GPU TECHNOLOGY CONFERENCE

20 Years of Excellence in Computational Science

OLCF

OAK RIDGE LEADERSHIP COMPUTING FACILITY

1992—2012

GPU-Accelerated Science on Titan

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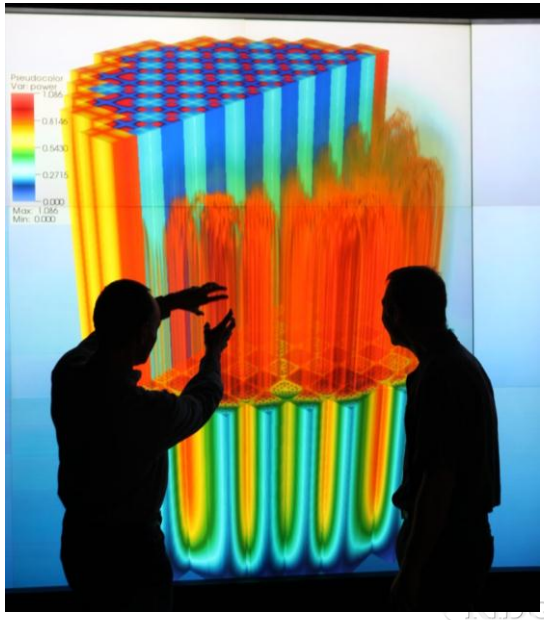
May 15, 2012

GTC 2012

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.



FOR IMMEDIATE RELEASE:

SANTA CLARA, Calif. —Sep. 30, 2009—Oak Ridge National Laboratory (ORNL) announced plans today for a new supercomputer that will use NVIDIA®'s next generation CUDA™ GPU architecture, codenamed "Fermi". Used to pursue research in areas such as energy and climate change, ORNL's supercomputer is expected to be 10-times more powerful than today's fastest supercomputer.

Jeff Nichols, ORNL associate lab director for Computing and Computational Sciences, joined NVIDIA co-founder and CEO Jen-Hsun Huang on stage during his keynote at NVIDIA's GPU Technology Conference. He told the audience of 1,400 researchers and developers that "Fermi" would enable substantial scientific breakthroughs that would be impossible without the new technology.

"This would be the first co-processing architecture that Oak Ridge has deployed for open science, and we are extremely excited about the opportunities it creates to solve huge scientific challenges," Nichols said.

Presentations of GPU-accelerated science

Jacqueline H. Chen (Sandia National Laboratories)
"Direct Numerical Simulation of Turbulence-Chemistry Interactions: Fundamental Insights Towards Predictive Models"

Ray Grout (National Renewable Energy Laboratory)
"S3D Direct Numerical Simulation - Preparations for the 10-100PF Era"

William Tang (Princeton Plasma Physics Laboratory (Princeton)
"Fusion Energy Sciences & Computing at the Extreme Scale"

John A. Turner (Oak Ridge National Laboratory)
"Transforming Modeling and Simulation for Nuclear Energy Applications"

Loukas Petridis (Oak Ridge National Laboratory)
"Computer Simulation of Lignocellulosic Biomass"

Jeroen Tromp (Princeton University)
"Toward Global Seismic Imaging based on Spectral-Element and Adjoint Methods"

Outline: Titan project overview

- Goals of Titan project
- Cray XK6 nodes
- Titan system
- Upgrade process
- Programming model
- Tools
- Early Performance Results

Titan System Goals: Deliver breakthrough science for DOE/SC, industry, and the nation

Earth System Science

Understanding our earth and the processes that impact it

- Sea level rise
- Regional climate change
- Geologic carbon sequestration
- Sustainability of biofuels
- Earthquakes and Tsunamis

Energy

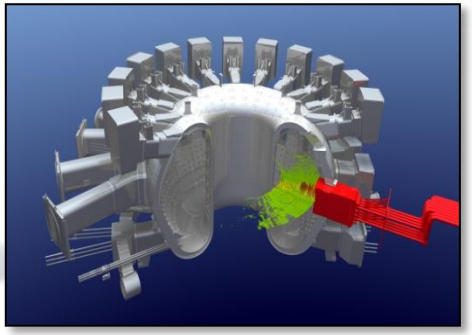
Reducing U.S. reliance on foreign energy & reducing carbon footprint of production

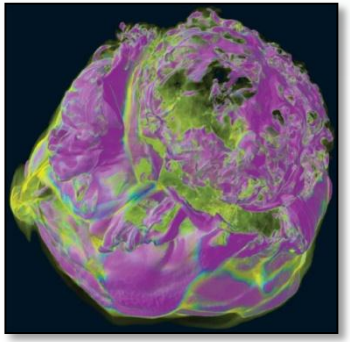
- Carbon free energy production from fusion, fission, solar, wind, and geothermal sources
- Improving the efficiency of combustion energy sources

Fundamental Science

Understanding the physical processes from the scale of subatomic particles to the universe

- Extend our knowledge of the natural world
- Deliver new technologies to advance energy mission





Accomplishing these missions requires the power of Titan

Titan System Goals: Promote application development for highly scalable architectures through the Center for Accelerated Application Readiness (CAAR)

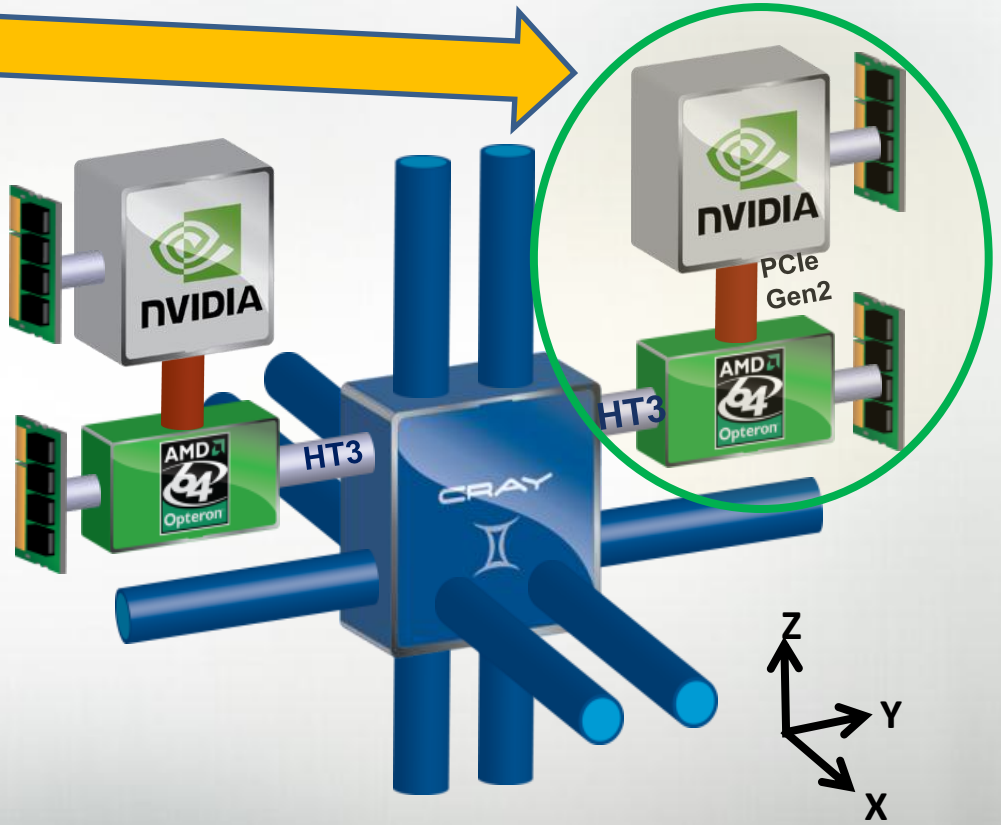
Using six representative apps to explore techniques to effectively use highly scalable architectures

- **CAM-SE** – Atmospheric model
- **Denovo** – Nuclear reactor neutron transport
- **wl-LSMS** - First principles statistical mechanics of magnetic materials
- **S3D** – Combustion model
- **LAMMPS** – Molelcular dynamics
- **NRDF** – Adaptive mesh refinement

- Data locality
- Explicit data management
- Hierarchical parallelism
- Exposing more parallelism through code refactoring and source code directives
- Highly parallel I/O
- Heterogeneous multi-core processor architecture

Cray XK6 Compute Node

XK6 Compute Node Characteristics
AMD Opteron 6200 Interlagos 16 core processor
Tesla X2090 @ 665 GF
Host Memory 16 or 32GB 1600 MHz DDR3
Tesla X090 Memory 6GB GDDR5 capacity
Gemini High Speed Interconnect
Upgradeable to NVIDIA's KEPLER many-core processor



Slide courtesy of Cray, Inc.

ORNL's "Titan" System

- Upgrade of Jaguar from Cray XT5 to XK6
- Cray Linux Environment operating system
- Gemini interconnect
  - 3-D Torus
  - Globally addressable memory
  - Advanced synchronization features
- AMD Opteron 6274 processors (Interlagos)
- New accelerated node design using NVIDIA multi-core accelerators
  - 2011: 960 NVIDIA x2090 "Fermi" GPUs
  - 2012: 14,592 NVIDIA "Kepler" GPUs
- 20+ PFlops peak system performance
- 600 TB DDR3 mem. + 88 TB GDDR5 mem

Titan Specs	
Compute Nodes	18,688
Login & I/O Nodes	512
Memory per node	32 GB + 6 GB
# of Fermi chips (2012)	960
# of NVIDIA "Kepler" (2013)	14,592
Total System Memory	688 TB
Total System Peak Performance	20+ Petaflops
Cross Section Bandwidths	X=14.4 TB/s Y=11.3 TB/s Z=24.0 TB/s

Two Phase Upgrade Process

- Phase 1: XT5 to XK6 without GPUs
  - Replace all XT5 nodes with XK6 nodes
  - 16-core processors, 32 GB/node, Gemini
  - 960 nodes (10 cabinets) have NVIDIA Fermi GPUs
  - Users ran on half of system while other half was upgraded
- Phase 2: Add NVIDIA Kepler GPUs
  - Cabinet Mechanical and Electrical upgrades
    - New air plenum bolts on to cabinet
    - Larger fan
    - Additional power supply
  - Rolling upgrade of node boards
    - Pull board, add 4 Kepler GPUs modules, replace board, test, repeat 3,647 times!
    - Keep most of the system available for users during upgrade
  - Acceptance test of system

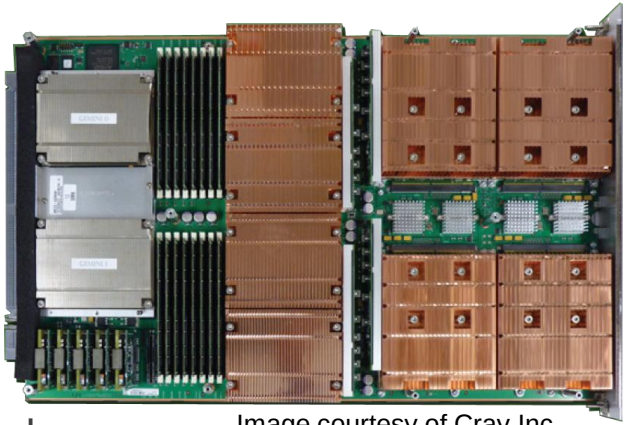


Image courtesy of Cray Inc.

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!***

How do you program these nodes?

- **Compilers**
  - OpenACC: Open standard for compiler directives that allows the expression of hierarchical parallelism in the source code so that the compiler can generate parallel code for the target platform, be it GPU, MIC, or vector SIMD on CPU
  - Cray compiler supports XK6 nodes and is OpenACC compatible
  - CAPS HMPP compiler supports C, C++ and Fortran compilation for heterogeneous nodes and is adding OpenACC support
  - PGI compiler supports OpenACC and CUDA Fortran
  - CrayPAT and Cray Apprentice support XK6 programming

How do you program these nodes?

- **Tools**
  - Allinea DDT debugger scales to full system size and with ORNL support will be able to debug heterogeneous (x86/GPU) apps
  - ORNL has worked with the Vampir team at TUD to add support for profiling codes on heterogeneous nodes
  - CrayPAT and Cray Apprentice support XK6 programming

Titan Tool Suite

Compilers	Performance Tools	GPU Libraries	Debuggers	Source Code
Cray PGI CAP-HMPP Pathscale NVIDIA CUDA GNU Intel	CrayPAT Apprentice Vampir VampirTrace TAU HPCToolkit CUDA Profiler	MAGMA CULA Trillinos libSCI	DDT NVIDIA Gdb	HMPP Wizard

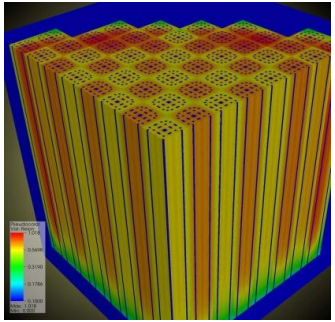
Titan: Early Applications & Stretch Goals

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

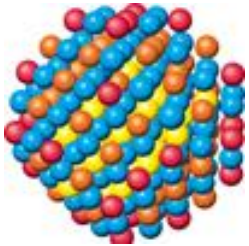
DENOVO: Neutron Transport in Reactor Core

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

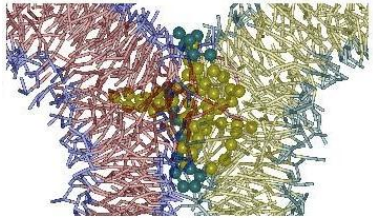


CAM-SE: Community Atmosphere Model – Spectral Elements

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

LAMMPS: Biological Membrane Fusion

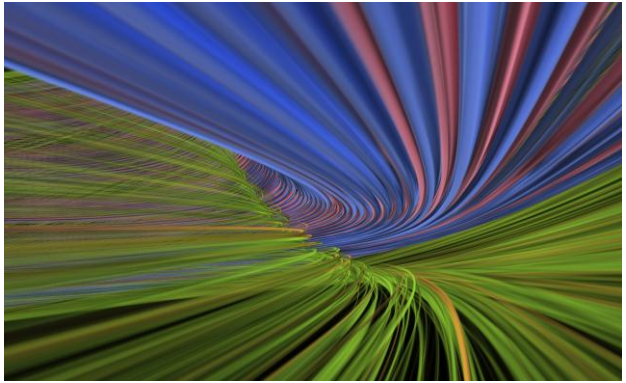
Coarse-grain MD simulation of biological membrane fusion in 5 wall clock days.

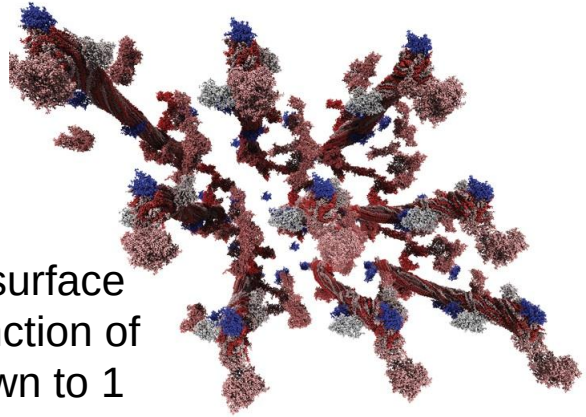


Additional Applications from Community Efforts

GTC: Magnetic confinement of fusion plasmas

Increasingly faster supercomputers enable new physics insights with GTC, the first fusion code delivering production simulations at petaflops in 2009.



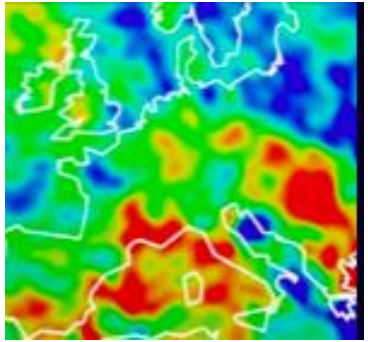


GROMACS: Biophysics and Biofuels

Understand the surface structure and function of lignin clumps down to 1 angstrom length scale

SPECFEM-3D: Seismological Imaging

Seismic inverse modeling and imaging to reveal seismic hotspots (red indicates fast seismic shear wave speeds whereas blue indicates slow wave speeds).



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 Interlagos CPU

XE6: AMD Dual Interlagos

Oak Ridge National Laboratory

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**

Oak Ridge National Laboratory

Access to Titan via INCITE

INCITE seeks computationally intensive, large-scale research projects with the potential to significantly advance key areas in science and engineering.

1 **Impact criterion**

High-impact science and engineering

2 **Computational leadership criterion**

Computationally intensive runs that cannot be done anywhere else

3 **Eligibility criterion**

- INCITE grants allocations regardless of funding source (ex. DOE, NSF, private, etc)
- Researchers at non-US institutions may apply

Email: INCITE@DOEleadershipcomputing.org
Web: http://hpc.science.doe.gov

Call for 2013 proposals open now through June 27, 2012

The INCITE program seeks proposals for high-impact science and technology research challenges that require the power of the leadership-class systems

In 2013 over 4 billion core-hours will be available through the INCITE program

Questions?

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