

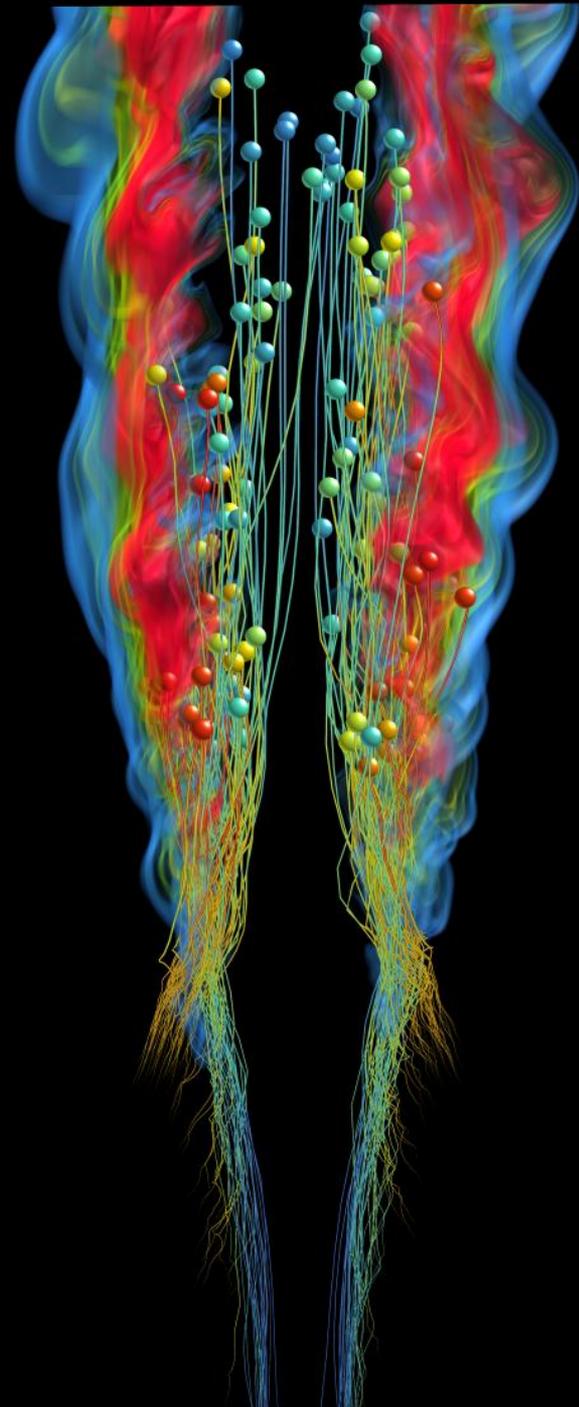
# *Keeneland: Toward Exascale Computational Science with Graphics Processors*

**Jeffrey Vetter**

Presented to

**SC09**

**NVIDIA**



# Contributors

- **Jeffrey Vetter, Jack Dongarra, Richard Fujimoto, Thomas Schulthess, Karsten Schwan, Sudha Yalamanchili, Kathlyn Boudwin, Jim Ferguson, Doug Hudson, Patricia Kovatch, Bruce Loftis, Jeremy Meredith, Jim Rogers, Philip Roth, Arlene Washington, Phil Andrews, Mark Fahey, Don Reed, Tracy Rafferty, Ursula Henderson, Terry Moore, and many others**
- NVIDIA
- HP



- Keeneland Sponsor: NSF
- Other sponsors: DOE, DOD, DARPA

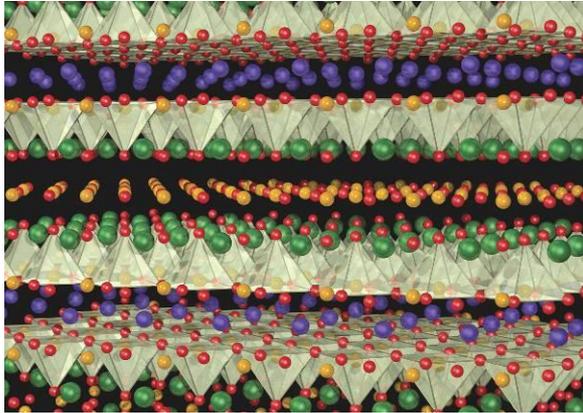
# Overview

- Predictive scientific simulation is important for scientific discovery
- HPC systems have been highly successful
- The HPC community has several (new) constraints
- Heterogeneous computing with GPUs offers some opportunities and challenges
- Newly awarded NSF partnership will provide heterogeneous supercomputing for open science
  - ORNL-Cray-NVIDIA announced system also using graphic processors

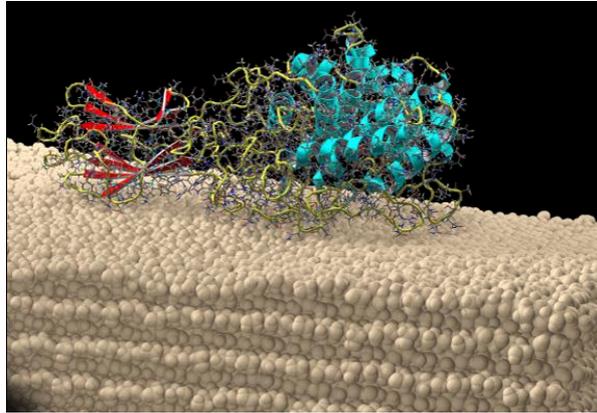
A satellite-style image of Earth, showing the Americas (North and South America) and surrounding oceans. The image features swirling cloud patterns and a dark blue ocean. The text "SCIENTIFIC SIMULATION" is overlaid in red, italicized, bold font across the lower portion of the image.

***SCIENTIFIC SIMULATION***

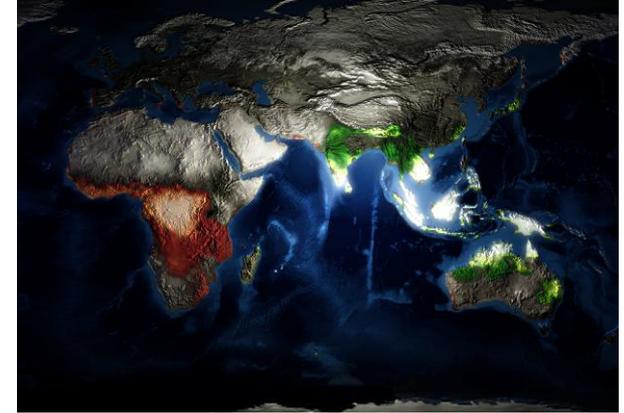
# Leadership computing is advancing scientific discovery



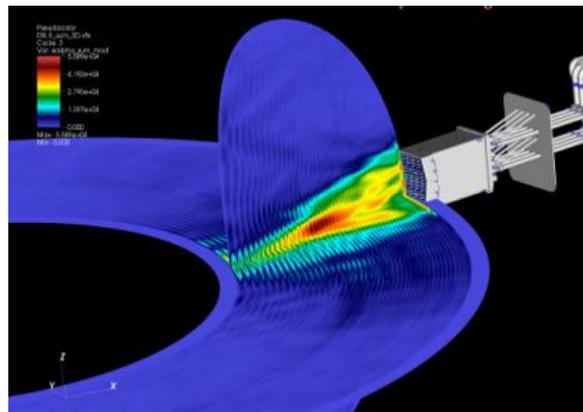
Resolved decades-long controversy about modeling physics of high temperature superconducting cuprates



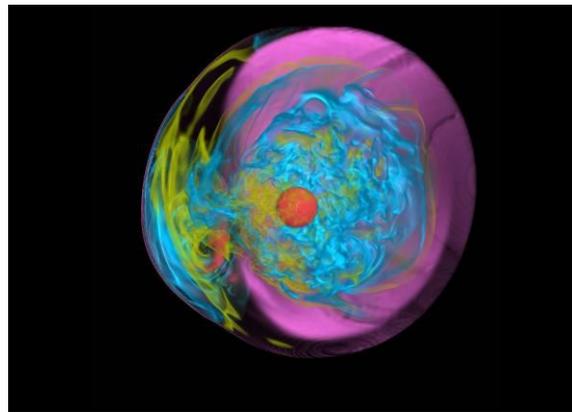
New insights into protein structure and function leading to better understanding of cellulose-to-ethanol conversion



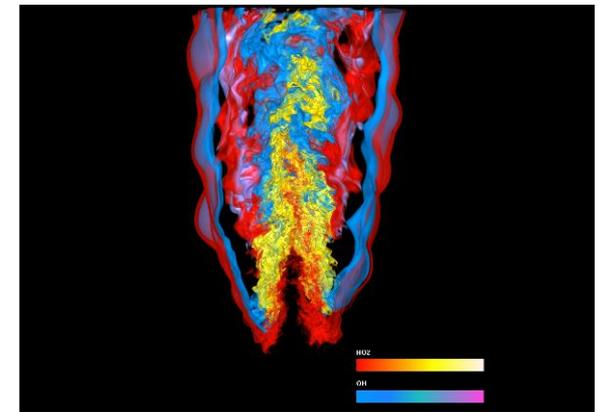
Addition of vegetation models in climate code for global, dynamic CO<sub>2</sub> exploration



First fully 3D plasma simulations shed new light on engineering superheated ionic gas in ITER



Fundamental instability of supernova shocks discovered directly through simulation

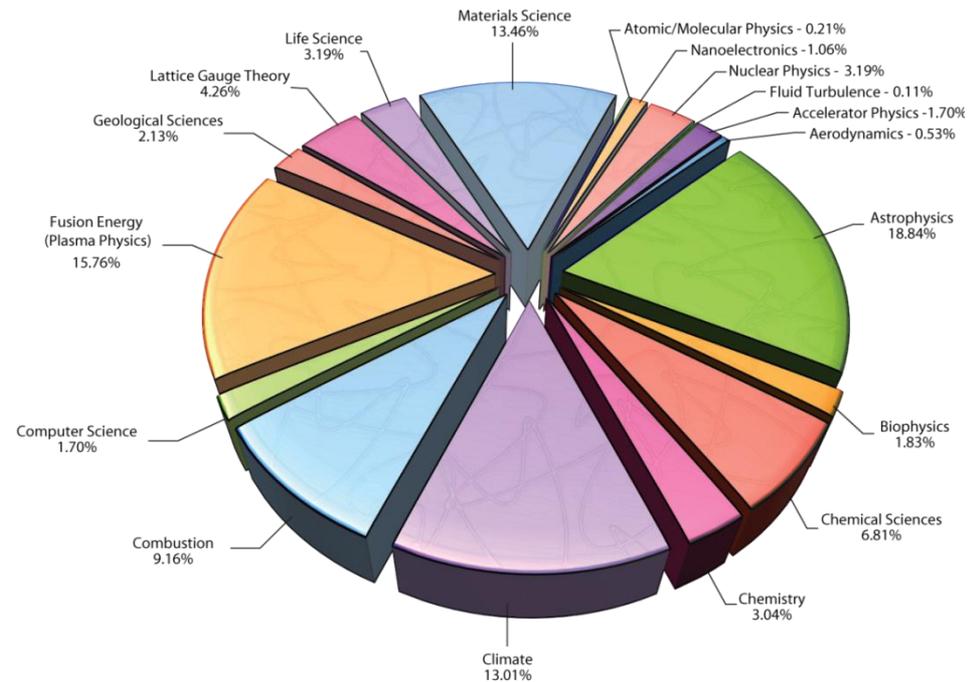
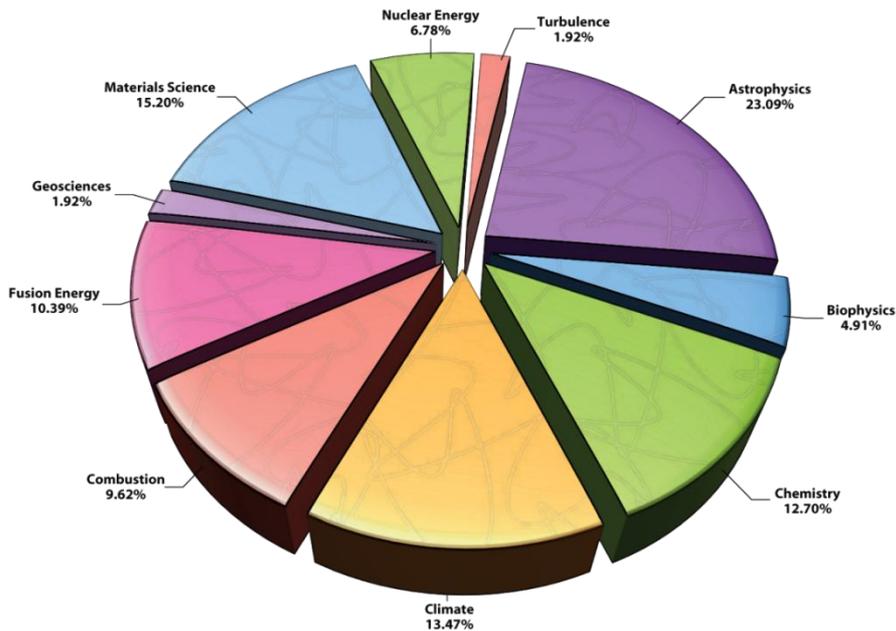


First 3-D simulation of flame that resolves chemical composition, temperature, and flow

# Jaguar XT5 science workload

- **Current: Transition to operations**
- **27 early-access projects, January–July**
  - > Total allocation: 540.8M hours
  - > Usage since January: 247M hours (159 users)
- **ALCC project: FY09 Joule metric applications**
  - > Total allocation: 25M hours
  - > Usage since January: 17M hours (17 users)

- **Fall 2009: General availability**
- **38 INCITE projects transitioned to system**
  - > Total allocation: 469M hours
  - > Usage (XT4) since January: 91M hours (448 users)
- **Discretionary projects: Climate AR5 production**
  - > Total allocation: 80M hours
  - > 2 projects: NCAR/DOE and NOAA (~50 users)



# Highly visible science output

PHYSICAL REVIEW LETTERS  
PRL 106, 23701 (2008)

**Dynamics of the Pairing Interaction in the Hubbard and  $t$ - $J$  Models of High-Temperature Superconductors**

T. A. Maier,<sup>1,2</sup> D. Poilblanc,<sup>2</sup> and D. J. Scalapino<sup>1</sup>

<sup>1</sup>Center for Nanophase Materials Science and Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6046, USA

<sup>2</sup>Laboratoire de Physique Théorique, CNRS & Université de Toulouse, F-31062 Toulouse, France

<sup>3</sup>Department of Physics, University of California, Santa Barbara, California 93106-5080, USA

(Received 28 January 2008; published 10 June 2008)

The question of whether one should speak of a "pairing glue" in the Hubbard and  $t$ - $J$  models is basically a question about the dynamics of the pairing interaction. If the dynamics of the pairing interaction arises from virtual states, whose energies compared to the  $d$ -band gap give rise to the exchange coupling  $J$ , the interaction is instantaneous on the relative time scales of interest. In this case,

## Physical Review Letters: High temperature superconductivity

turning  $D$ - $\pi$  and infrared conductivity [10,11] studies, ...

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ScienceDirect  
Combustion and Flame

Three-dimensional direct numerical simulation of soot formation and transport in a temporally evolving nonpremixed ethylene jet flame

David O. Lignell<sup>a,b,\*</sup>, Jacqueline H. Chen<sup>b</sup>, Philip J. Smith<sup>a</sup>

<sup>a</sup>Department of Chemical Engineering, University of Utah, Salt Lake City, UT 84098, USA

ELSEVIER

Combustion and Flame

www.elsevier.com/locate/combustionandflame

## Combustion and Flame: 3D flame simulation

Three-dimensional direct numerical simulation of soot formation and transport in a temporally evolving nonpremixed ethylene jet flame

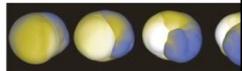
LETTERS

**Pulsar spins from an instability in the accretion shock of supernovae**

John M. Blondin<sup>a</sup> & Anthony Mezzacappa<sup>a</sup>

Rotation-powered radio pulsars are born with inferred initial rotation periods of order 500 ms (some as short as 20 ms) in core-collapse supernovae. In the traditional picture, this fast rotation is the result of conservation of angular momentum during the collapse of a rotating stellar core. This leads to the inevitable conclusion that pulsar spins are directly correlated with the rotation of the progenitor star. So far, however, stellar theory has not been able to explain the distribution of pulsar spins, suggesting that the birth rotation is either too slow or too fast. Here we report a robust instability of the stalled accretion shock in core-collapse supernovae that is able to generate a strong rotational flow in the vicinity of the accreting proto-neutron star. Sufficient angular momentum is deposited on the proto-neutron star to generate a final spin period consistent with observations, even beginning with spherically symmetrical initial conditions. This provides a new mechanism for the generation of rotation rates in supernovae. Our fast breaks, the assumed correlation between the period of supernova progenitor cores and pulsar spin, is followed by a brief epoch of fast spins in which the momentary accretion shock wave stalls at a radius  $R_{\text{stall}}$  and is revived, and the supernova initiates an "underdriven mechanism". Hydrodynamic simulations show that this quasi-steady shock is subject to the stall from shock instability, or SASI. However, these two simulations admit only axisymmetric modes and, long-term dynamics cannot affect the rotation of the accreting shock here, in three dimensions non-axisymmetric modes can affect the angular momentum of the collapsed core.

We have performed on a three-dimensional cartesian grid a series of simulations of a steady accretion shock, following the numerical approach described in ref. 4 and in the Supplementary Information. We found that the combined evolution of the SASI is dominated by a low-order non-axisymmetric mode characterized by a spiral flow



**Figure 1** The evolution of the accretion shock illustrates the rotation of the spiral mode of the SASI. The color gradient of the shock surface represents the leading portion of the spiral SASI wave, with flow propagating from right to left across the front face of the shock. The

ated pairing, one says that the spin fluctuations provide the positive glue. On the other hand, whether there is a pairing interaction, different pairing interaction techniques we refer to the pairing interaction region characteristic signature that the system is driven by inelastic neutrons or frequency dependence of the Nambu self-energy  $\Sigma(\omega, \mathbf{k}) = \Delta(\omega, \mathbf{k})/i\omega$ , (1)

LETTERS

**Clumps and streams in the local dark matter distribution**

J. Diemand, M. Kuhlen<sup>a</sup>, P. Madaam<sup>a</sup>, M. Zemp<sup>b</sup>, B. Moore<sup>c</sup>, D. Potter<sup>d</sup> & J. Stadel<sup>d</sup>

In cold dark matter cosmological models, structures form and grow hierarchically. Numerical simulations of the local area indicate that the local dark matter distribution is highly inhomogeneous, with a complex structure even in the immediate vicinity of the Sun. We present a new method for measuring the local dark matter distribution and show that the local dark matter distribution is highly inhomogeneous, with a complex structure even in the immediate vicinity of the Sun. We present a new method for measuring the local dark matter distribution and show that the local dark matter distribution is highly inhomogeneous, with a complex structure even in the immediate vicinity of the Sun.



**Figure 2** Via Lactea II projected dark matter spatial density map. A cube of 100 pc on each side, centered on the Sun, is shown. The color scale ranges from 0.05 to 0.15 GeV cm<sup>-3</sup>. The map shows the local dark matter distribution and properties. We used the

decided mechanism. A four-step, three-moment, semiempirical soot model is employed. Previous two-dimensional soot models have shown the importance of multidimensional flame dynamic effects on soot formation. Here, we show that the importance of multidimensional flame dynamic effects on soot formation is strongly impacted by the diffusive motion of the flame relative to soot (which is convective), resulting in soot being differentially transported toward or away from the flame. We show that the importance of multidimensional flame dynamic effects on soot formation is strongly impacted by the diffusive motion of the flame relative to soot (which is convective), resulting in soot being differentially transported toward or away from the flame. We show that the importance of multidimensional flame dynamic effects on soot formation is strongly impacted by the diffusive motion of the flame relative to soot (which is convective), resulting in soot being differentially transported toward or away from the flame.

**I. Introduction**

Soot formation in turbulent hydrocarbon combustion is of great practical importance. Soot emission is a known health hazard, and its presence indicates reduced combustion efficiency. Soot formation is responsible for the bulk of flame luminosity and radiative heat transfer. For these reasons, and others, soot formation in laminar and turbulent flames is a subject of intense research interest.

The cold dark matter (CDM) model has been remarkably successful at describing the large-scale mass distribution of our Universe from the hot Big Bang to the present. However, the nature of the dark matter particles is not known, and this is a major challenge in particle physics. The CDM model is a simple extension of the Standard Model of particle physics, and it is a major challenge in particle physics. The CDM model is a simple extension of the Standard Model of particle physics, and it is a major challenge in particle physics.

**Figure 1** Via Lactea II projected dark matter spatial density map. A cube of 100 pc on each side, centered on the Sun, is shown. The color scale ranges from 0.05 to 0.15 GeV cm<sup>-3</sup>. The map shows the local dark matter distribution and properties. We used the

JULY 2008 VOLUME 16 NUMBER 7

# PHYSICS OF PLASMAS

Simulation of high-power electromagnetic wave heating in the ITER burning plasma by E. F. Jaeger, I. A. Berry, E. F. D'Arco, R. F. Barrett, S. D. Barab, D. W. Swain, D. B. Batchelor, R. W. Harvey, J. R. Myra, D. A. D'ippolito, C. K. Phillips, E. Valeo, D. A. Smith, P. T. Bonoli, J. C. Wright, and M. Chen

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AMERICAN INSTITUTE OF PHYSICS

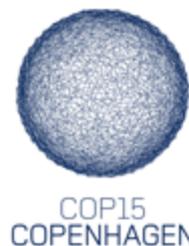
## Physics of Plasmas: ICRF heating in ITER

Transformational science enabled by advanced scientific computing

# Examples: Climate Modeling



- **Assess scientific basis, impact, adaptation, vulnerability, mitigation**
  - > Observation and simulation play critical roles
- ***Profound impact on worldwide socioeconomic policy, energy, etc***
  - > UN Conference - Sep 09
  - > Copenhagen Climate conference – Dec 09
- **Intergovernmental Panel On Climate Change**
  - > Sponsored by UNEP and WMO
  - > Thousands of scientists from around the world



UNITED NATIONS  
CLIMATE CHANGE  
CONFERENCE  
DEC 7-DEC 18  
2009

<http://www.ipcc.ch>

<http://en.cop15.dk/>

# Application Complexity

- Today's applications are quickly becoming more complex than earlier applications
  - > Exascale Town Hall report [1]
- Increased fidelity
- Answering more complex questions
  - > Scientists [2,3] working on model that combines
    - Climate model
    - Energy economics
    - Population movements, demographics

**New physics capabilities are continuously integrated into ALE3D**

- Dates are approximate, and represent *initial* capability
- List does not include computer science advancements (e.g. new databases, parsers, objects, etc...)

Initial Capability	Physics package
1994	ALE explicit hydro w/ advection and slide surfaces (ASC code)
1995	Thermal transport (Topaz)
1996	Chemical reactions
1997	Implicit time stepping
1998	Shell (structural) elements
1999	Species diffusion of chemicals
2000	Incompressible flow
2001	Compressible flow
2002	MS material model library
2002	Particle tracking

2003	Built-in mesh generator
2004	Dislocation dynamics
2004	Beam elements
2005	Multiple implicit element types
2005	Multiphase flow hydro
2005	2D axisymmetric
2005	Detonation Shock Dynamics (DSD)
2006	Magneto Hydrodynamics (MHD)
2007	Adaptive Mesh Refinement (AMR)
2008	Multiple time-integration options
2008	Auto contact
2009?	Embedded grids
2009?	Discrete Element Methods (DEM)
2010?	Fully coupled AMR

Still work in progress
Future plans

S&T / Comp / WCI

11

Source: LLNL ALE3D Team

Applications design and implementation are already complex!!  
 Writing and optimizing code for each new architecture and programming model is impractical (and only going to happen w/ heroic efforts/funding.)

[1] H. Simon, T. Zacharia, and R. Stevens, Eds., Modeling and Simulation at the Exascale for Energy and the Environment, 2007.

[2] S.W. Hadley, D.J. Erickson et al., "Responses of energy use to climate change: A climate modeling study," *Geophysical Research Letters*, 33(17), 2006.

[3] D. Vergano, "Air conditioning fuels warming," in USA Today, 2006.

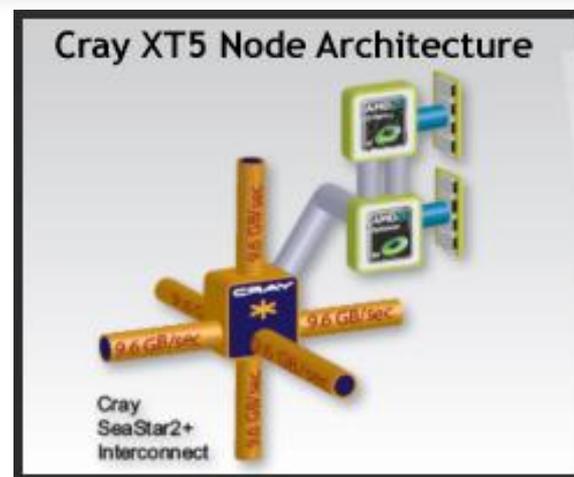
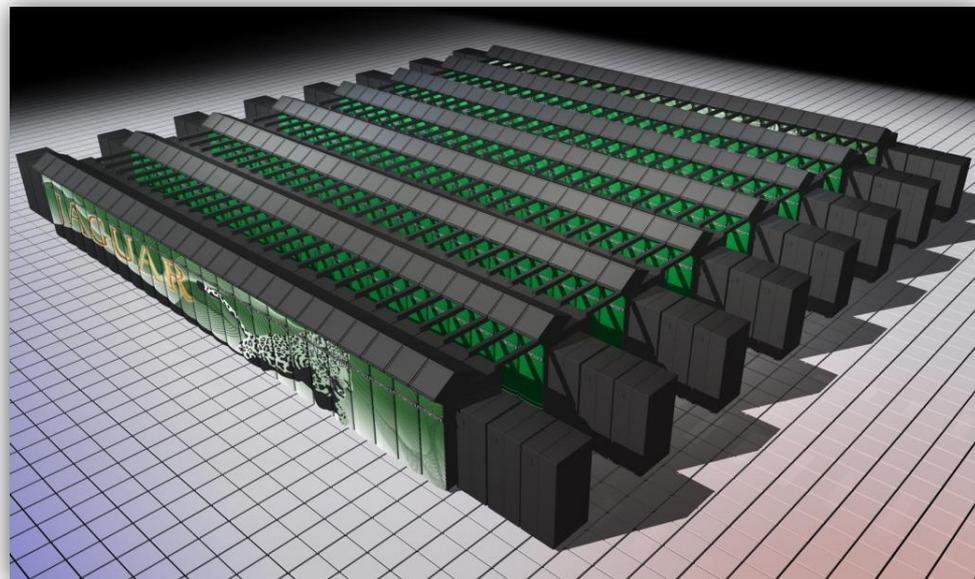


***HPC LANDSCAPE TODAY***  
***JAGUAR AT ORNL***

# HPC Landscape Today

- 2.3 PF Peak
- 1.7 PF announced yesterday

Jaguar Specifications	Total	XT5	XT4
Peak Teraflops	1,645	1,382	263
Quad-Core AMD Opterons	45,376	37,544	7,832
AMD Opteron Cores	181,504	150,176	31,328
Compute Nodes	26,604	18,772	7,832
Memory (TB)	362	300	62
Disk Bandwidth (GB/s)	284	240	44
Disk Space (TB)	10,750	10,000	750
Interconnect Bandwidth (TB/s)	532	374	157
Floor Space (feet <sup>2</sup> )	5,800	4,400	1,400
Cooling Technology		Liquid	Air



# ***Science applications are scaling on Jaguar***

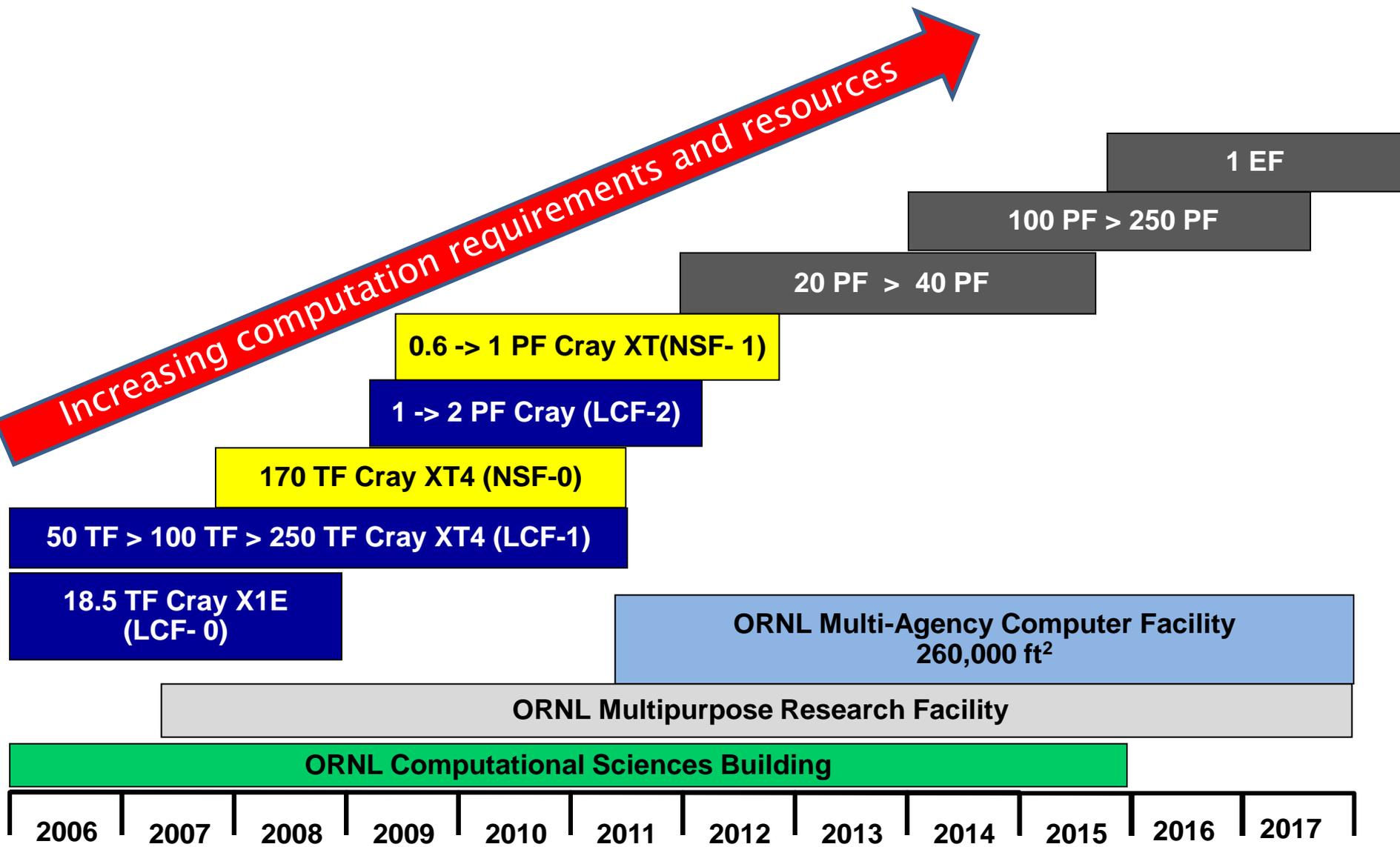
<b>Science area</b>	<b>Code</b>	<b>Contact</b>	<b>Cores</b>	<b>Performance</b>
<b>Materials</b>	<b>DCA++</b>	<b>Schulthess</b>	<b>150,144</b>	<b>1.3 PF MP</b>
Materials	LSMS	Eisenbach	149,580	1.05 PF
<b>Seismology</b>	<b>SPECFEM3D</b>	<b>Carrington</b>	<b>149,784</b>	<b>165 TF</b>
Weather	WRF	Michalakes	150,000	50 TF
Climate	POP	Jones	18,000	20 simulation years/day
Combustion	S3D	Chen	144,000	83 TF
Fusion	GTC	PPPL	102,000	20 billion particles/second
<b>Materials</b>	<b>LS3DF</b>	<b>Lin-Wang Wang</b>	<b>147,456</b>	<b>442 TF</b>
Chemistry	NWChem	Apra	96,000	480 TF
Chemistry	MADNESS	Harrison	140,000	550+ TF

More apps to come in this year's Gordon Bell contest

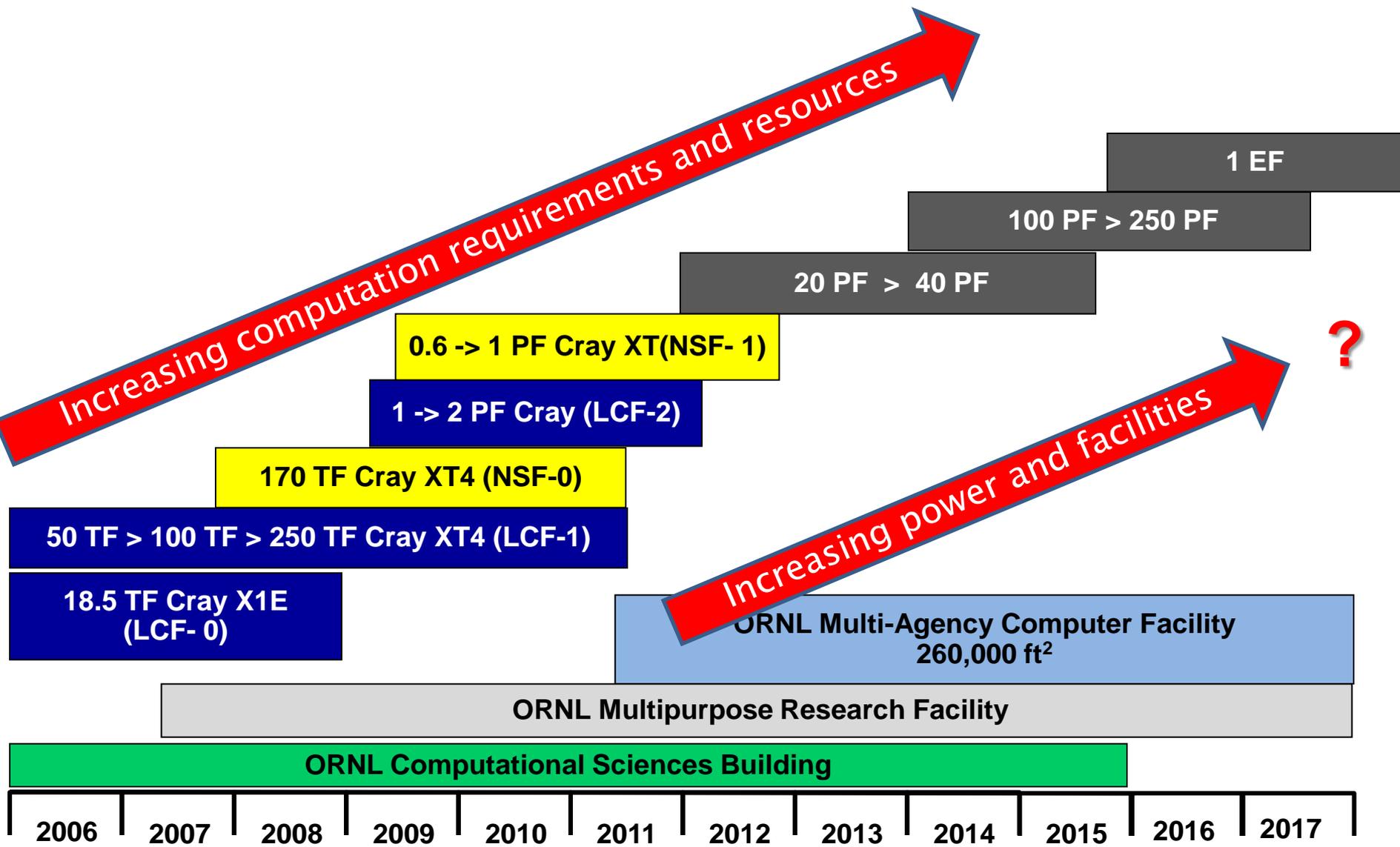


***THE ROAD AHEAD***

# Representative Roadmap to Exascale from ORNL



# ... facilities and cost issue ???



# ***Reality: Facilities and Power for Exascale Computing are growing at an unsustainable rate***



## Open Science Center (40k ft<sup>2</sup>)

- Upgrading building power to 15 MW
- 210 MW substation, upgradeable to 280 MW
- Deploying a 6,600 ton chiller plant
- Tripling UPS and generator capability



## National Security Center (32k ft<sup>2</sup>)

- Capability computing for national defence
- 25 MW of power and 8,000+ ton chillers



## New Computer Facility (260k ft<sup>2</sup>)

- 110 ft<sup>2</sup> raised floor classified; same unclassified
- Shared mechanical and electrical
- Lights out facility
- Capable of greater than 100 MW power

# Power, cooling, and floorspace are fundamental challenges for the entire community over the next decade

## ExaScale Computing Study: Technology Challenges in Achieving Exascale Systems

Peter Kogge, Editor & Study Lead

Keren Bergman  
Shekhar Borkar  
Dan Campbell  
William Carlson  
William Dally  
Monty Denneau  
Paul Franzon  
William Harrod  
Kerry Hill  
Jon Hiller  
Sherman Karp  
Stephen Keckler  
Dean Klein  
Robert Lucas  
Mark Richards  
Al Scarpelli  
Steven Scott  
Allan Snaveley  
Thomas Sterling  
R. Stanley Williams  
Katherine Yelick

September 28, 2008

This work was sponsored by DARPA IPTO in the ExaScale Computing Study with Dr. William Harrod as Program Manager; AFRL contract number FA8650-07-C-7724. This report is published in the interest of scientific and technical information exchange and its publication does not constitute the Government's approval or disapproval of its ideas or findings

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- **Energy, Power, and Facilities**
  - > Exascale system cannot use 1 GW!!
  - > Can we do Exascale in 20 MW??
- **Memory and Storage**
- **Concurrency and Locality**
- **Resiliency**

# Decisions for Managing Power and Facilities Demands

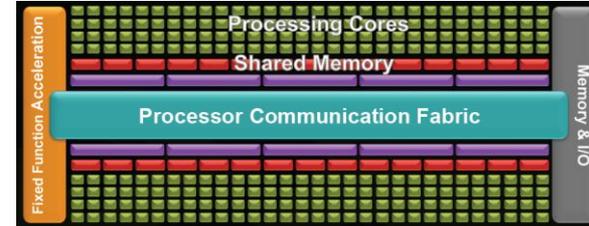
- Build bigger buildings near power stations, and allocate large budget for power



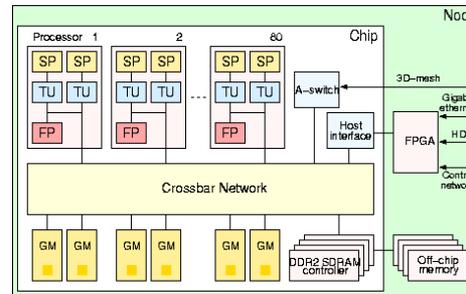
- Improve efficiencies
  - > Power distribution
  - > Workload scheduling
  - > Software
- Design new underlying technologies
  - > Optical networks
  - > 3D stacking
  - > MRAM, PCM, nanotubes
- Use different architectures (that match your workload)
- Or, build bigger buildings and plan to pay \$\$\$ for ops

# Scaling dimension seems straightforward ...

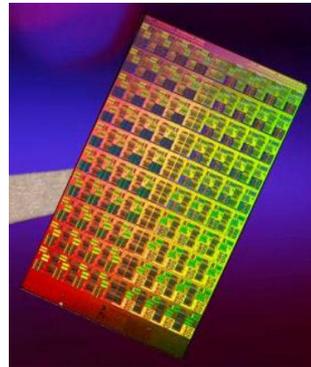
240 cores, 30k threads...



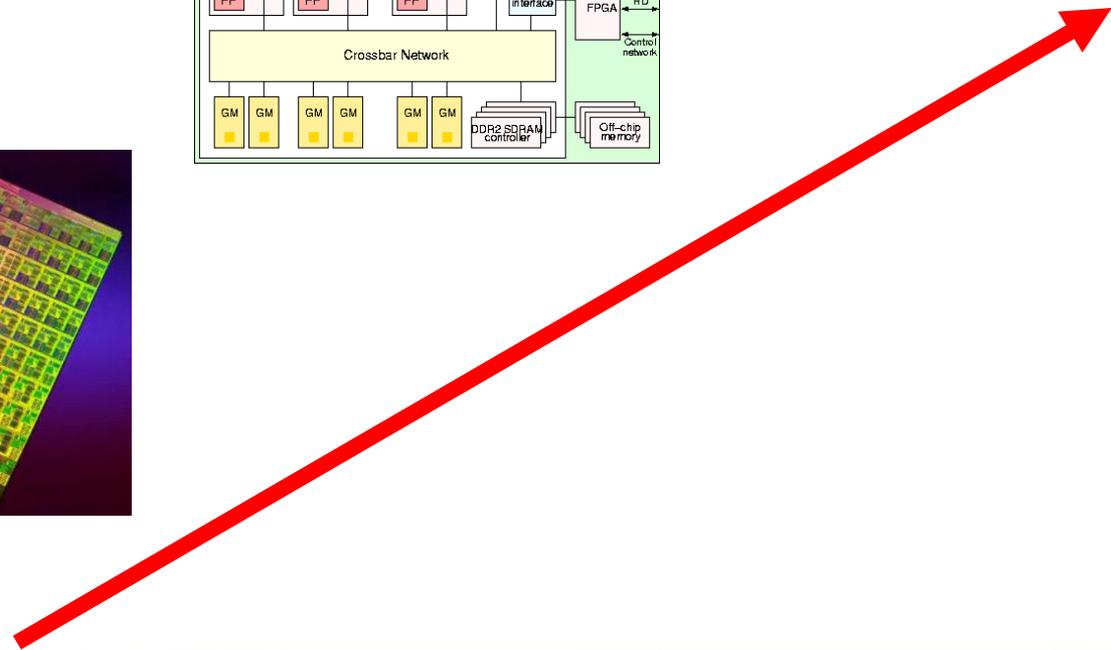
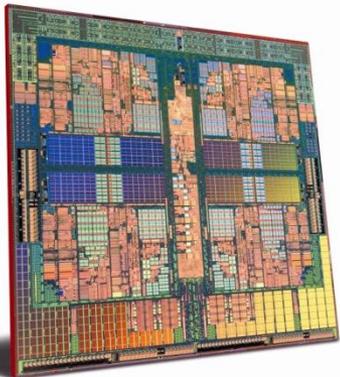
160...



80...

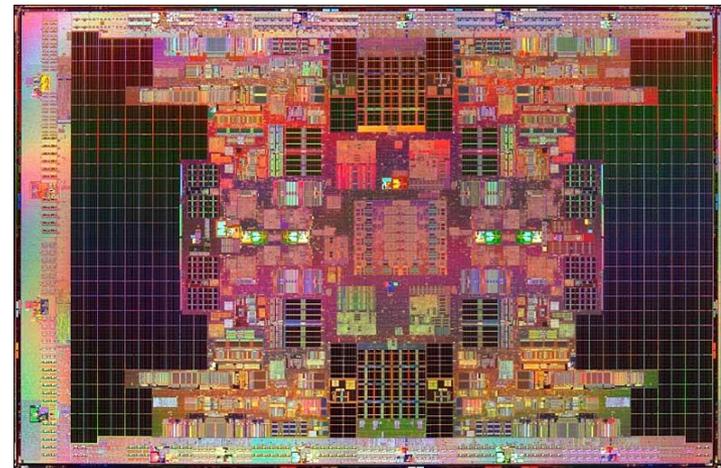


4...



# Another dimension: Several Factors Motivate Heterogeneity

- **Sacrifice generality and compatibility to address specific algorithms**
- **Computational power**
  - > Asymmetric, dynamic cores can provide performance advantages [1]
  - > Use transistors differently
- **Tukwila – First 2 billion transistor chip**
  - > 80486 had ~1.2M transistors, ~50MHz, 1989
  - > Specialization can be free
- **Power**
  - > Combination of these features provide more ops per watt for your targeted application
- **Memory**
  - > Include different cache or memory organization tuned for data access patterns
- **Performance of general purpose processors de-accelerating**



ISSCC 2008.

[1] M.D. Hill and M.R. Marty, "Amdahl's Law in the Multicore Era," *IEEE Computer*, to appear, 2008.



# ***ENABLING HETEROGENEOUS COMPUTING FOR THE OPEN SCIENCE COMMUNITY***

# National Science Foundation Office of Cyberinfrastructure

- NSF OCI HPC Strategy
  - Track 1, BlueWaters
  - Track 2, TACC Ranger, NICS Kraken
- NSF 08-573 OCI Track 2D RFP in Fall 2008
  - Data Intensive
  - Experimental Grid testbed
  - Pool of loosely coupled grid-computing resources
  - **Experimental HPC System of Innovative Design**

**An experimental high-performance computing system of innovative design.** Proposals are sought for the development and deployment of a system with an architectural design that is outside the mainstream of what is routinely available from computer vendors. Such a project may be for a duration of up to five years and for a total award size of up to \$12,000,000. It is not necessary that the system be deployed early in the project; for example, a lengthy development phase might be included. Proposals should explain why such a resource will expand the range of research projects that scientists and engineers can tackle and include some examples of science and engineering questions to which the system will be applied. It is not necessary that the design of the proposed system be useful for all classes of computational science and engineering problems. When finally deployed, the system should be integrated into the TeraGrid. It is anticipated that the system, once deployed, will be an experimental TeraGrid resource, used by a smaller number of researchers than is typical for a large TeraGrid resource. (Up to 5 years duration. Up to \$12,000,000 in total budget to include development and/or acquisition, operations and maintenance, including user support. First-year budget not to exceed \$4,000,000.)

# Large Scale Computational Science Demands Performance, Programmability, Precision, Reliability, Cost from HPC Platforms

- Performance
  - Must show reasonable performance improvements at scale on real scientific applications of interest
- Programmability
  - Must be easy to re-port and re-optimize applications for each new architecture (generation) without large effort, delays
- Precision - Accuracy
  - Must provide impressive performance accurately
- Reliability
  - Must get high scientific throughput without job failures or inaccurate results
- Power and Facilities Cost
  - Must be reasonably affordable in terms of power and facilities costs

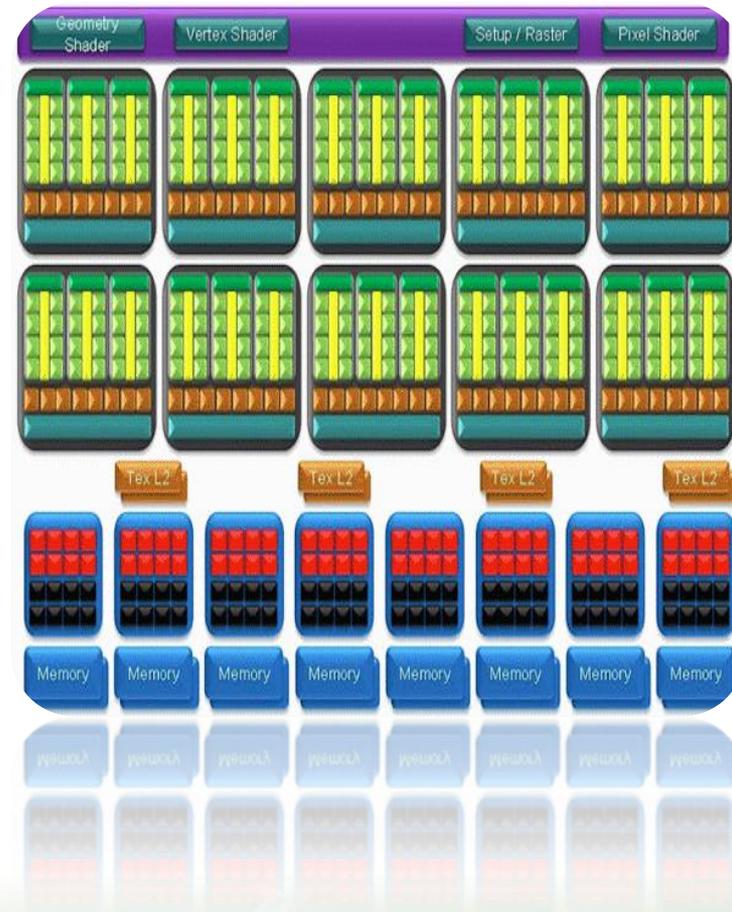
# Oct 2008 – Alternatives Analysis

- STI Cell
- FGPA's
- Cyclops64
- Cray XMT
- Sun Rock/Niagara
- ClearSpeed
- Tensilica
- Tiler
- Anton
- SGI Molecule
- Intel Larrabee
- Graphics processors
  
- Others...

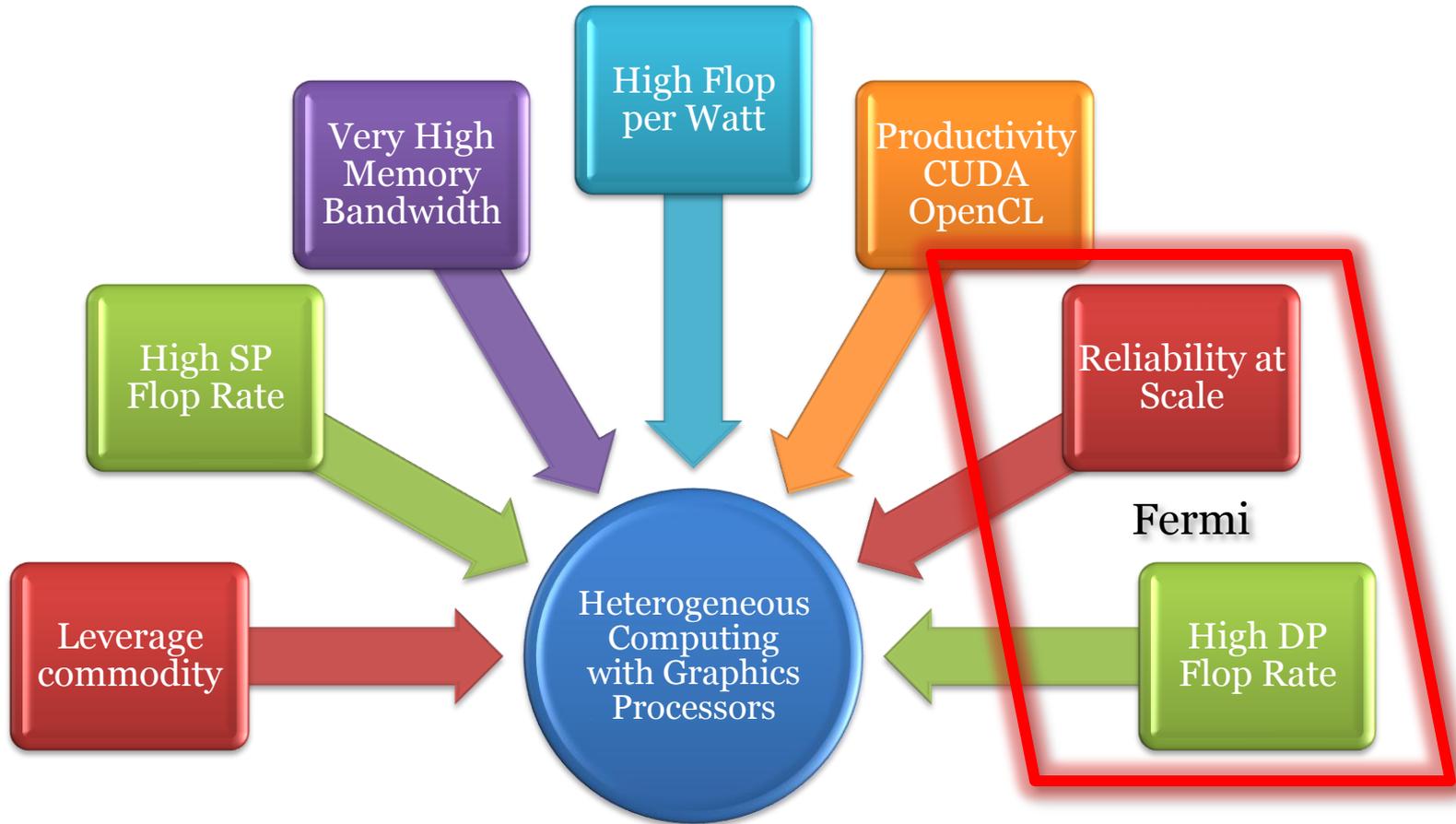
# Alternatives analysis concluded GPUs were a competitive solution

- Success with various applications at DOE, NSF, government, industry
  - Signal processing, image processing, etc.
  - DCA++, S3D, NAMD, many others
- Commodity solution
  - Certified GPGPU clusters widely available this past quarter from multiple vendors
- Improving programmability
  - Widespread adoption of CUDA
  - OpenCL ratification
- Community application experiences also positive
  - Frequent workshops, tutorials, software development, university classes
  - Many apps teams are excited about using GPGPUs

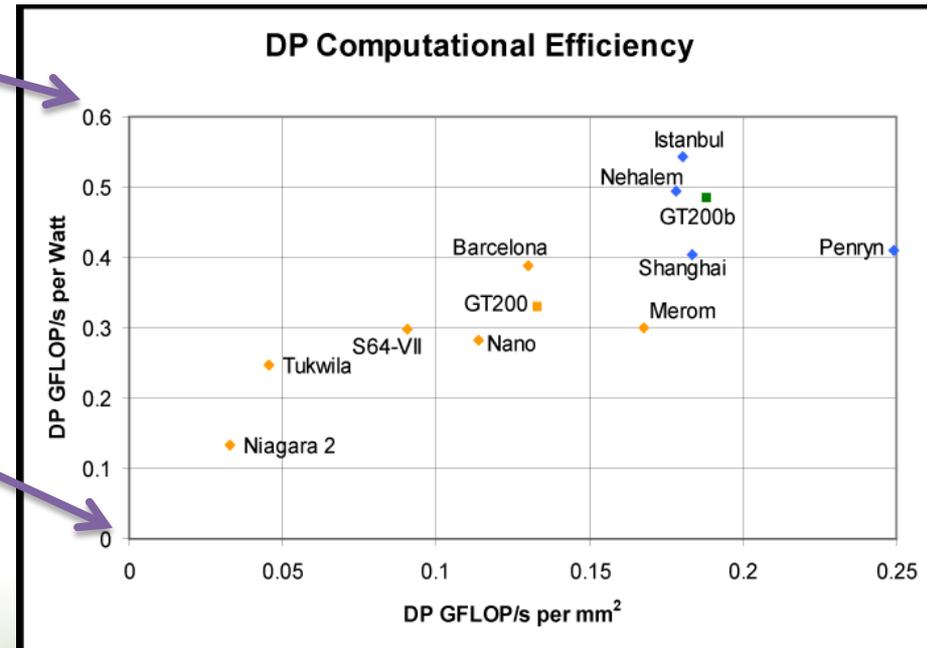
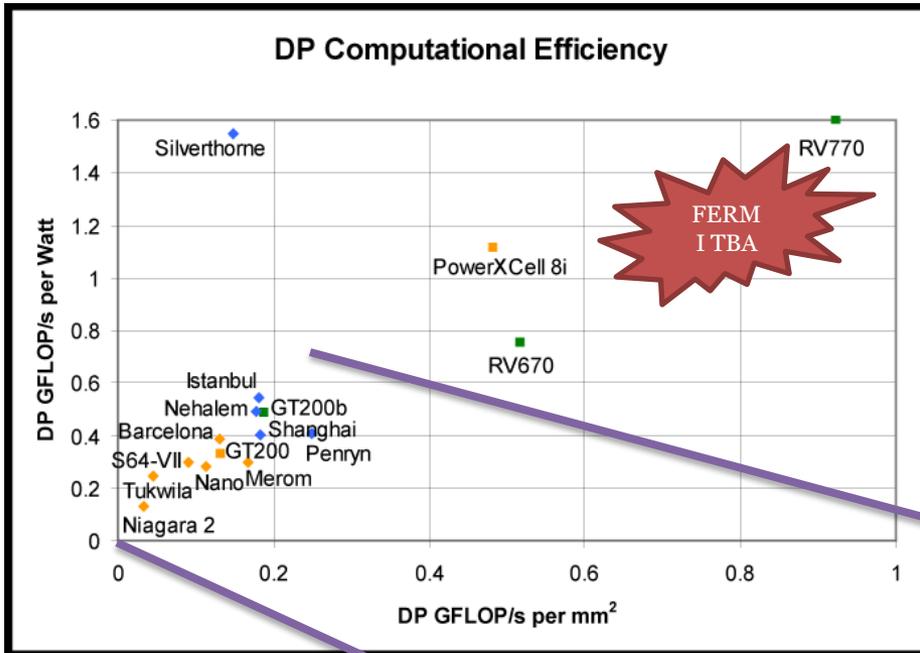
- NVIDIA GT200 - 240



# GPU Rationale – What's different now?



# GPU Rationale - Power Efficiency!

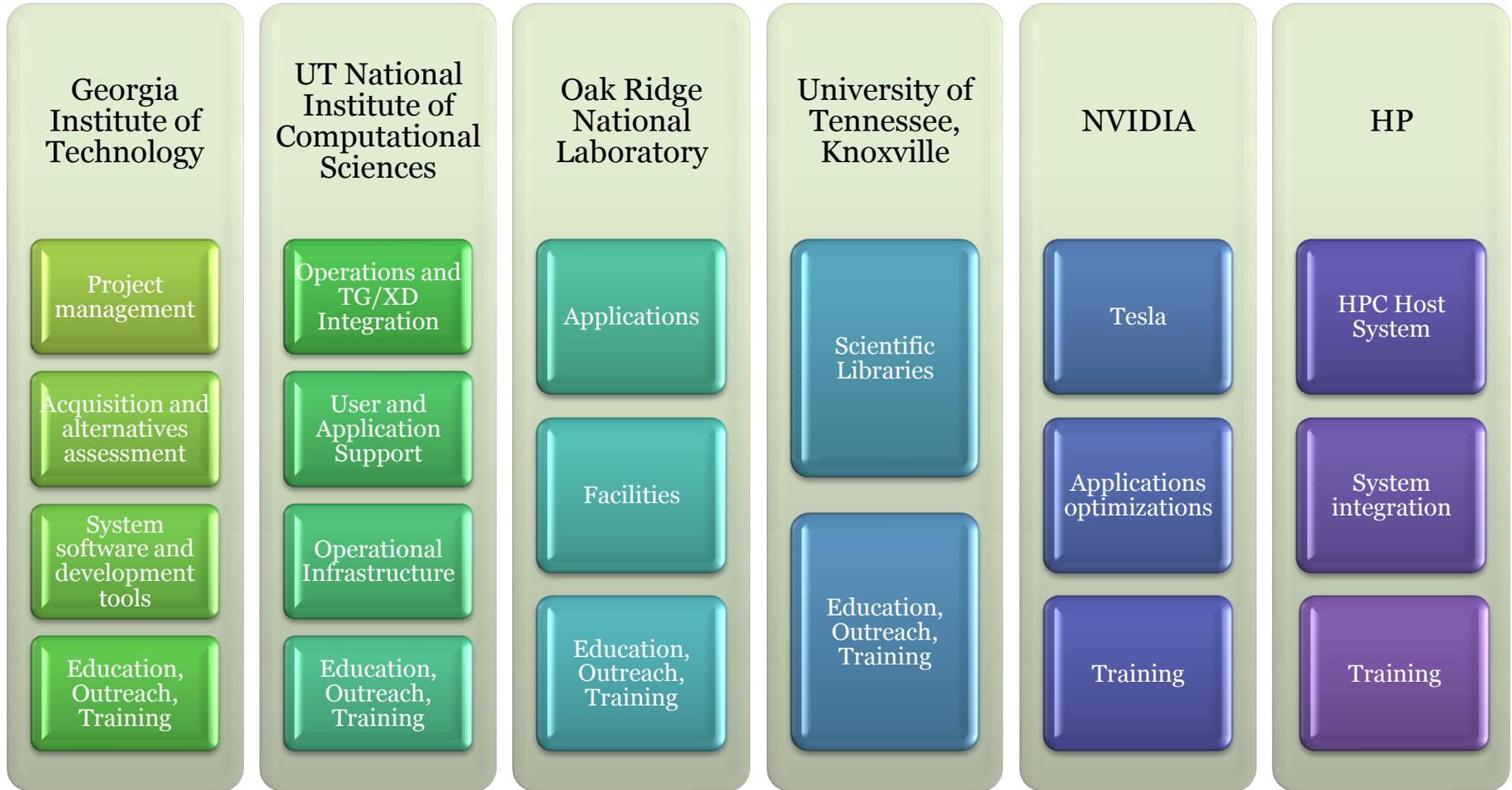


# Keeneland – An NSF-Funded Partnership to Enable Large-scale Computational Science on Heterogeneous Architectures

- Track 2D System of Innovative Design
  - Large GPU cluster
    - Initial delivery system – Spring 2010
    - Full scale system – Spring 2012
- Software tools, application development
- Operations, user support
- Education, Outreach, Training for scientists, students, industry

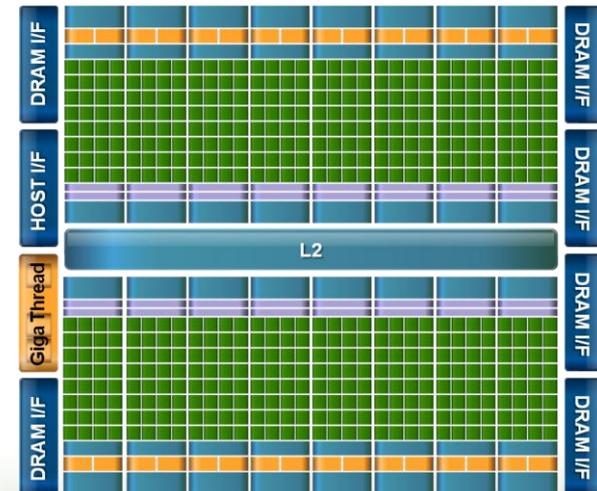
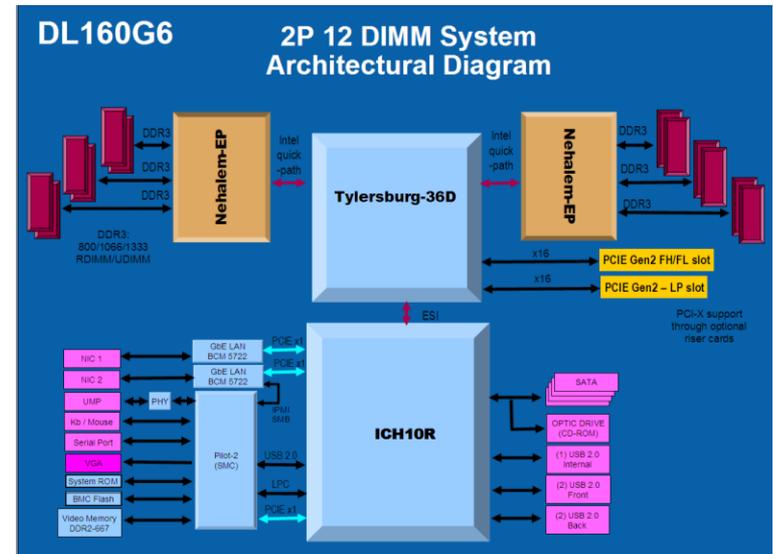
Jeffrey	Vetter
Jack	Dongarra
Richard	Fujimoto
Thomas	Schulthess
Karsten	Schwan
Sudha	Yalamanchili
Kathlyn	Boudwin
Jim	Ferguson
Doug	Hudson
Patricia	Kovatch
Bruce	Loftis
Jeremy	Meredith
Jim	Rogers
Philip	Roth
Arlene	Washington
Phil	Andrews
Mark	Fahey
Don	Reed
Tracy	Rafferty
Ursula	Henderson
Terry	Moore

# Keeneland Partners



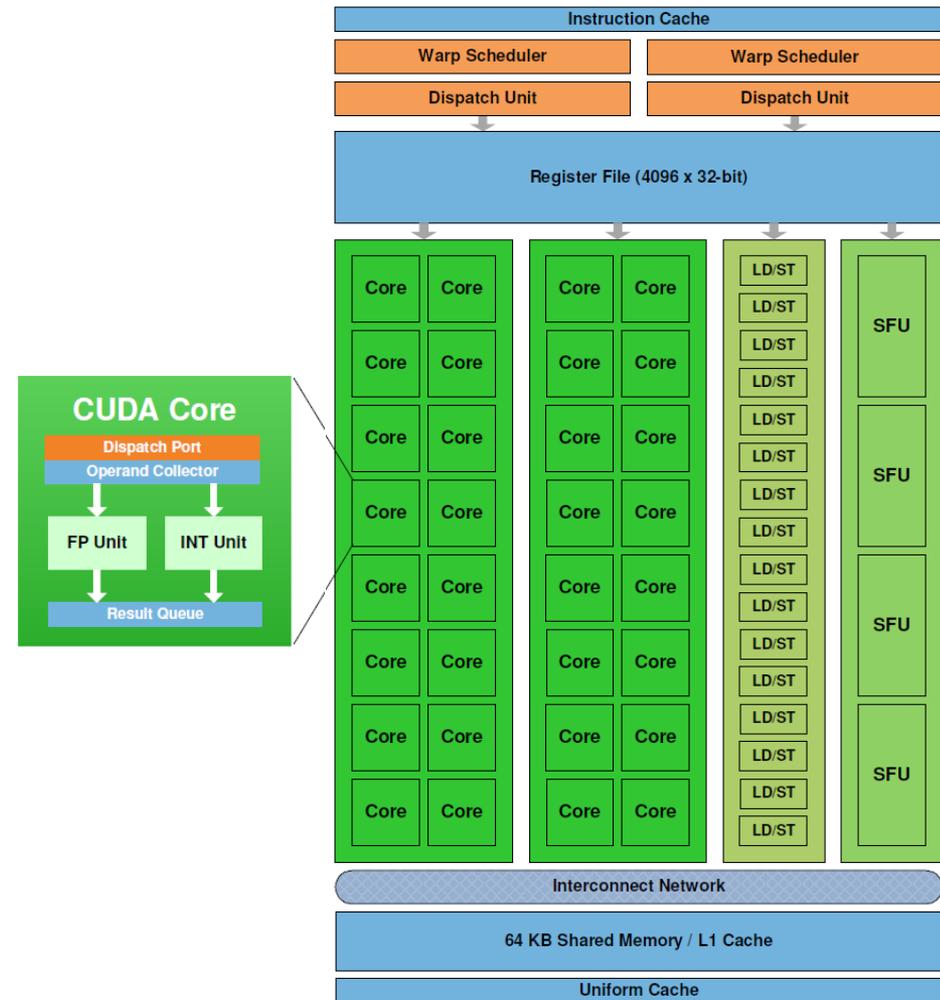
# Keeneland Initial Delivery (ID) System

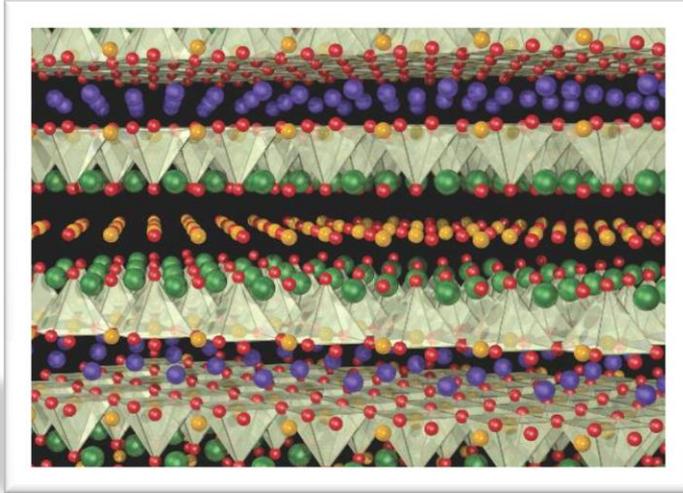
- Hewlett Packard Nodes
  - Dual socket Intel 2.8 GHz Nehalem-EP
  - 24 GB Main memory per node
- NVIDIA Servers
  - Fermi GPUs
- InfiniBand 4x QDR w/ full bisection interconnect
- Traditional Linux software stack augmented with GPU compilers, software tools, libraries
- Hundreds of Fermi processors
- Delivery and acceptance in Spring 2010



# ID system will use NVIDIA's Fermi

- “The soul of a supercomputer in the body of a GPU.”
- 3B transistors
- ECC
- 8x the peak double precision arithmetic performance over NVIDIA's last generation GPU.
- 512 CUDA Cores featuring the new IEEE 754-2008 floating-point standard
- NVIDIA Parallel DataCache
- NVIDIA GigaThread Engine
- CUDA and OpenCL support
- Debuggers, language support

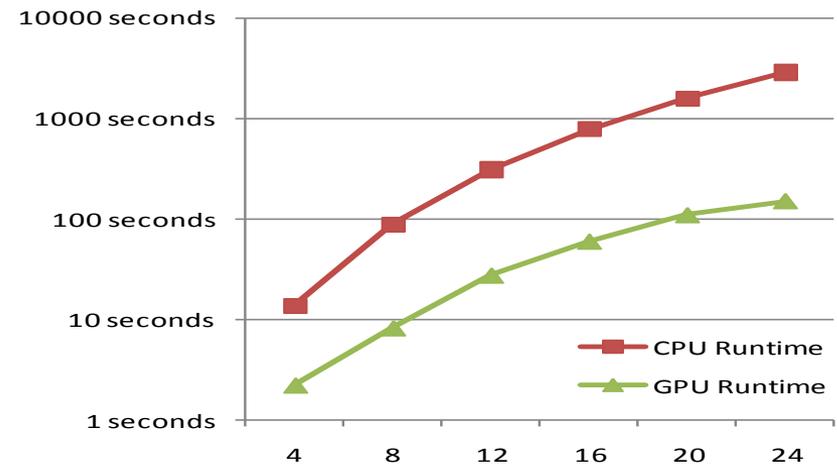
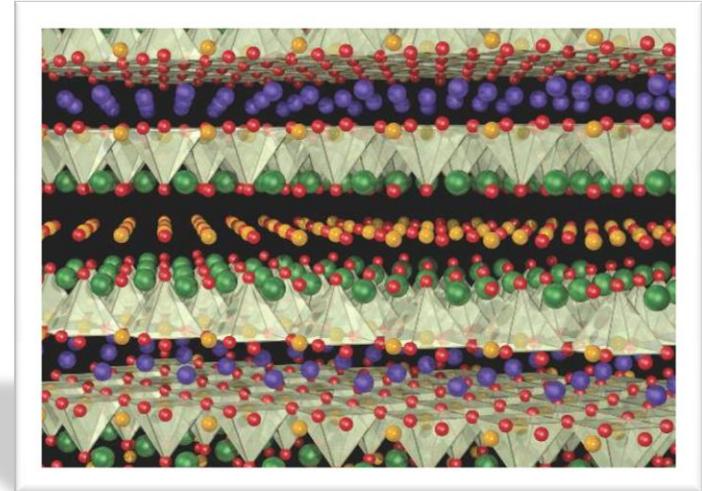




# ***APPLICATIONS***

# Computational Materials - Case Study

- Quantum Monte Carlo simulation
  - High-temperature superconductivity and other materials science
  - 2008 Gordon Bell Prize
- GPU acceleration speedup of 19x in main QMC Update routine
  - Single precision for CPU and GPU: target single-precision only cards
  - Required detailed accuracy study and mixed precision port of app
- Full parallel app is 5x faster, start to finish, on a GPU-enabled cluster

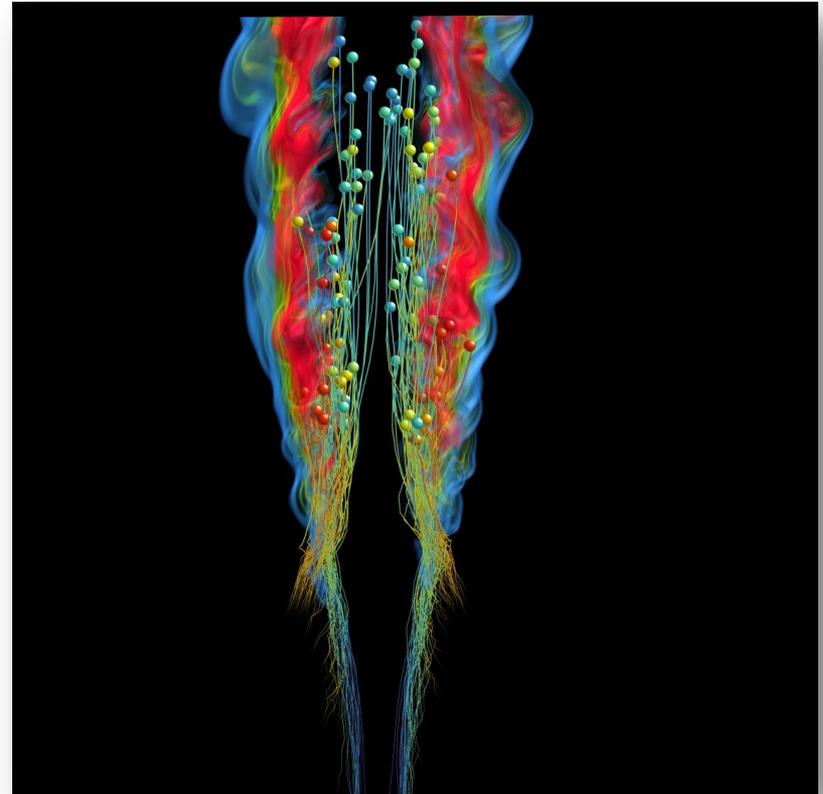


GPU study: J.S. Meredith, G. Alvarez, T.A. Maier, T.C. Schulthess, J.S. Vetter, "Accuracy and Performance of Graphics Processors: A Quantum Monte Carlo Application Case Study", *Parallel Comput.*, 35(3):151-63, 2009.

Accuracy study: G. Alvarez, M.S. Summers, D.E. Maxwell, M. Eisenbach, J.S. Meredith, J. M. Larkin, J. Levesque, T. A. Maier, P.R.C. Kent, E.F. D'Azevedo, T.C. Schulthess, "New algorithm to enable 400+ TFlop/s sustained performance in simulations of disorder effects in high-Tc superconductors", *SuperComputing*, 2008. [Gordon Bell Prize winner]

# Combustion with S3D – Case Study

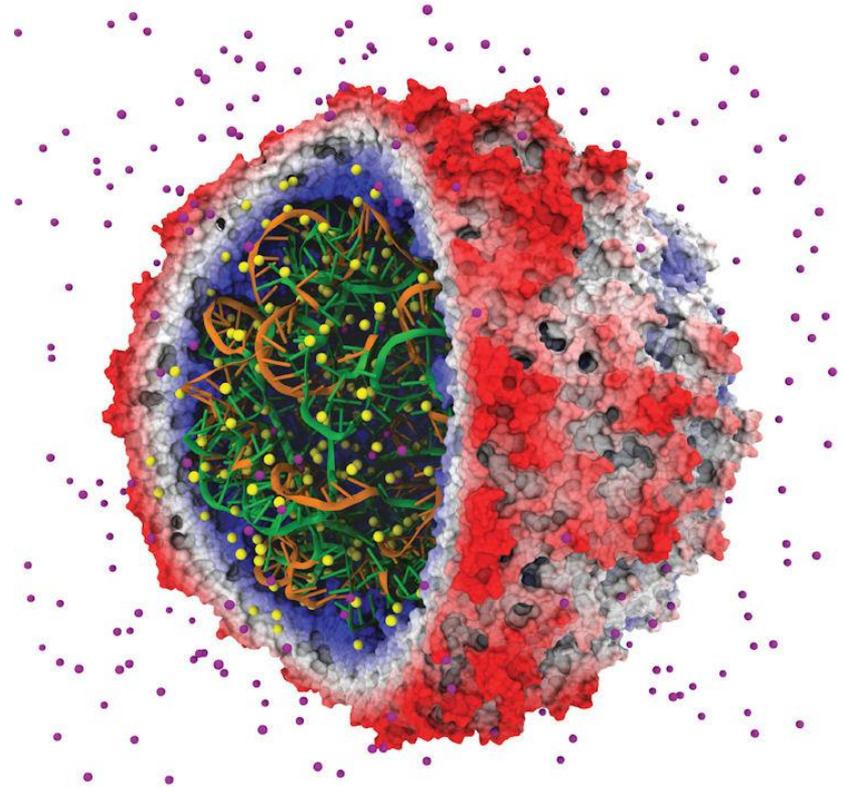
- Application for combustion - S3D
  - Massively parallel direct numerical solver (DNS) for the full compressible Navier-Stokes, total energy, species and mass continuity equations
  - Coupled with detailed chemistry
  - Scales to 150k cores on Jaguar
- Accelerated version of S3D's Getrates kernel in CUDA
  - 14.3x SP speedup
  - 9.32x DP speedup



K. Spafford, J. Meredith, J. S. Vetter, J. Chen, R. Grout, and R. Sankaran. Accelerating S3D: A GPGPU Case Study. Proceedings of the Seventh International Workshop on Algorithms, Models, and Tools for Parallel Computing on Heterogeneous Platforms (HeteroPar 2009) Delft, The Netherlands.

# Biomolecular systems from NAMD Team – Not just us

- NAMD, VMD
  - Study of the structure and function of biological molecules
- Calculation of non-bonded forces on GPUs leads to 9x speedup
- Framework hides most of the GPU complexity from users



J.C. Phillips and J.E. Stone, “Probing biomolecular machines with graphics processors,” *Commun. ACM*, 52(10):34-41, 2009. (fig)

# KEENELAND SOFTWARE

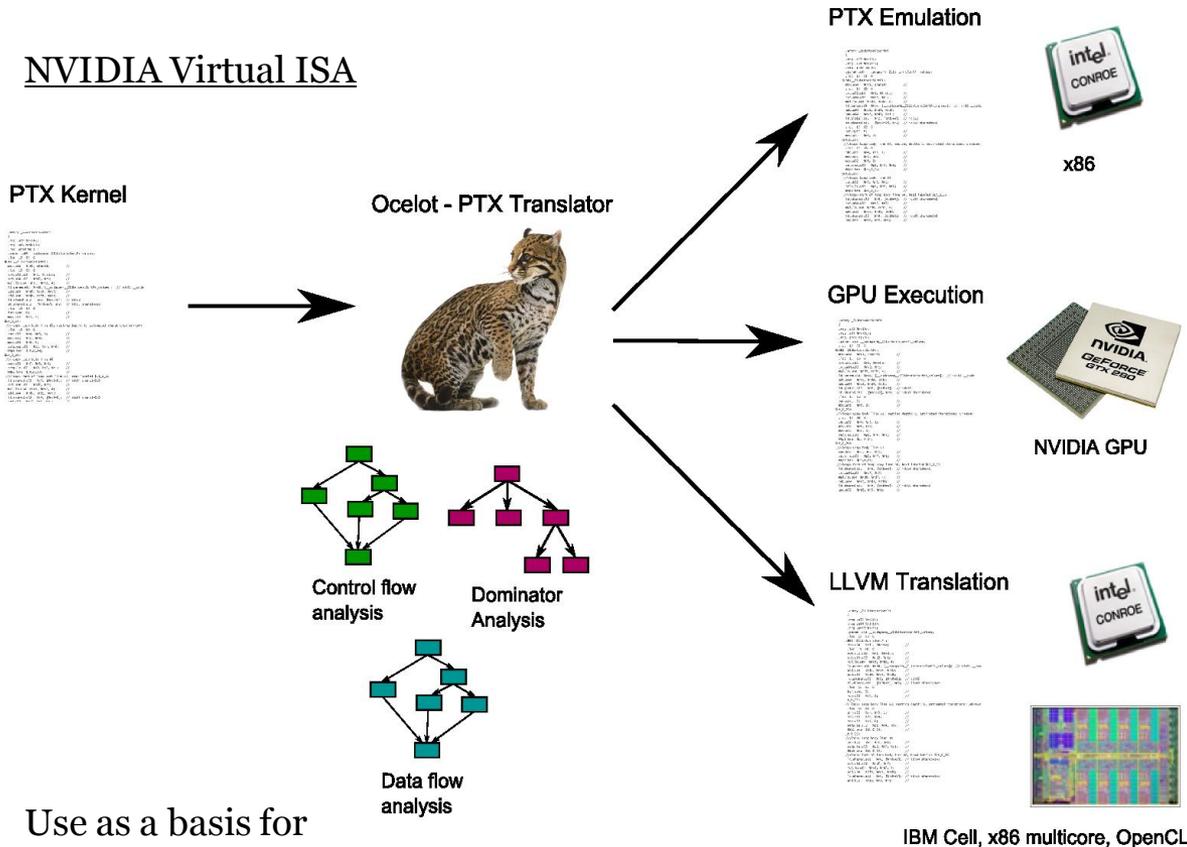


# Keeneland Software Environment

- Integrated with NSF TeraGrid/XD
  - Including TG and NICS software stack
- Programming models
  - CUDA
  - OpenCL
  - PGI w/ accelerate
  - OpenMP 3.0
  - MPI
- Additional software activities
  - Performance and correctness tools
  - Scientific libraries
  - Virtualization
  - Benchmarks

# Ocelot: Dynamic Execution Infrastructure

## NVIDIA Virtual ISA



- PTX 1.4 compliant Emulation
- Validated on full CUDA SDK
- Open Source version released

<http://code.google.com/p/gpuocelot/>

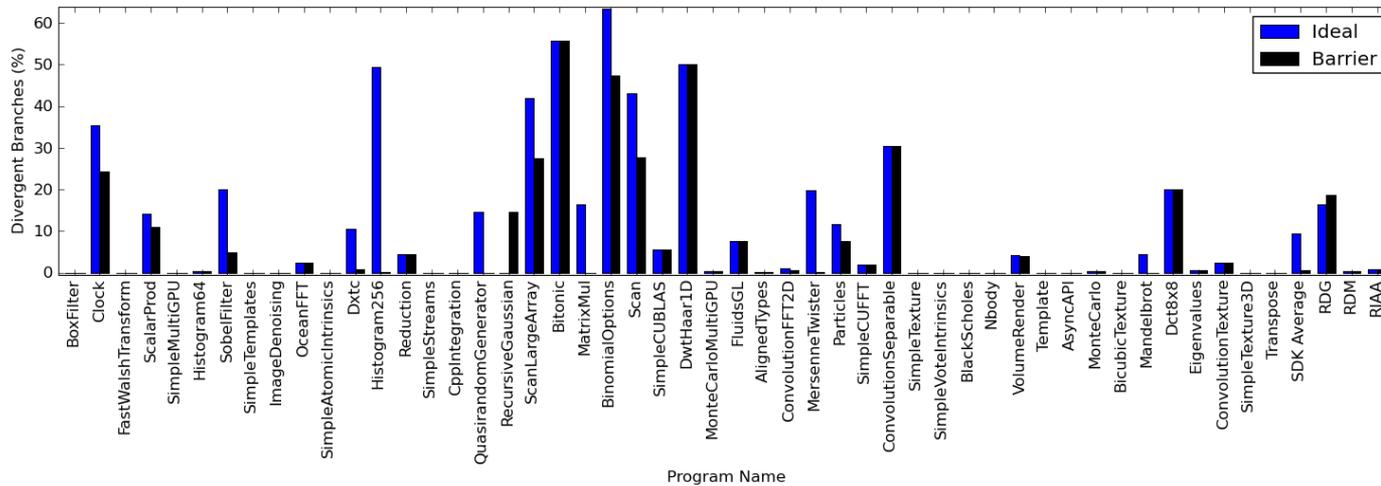
Use as a basis for

- Insight → workload characterization
- Performance tuning → detecting memory bank conflicts
- Debugging → illegal memory accesses, out of bounds checks, etc.

*Gregory Damos, Dhruv Choudhary, Andrew Kerr, Sudhakar Yalamanchili*

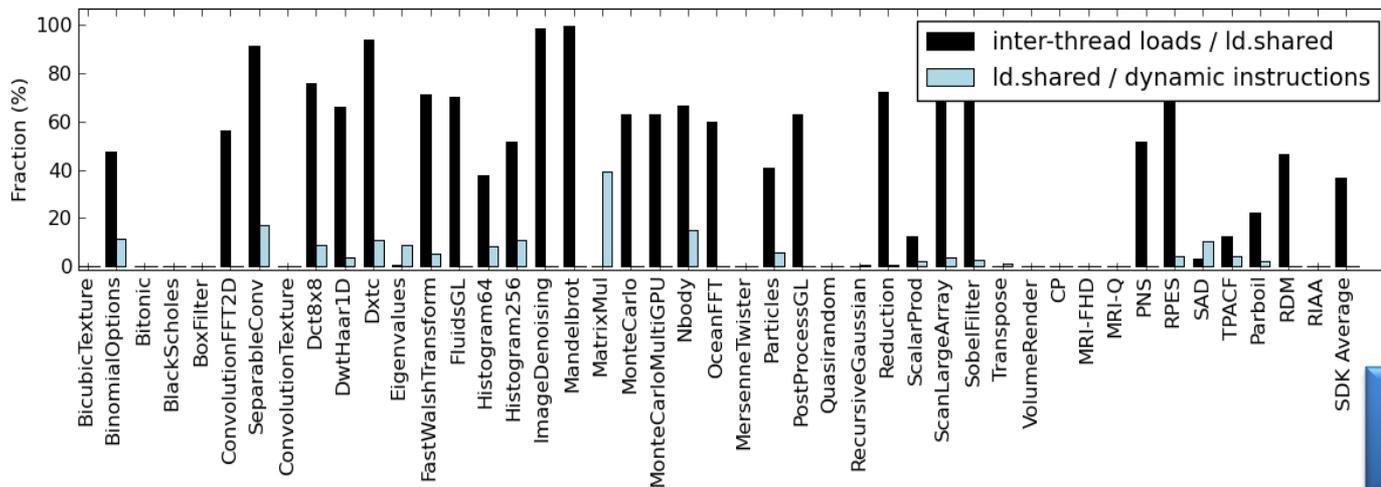
*Gregory Damos recently awarded NVIDIA Fellowship*

# Workload Analysis: Examples



## Branch Divergence

- Study of control Flow behavior
- Motivate synchronization support



## Inter-thread Data Flow

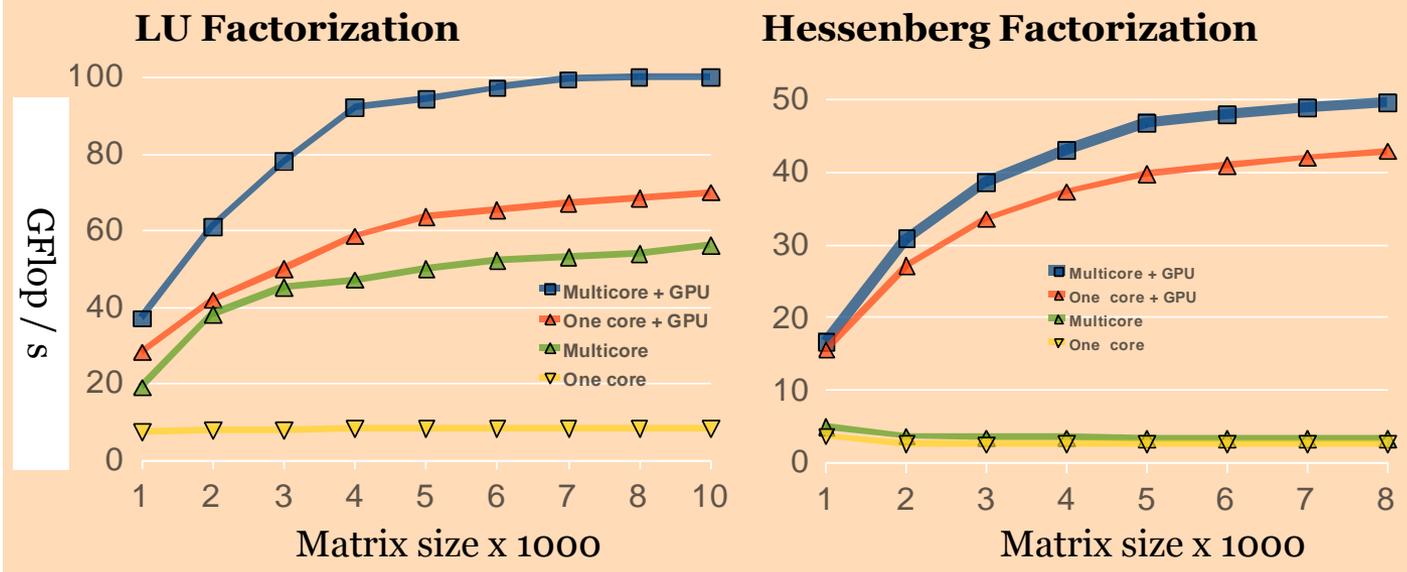
- Study of data sharing patterns
- Motivate architectural support

Gregory Diamos, Dhruv Choudhary, Andrew Kerr, Sudhakar Yalamanchili

# One and two-sided Multicore+GPU Factorizations

- These will be included in up-coming MAGMA releases
- Two-sided factorizations can not be efficiently accelerated on homogeneous x86-based multicores (above) because of memory-bound operations
  - MAGMA provided hybrid algorithms that overcome those bottlenecks (16x speedup!)

## Multicore + GPU Performance in double precision



Jack  
Dongarra,  
Stan Tomov,  
and Rajib  
Nath

**GPU** : NVIDIA GeForce GTX 280

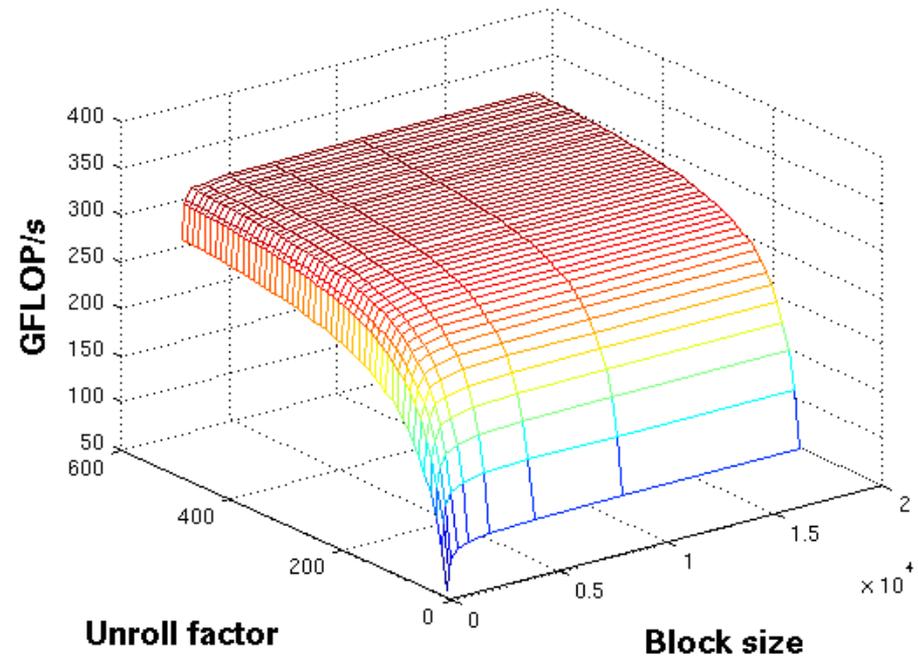
**CPU** : Intel Xeon dual socket quad-core @2.33 GHz

**GPU BLAS** : CUBLAS 2.2, dgemm peak: 75 GFlop/s

**CPU BLAS** : MKL 10.0 , dgemm peak: 65 GFlop/s

# Scalable Heterogeneous Computing (SHOC) Benchmark Suite

- Problem: we don't yet understand overheads and performance benefits of GPU versus CPU, and trade-offs between different programming approaches
  - Systems can differ greatly
  - Need procurement and acceptance tests
- Antero: a collection of benchmark programs for quantifying those overheads and trade-offs
- Multiple levels
  - Level 0: low-level, feeds and speeds
  - Level 1: higher-level, problem kernels
- Multiple test categories
  - Performance
  - Stability
- Support for both single-node and clusters like Keeneland (MPI-based)



Jeremy Meredith, Phil Roth, Kyle Spafford,  
Anthony Danalis, Gabriel Marin, Vinod  
Tippiraju, Jeffrey Vetter

# Summary

- Predictive scientific simulation is important for scientific discovery
  - Advancing science, informing policymakers
- HPC systems have been highly successful
  - Decades of improvement
- The HPC community has several (new) constraints
  - Power, Facilities, Cost
- Heterogeneous computing with GPUs offers some opportunities and challenges
  - High performance; good performance per watt
  - Programmability; limited applicability
- Keeneland - Newly awarded NSF partnership will provide heterogeneous supercomputing for open science

# Thank You!

## Thanks to contributors, sponsors

Many collaborators across apps  
teams, academia, labs, and  
industry

DOE, NSF, ORNL, DARPA, DOD

## More information

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<http://keeneland.gatech.edu>

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<http://www.cercs.gatech.edu>

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<http://www.nics.tennessee.edu/>

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