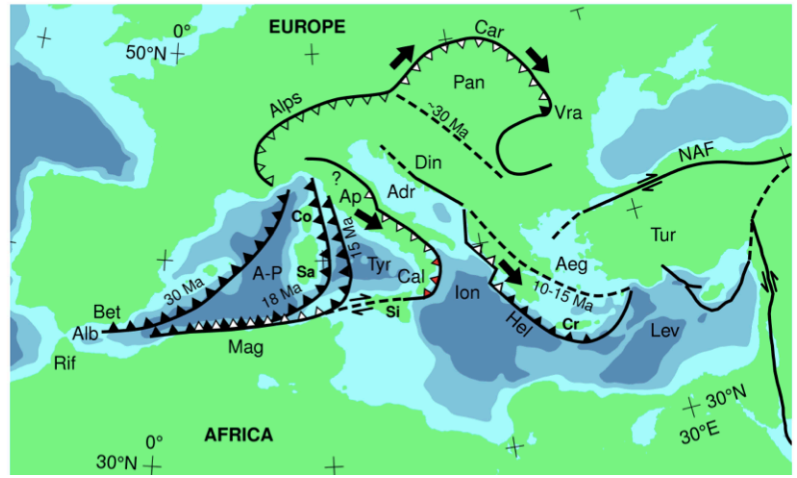

Analysis of 190 European quakes revealed seismic hotspots in the upper mantle. The imaging detailed the subduction of Africa, volcanism in the Czech Republic, a "hole" under Bulgaria, and Italy's counterclockwise rotation over the past 6 million years. J. Tromp, ACSS Symposium

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Additional Applications from Community Efforts
Current performance measurements on TitanDev

Application	XK6 vs. XE6 Performance Ratio Titan Dev : Monte Rosa
NAMD High-performance molecular dynamics	**1.4**
Chroma High-energy nuclear physics	**6.1**
QMCPACK Electronic structure of materials	**3.0**
SPECFEM-3D Seismology	**2.5**
GTC Plasma physics for fusion-energy	**1.6**
CP2K Chemical physics	**1.5**

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Titan milestones

- Jaguar to Titan hardware upgrade complete
- Currently in acceptance process
- 4x to 8x improvement in many scientific applications

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Questions & Discussion