Living at the Top of the Top500: Myopia from Being at the Bleeding Edge

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Oak Ridge Leadership Computing Facility &
Theoretical Astrophysics Group
Oak Ridge National Laboratory

Department of Physics & Astronomy
University of Tennessee
Outline

• Statements made without proof
• OLCF’s Center for Accelerated Application Readiness
• Speculations on task-based approaches for multiphysics applications in astrophysics (e.g. blowing up stars)
Riffing on Hank’s fable...
The Effects of Moore’s Law and Slacking $^1$ on Large Computations

Chris Gottbrath, Jeremy Bailin, Casey Meakin, Todd Thompson, J.J. Charfman
Steward Observatory, University of Arizona

Abstract

We show that, in the context of Moore’s Law, overall productivity can be increased for large enough computations by ‘slacking’ or waiting for some period of time before purchasing a computer and beginning the calculation.

$^1$This paper took 2 days to write
Some realities

• The future is now: if you go from franklin to hopper at the same size, you lose.

Franklin - Cray XT4

- 38,288 compute cores
- 9,572 compute nodes
- One quad-core AMD 2.3 GHz Opteron processors (Budapest) per node
- 4 processor cores per node
- 8 GB of memory per node
- 78 TB of aggregate memory
- 1.8 GB memory / core for applications
- /scratch disk default quota of 750 GB

Light-weight Cray Linux operating system
No runtime dynamic, shared-object libs
PGI, Cray, Pathscale, GNU compilers

NERSC-6
Grace “Hopper”

Cray XE6
Performance
1.2 PF Peak
1.05 PF HPL (#5)
Processor
AMD Magny Cours
2.1 GHz 12-core
6.4 GFLOPs/core
24 cores/node
32-64 GB DDR3-1333 per node
System
Gemini Interconnect (3D torus)
6392 nodes
153,408 total cores
I/O
2PB disk space
70GB/s peak I/O Bandwidth

Franklin - Cray XT4

Use Franklin for all your computing jobs, except those that need a full Linux operating system.
Some realities

• If you use primarily IBM platforms, you have a bit longer.
  – scp+make on Blue Waters will likely give you a speedup.
  – BG/P --> BG/Q brings an increased clock, and you probably aren’t engaging the Double Hummer now anyway.
Some realities

• It doesn’t matter if you are gonna use GPU-based machines or not
  — GPUs [CUDA, OpenCL, directives]
  — FPUs on Power [xlf, etc.]
  — Cell [SPE]
  — SSE/AVX; MIC (Knights Ferry, Knights Corner)[?]

• Exposing the maximum amount of node-level parallelism and increasing data locality are the only way to get performance from any of these things
ORNL’s “Titan” System Goals

- Similar number of cabinets, cabinet design, and cooling as Jaguar
- Operating system upgrade of today’s Linux operating system
- Gemini interconnect
  - 3-D Torus
  - Globally addressable memory
  - Advanced synchronization features
- AMD Opteron 6200 processor (Interlagos)
- New accelerated node design using NVIDIA multi-core accelerators
- 10-20 PF peak performance
  - Performance based on available funds
- Larger memory - more than 2x more memory per node than Jaguar
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.
# OLCF-3 Applications Requirements

developed by surveying science community

## OLCF Application Requirements Document

- Elicited, analyzed, and validated using a new comprehensive requirements questionnaire
- Project overview, science motivation and impact, application models, algorithms, parallelization strategy, software, development process, SQA, V&V, usage workflow, performance
- Results, analysis, and conclusions documented in 2009 OLCF application requirements document

## Science Driver Survey

- Developed in consultation with 50+ leading scientists in many domains
- Key questions
  - What are the science goals and does OLCF-3 enable them?
  - What might the impact be if the improved science result occurs?
  - What does it matter if this result is delivered in the 2012 timeframe?

## Science Driver Survey

- Science driver
  - What science will be pursued on this system and how is it different (in fidelity/quality/predictability and/or productivity/throughput) from the current system
- Science impact
  - What might the impact be if this improved science result occurs? Who cares, and why?
- Science timeliness
  - If this result is delivered in the 2010 timeframe, what does it matter as opposed to coming 5 years later (or never at all)? What other programs agencies, stakeholders, and/or facilities are dependent on the timely delivery of this result, and why?
# OLCF-3 Applications Analyzed

Science outcomes were elicited from a broad range of applications

<table>
<thead>
<tr>
<th>Application area</th>
<th>Application codes</th>
<th>Science target</th>
</tr>
</thead>
<tbody>
<tr>
<td>Astrophysics</td>
<td>Chimera, GenASiS</td>
<td>• Core-collapse supernovae simulation; validation against observations of neutrino signatures, gravitational waves, and photon spectra</td>
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<td></td>
<td>MPA-FT, MAESTRO</td>
<td>• Full-star type Ia supernovae simulations of thermonuclear runaway with realistic subgrid models</td>
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<tr>
<td>Bioenergy</td>
<td>LAMMPS, GROMACS</td>
<td>• Cellulosic ethanol: dynamics of microbial enzyme action on biomass</td>
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<tr>
<td>Biology</td>
<td>LAMMPS</td>
<td>• Systems biology</td>
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<td></td>
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<td>• Genomic structure</td>
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<tr>
<td>Chemistry</td>
<td>CP2K, CPMD</td>
<td>• Interfacial chemistry</td>
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<td></td>
<td>GAMESS</td>
<td>• Atmospheric aerosol chemistry</td>
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<td></td>
<td></td>
<td>• Fuels from lignocellulosic materials</td>
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<tr>
<td>Combustion</td>
<td>S3D</td>
<td>• Combustion flame front stability and propagation in power and propulsion engines</td>
</tr>
<tr>
<td></td>
<td>RAPTOR</td>
<td>• Internal combustion design in power and propulsion engines: bridge the gap between device- and lab-scale combustion</td>
</tr>
<tr>
<td>Energy Storage</td>
<td>MADNESS</td>
<td>• Electrochemical processes at the interfaces; ionic diffusion during charge-discharge cycles</td>
</tr>
</tbody>
</table>
## OLCF-3 Applications Analyzed
Science outcomes were elicited from a broad range of applications

<table>
<thead>
<tr>
<th>Application area</th>
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<th>Science target</th>
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</thead>
<tbody>
<tr>
<td><strong>Fusion</strong></td>
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<tr>
<td></td>
<td>GTC</td>
<td>• Energetic particle turbulence and transport in ITER</td>
</tr>
</tbody>
</table>
|                   | GTS               | • Electron dynamics and magnetic perturbation (finite-beta) effects in a global code environment for realistic tokamak transport  
• Improved understanding of confinement physics in tokamak experiments  
• Address issues such as the formations of plasma critical gradients and transport barriers |
|                   | XGC1              | • First-principles gyrokinetic particle simulation of multiscale electromagnetic turbulence in whole-volume ITER plasmas with realistic diverted geometry |
|                   | AORSA, CQL3D      | • Tokamak plasma heating and control |
|                   | FSP               | • MHD scaling to realistic Reynolds numbers  
• Global gyrokinetic studies of core turbulence encompassing local & nonlocal phenomena and electromagnetic electron dynamics |
|                   | GYRO, TGYRO       | • Predictive simulations of transport iterated to bring the plasma into steady-state power balance; radial transport balances power input |
| **Geoscience**    |                   |                |
|                   | PFLOTRAN           | • Stability and viability of large-scale CO₂ sequestration  
• Predictive contaminant ground water transport |
### OLCF-3 Applications Analyzed

Science outcomes were elicited from a broad range of applications

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<thead>
<tr>
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</thead>
<tbody>
<tr>
<td>Nanoscience</td>
<td>OMEN</td>
<td>• Electron-lattice interactions and energy loss in full nanoscale transistors</td>
</tr>
<tr>
<td></td>
<td>LS3DF</td>
<td>• Full device simulation of a nanostructure solar cell</td>
</tr>
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<td></td>
<td>DCA++</td>
<td>• Magnetic/superconducting phase diagrams including effects of disorder&lt;br&gt;• Effect of impurity configurations on pairing and the high-T superconducting gap&lt;br&gt;• High-T superconducting transition temperature materials dependence in cuprates</td>
</tr>
<tr>
<td></td>
<td>WL-LSMS</td>
<td>• To what extent do thermodynamics and kinetics of magnetic transition and chemical reactions differ between nano and bulk?&lt;br&gt;• What is the role of material disorder, statistics, and fluctuations in nanoscale materials and</td>
</tr>
<tr>
<td>Nuclear energy</td>
<td>Denovo</td>
<td>• Predicting, with UQ, the behavior of existing and novel nuclear fuels and reactors in transient and nominal operation</td>
</tr>
<tr>
<td></td>
<td>UNIQ</td>
<td>• Reduce uncertainties and biases in reactor design calculations by replacing existing multi-level homogenization techniques with more direct solution methods</td>
</tr>
<tr>
<td>Nuclear Physics</td>
<td>NUCCOR</td>
<td>• Limits of nuclear stability, static and transport properties of nucleonic matter&lt;br&gt;• Predict half-lives, mass and kinetic energy distribution of fission fragments and fission cross sections</td>
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<td></td>
<td>MFDn</td>
<td></td>
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<tr>
<td></td>
<td>MILC,Chroma</td>
<td>• Achieving high precision in determining the fundamental parameters of the Standard Model (masses and mixing strengths of quarks)</td>
</tr>
<tr>
<td>Turbulence</td>
<td>DNS</td>
<td>• Stratified and unstratified turbulent mixing at simultaneous high Reynolds and Schmidt numbers</td>
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<tr>
<td></td>
<td>Hybrid</td>
<td>• Nonlinear turbulence phenomena in multi-physics settings</td>
</tr>
</tbody>
</table>
# Evaluation Criteria for Selection of Six Representative Applications

<table>
<thead>
<tr>
<th>Task</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Science</td>
<td>• Science results, impact, timeliness&lt;br&gt; • Alignment with DOE and U.S. science mission (CD-0)&lt;br&gt; • Broad coverage of science domains</td>
</tr>
<tr>
<td>Implementation (models, algorithms, software)</td>
<td>• Broad coverage of relevant programming models, environment, languages, implementations&lt;br&gt; • Broad coverage of relevant algorithms and data structures (motifs)&lt;br&gt; • Broad coverage of scientific library requirements</td>
</tr>
<tr>
<td>User community (current and anticipated)</td>
<td>• Broad institutional and developer/user involvement&lt;br&gt; • Good representation of current and anticipated INCITE workload</td>
</tr>
<tr>
<td>Preparation for steady state (“INCITE ready”) operations</td>
<td>• Mix of low (“straightforward”) and high (“hard”) risk porting and readiness requirements&lt;br&gt; • Availability of OLCF liaison with adequate skills/experience match to application&lt;br&gt; • Availability of key code development personnel to engage in and guide readiness activities</td>
</tr>
</tbody>
</table>
Center for Accelerated Application Readiness

WL-LSMS
Role of material disorder, statistics, and fluctuations in nanoscale materials and systems.

S3D
Understanding turbulent combustion through direct numerical simulation with complex chemistry.

PFLOTRAN
Stability and viability of large scale CO₂ sequestration; predictive containment groundwater transport.

CAM-SE
Answer questions about specific climate change adaptation and mitigation scenarios; realistically represent features like precipitation patterns/statistics and tropical storms.

LAMMPS
Biofuels: An atomistic model of cellulose (blue) surrounded by lignin molecules comprising a total of 3.3 million atoms.

Denovo
Discrete ordinates radiation transport calculations that can be used in a variety of nuclear energy and technology applications.

CAAR apps will form the vanguard of ‘day-one’ science on OLCF-3, but additional science teams will be granted friendly-user access as well (cf. our Petascale Early Science Period). Call for proposals will be forthcoming this summer.
## CAAR Application Summary

<table>
<thead>
<tr>
<th>Code</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAM-HOMME</td>
<td>• Spectral finite element method&lt;br&gt;• High leverage in physics packages&lt;br&gt;• Scalable dynamical core of choice for future CCSM&lt;br&gt;• Hard rating: Low compute intensity and high data movement in physics kernels</td>
</tr>
<tr>
<td>S3D</td>
<td>• DNS of combustion processes for specific fuels&lt;br&gt;• Compressible Navier-Stokes flow solver for the full mass, momentum, energy and species conservation equations with structured grid written in F90&lt;br&gt;• Moderate rating: Complex rate equations, thermodynamics, and transport properties modules; no compute libraries used</td>
</tr>
<tr>
<td>LAMMPS</td>
<td>• Critical to development of alternative energy sources, including second-generation cellulosic ethanol&lt;br&gt;• Easily broken up into components available to other MD codes&lt;br&gt;• Broad open community MD code owned by a DOE national laboratory: Large user and developer groups&lt;br&gt;• Moderate rating: Data non-locality due to calculation of long-range Coulomb force (common to all MD codes) – these changes will be made available as library</td>
</tr>
</tbody>
</table>
### CAAR Application Summary (continued)

<table>
<thead>
<tr>
<th>Code</th>
<th>Description</th>
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</thead>
</table>
| gWL-LSMS   | • Enables first-principles studies of magnetic materials with broad relevance to DOE energy mission  
            • Uses a workhorse approach (F77/90, C++, MPI) common to many applications  
            • Straightforward rating: Main kernel based on dense linear algebra of complex numbers (LAPACK, CULA, MAGMA)                                                                                     |
| Denovo     | • Key application for neutron transport and power distribution prediction in nuclear reactor cores  
            • Moderate rating: Huge potential for exploiting untapped concurrency along “energy dimension” helps port, while heavy use of C++ and advanced programming models will tax GPU software and tool environment |
| PFLOTRAN   | • Full featured finite element application with both structured and unstructured versions written in F90  
            • PETSc solver technology used extensively  
            • Hard rating: Non-data locality caused by implicit nonlinear PDE solutions with indirect addressing and data movement caused by AMR (via SAMRAI)                         |
## CAAR Algorithmic Coverage

<table>
<thead>
<tr>
<th>Code</th>
<th>FFT</th>
<th>Dense linear algebra</th>
<th>Sparse linear algebra</th>
<th>Particles</th>
<th>Monte Carlo</th>
<th>Structured grids</th>
<th>Unstructured grids</th>
</tr>
</thead>
<tbody>
<tr>
<td>S3D</td>
<td></td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>CAM</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
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<tr>
<td>LSMS</td>
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<td>X</td>
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<tr>
<td>LAMMPS</td>
<td>X</td>
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<td>X</td>
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<tr>
<td>Denovo</td>
<td></td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
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<tr>
<td>PFLOTRAN</td>
<td></td>
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<td>X (AMR)</td>
</tr>
</tbody>
</table>

- Selected applications represented bulk of use for 6 INCITE allocations totaling 212M cpu-hours (2009)
  - Represented 35% of 2009 INCITE allocations
  - 23% of 2010 INCITE allocations (in cpu-hours)
<table>
<thead>
<tr>
<th>App</th>
<th>Science Area</th>
<th>Algorithm(s)</th>
<th>Grid type</th>
<th>Programming Language(s)</th>
<th>Compiler(s) supported</th>
<th>Communication Libraries</th>
<th>Math Libraries</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAM-HOMME</td>
<td>climate</td>
<td>spectral finite elements, dense &amp; sparse linear algebra, particles</td>
<td>structured</td>
<td>F90</td>
<td>PGI, Lahey, IBM</td>
<td>MPI</td>
<td>Trilinos</td>
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<tr>
<td>LAMMPS</td>
<td>biology/materials</td>
<td>molecular dynamics, FFT, particles</td>
<td>N/A</td>
<td>C++</td>
<td>GNU, PGI, IBM, Intel</td>
<td>MPI</td>
<td>FFTW</td>
</tr>
<tr>
<td>S3D</td>
<td>combustion</td>
<td>Navier-Stokes, finite diff, dense &amp; sparse linear algebra, particles</td>
<td>structured</td>
<td>F77, F90</td>
<td>PGI</td>
<td>MPI</td>
<td>None</td>
</tr>
<tr>
<td>Denovo</td>
<td>nuclear energy</td>
<td>wavefront sweep, GMRES</td>
<td>structured</td>
<td>C++, Fortran, Python</td>
<td>GNU, PGI, Cray, Intel</td>
<td>MPI</td>
<td>Trilinos, LAPACK, SuperLU, Metis</td>
</tr>
<tr>
<td>WL-LSMS</td>
<td>nanoscience</td>
<td>density functional theory, Monte Carlo</td>
<td>N/A</td>
<td>F77, F90, C, C++</td>
<td>PGI, GNU</td>
<td>MPI</td>
<td>LAPACK (ZGEMM, ZGTRF, ZGTRS)</td>
</tr>
<tr>
<td>PFLOTRAN</td>
<td>geoscience</td>
<td>Richards’ equation coupled to transport and chemistry, finite-volume hydrodynamics</td>
<td>AMR</td>
<td>F90</td>
<td>PGI, GNU</td>
<td>MPI, SAMRAI</td>
<td>BLAS, PETSc</td>
</tr>
</tbody>
</table>

- Algorithm and implementation coverage extends applicability well beyond the science domains immediately represented.

- Much of the development work will also be pushed out to broader communities (e.g., in use of ChemKin)
Tactics

- Comprehensive team assigned to each app
  - OLCF application lead
  - Cray engineer
  - NVIDIA developer
  - Other: other application developers, local tool/library developers

- Particular plan-of-attack different for each app
  - WL-LSMS – dependent on accelerated ZGEMM
  - CAM-HOMME – pervasive and widespread custom acceleration required

- Multiple acceleration methods explored
  - WL-LSMS – CULA, MAGMA, custom ZGEMM
  - CAM-HOMME – CUDA, PGI directives
  - Two-fold aim
    - Maximum acceleration for model problem
    - Determination of optimal, reproducible acceleration path for other applications

- Constant monitoring of progress
  - Status of each app discussed weekly

Friday, July 1, 2011
# Application Teams

<table>
<thead>
<tr>
<th>Application</th>
<th>OLCF Lead</th>
<th>Cray</th>
<th>NVIDIA</th>
<th>Science &amp; Tools</th>
</tr>
</thead>
<tbody>
<tr>
<td>S3D</td>
<td>Ramanan Sankaran</td>
<td>John Levesque</td>
<td>Gregory Ruetsch</td>
<td>Ray Grout (NREL)</td>
</tr>
<tr>
<td>WL-LSMS</td>
<td>Markus Eisenbach</td>
<td>Jeff Larkin</td>
<td>Massimiliano Fatica</td>
<td>Yang Wang (PSC)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Adrian Tate</td>
<td>Peng Wang</td>
<td>Aurelian Rusanu (ORNL/UTK)</td>
</tr>
<tr>
<td>CAM-HOMME</td>
<td>Ilene Carpenter (NREL)</td>
<td>Jeff Larkin</td>
<td>Paulius Micikevicius</td>
<td>Matt Norman, Kate Evans,</td>
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<td>Rick Archibald, Jim Hack,</td>
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<td>Oscar Hernandez (ORNL)</td>
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<td>Mark Taylor (SNL)</td>
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<td>JF Lamarque, John Dennis (NCAR)</td>
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<td>Jim Rosinski (NOAA)</td>
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<tr>
<td>LAMMPS</td>
<td>Arnold Tharrington</td>
<td>Sarah Anderson</td>
<td>Peng Wang</td>
<td>Steve Plimpton, Paul Crozier (SNL)</td>
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<td></td>
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<td>Scott Le Grande</td>
<td>Mike Brown (ORNL)</td>
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<td>Axel Kohlmeyer (Temple)</td>
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<td></td>
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<td></td>
<td></td>
<td>Mike Brown (OLCF)</td>
</tr>
<tr>
<td>Denovo</td>
<td>Wayne Joubert</td>
<td>Kevin Thomas</td>
<td>Cyril Zeller</td>
<td>Tom Evans, Chris Baker (ORNL)</td>
</tr>
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<td></td>
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<td>John Roberts</td>
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<tr>
<td>PFLOTRAN</td>
<td>Bobby Philip</td>
<td>Nathan Wichmann</td>
<td>Peng Wang</td>
<td>Peter Lichtner (LANL)</td>
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<td>Rebecca Hartmann-Baker (ORNL)</td>
</tr>
</tbody>
</table>
Complications

• All of the chosen apps are under constant development
  – Groups have, in many cases, already begun to explore GPU acceleration “on their own.”

• Production-level tools, compilers, libraries, etc. are just beginning to become available
  – Multiple paths are available, with multifarious trade-offs
    – ease-of-use
    – (potential) portability
    – performance
What Are We Trying First?

- WL-LSMS
  - Primarily Library-based
- S3D
  - Directives and CUDA
- LAMMPS
  - CUDA
- CAM-SE
  - CUDA Fortran & Directives
- Denovo
  - CUDA
- PFLOTRAN
  - Directives
Hierarchical Parallelism

- MPI parallelism between nodes (or PGAS)
- On-node, SMP-like parallelism via threads (or subcommunicators, or…)
- Vector parallelism
  - SSE/AVX on CPUs
  - GPU threaded parallelism

- Exposure of unrealized parallelism is essential to exploit all near-future architectures.
- Uncovering unrealized parallelism and improving data locality improves the performance of even CPU-only code.
Some Lessons Learned

• Exposure of unrealized parallelism is essential.
  – Figuring out where is often straightforward
  – Making changes to exploit it is hard work (made easier by better tools)
  – Developers can quickly learn, e.g., CUDA and put it to effective use
  – A directives-based approach offers a straightforward path to portable performance

• For those codes that already make effective use of scientific libraries, the possibility of continued use is important.
  – HW-aware choices
  – Help (or, at least, no hindrance) to overlapping computation with device communication

• Ensuring that changes are communicated back and remain in the production “trunk” is every bit as important as we initially thought.
  – Other development work taking place on all CAAR codes could quickly make acceleration changes obsolete/broken otherwise

• How much effort is this demanding?
  – All 6 CAAR teams have converged (independently) to 2 ± 0.5 FTE-years
Global circulation solar model with resolved, turbulent tachocline

3D supernova progenitors including iron core and overlying silicon burning shell up to core collapse including the effects of rotation

3D supernova progenitors from the end of silicon core burning up to core collapse

1st-gen 2D supernova progenitor including all dynamically active layers

1st-gen 3D AGB model including convective red giant envelope

3D AGB model with convective envelope and resolved turbulent boundary layer mixing between active burning layers and envelope

3d supernova progenitor including all dynamically active layers

Global circulation solar model with techocline and surface granulation

3d AGB model including the effects of rotation on the global circulation and mass mixing properties

Exa-flop year sustained

Core-Collapse Supernovae

Decades of core-collapse supernovae simulations have led to a challenging opposition for the eventual description of the explosion mechanism and the associated phenomenology. It is now known that three-dimensional hydrodynamics in general relativistic gravity must be coupled to nuclear kinetics capable of accurate estimation of energy release and compositional changes, and to spectral neutrino transport of all flavors (requiring a fourth, neutrino energy, dimension) to reliably determine the nature of the explosion mechanism. Moreover, the inclusion of neutrino masses and oscillations, as well as magnetic fields—both of which may be important effects—make the problem even more difficult. All of these effects, familiar in some sense from the earlier life of the star, operate on very short (millisecond) timescales and at extremes in density (as high as three to four times nuclear matter density) and neutron richness (the ratio of protons to neutrons in the matter can be several times smaller than what is accessible in terrestrial experiments). The rich interplay of all these physical phenomena in core-collapse supernovae ultimately leads to the realization that only through simulation will scientists be able to fully understand these massive stellar explosions. The relative complexity of the germane physics also means the requisite physical fidelity for these simulations will only be realized at the extreme scale.

Source: Messer et al. (2009).

Image courtesy of Bronson Messer (Oak Ridge National Laboratory).

Rendering of the matter entropy in the core of a massive star at approximately 100 ms following core bounce. Multidimensional fluid effects, coupled to heating and cooling via neutrino emission and absorption, have served to form large, asymmetric structures in the flow. Much of this complicated flow pattern occurs between the surface of the nascent neutron star at the center of the star and the position of the original supernova shock (demarcated by the faint blue circle near the edge of the figure). These first four-dimensional simulations have already consumed tens of millions of central processing unit hours on leadership computing platforms and will require tens of millions of additional central processing unit hours to follow the evolution to the requisite one second of physical time.
3-D whole-star simulations with nuclear kinetics and resolution to treat turbulent nuclear burning.

3-D whole-star simulations with resolution to capture turbulent burning dynamics and convection in the stellar core.

3-D whole-star simulations with resolution sufficient to capture initiation of a detonation.

10x Tera | 100x Tera | Peta | 10x Peta | 100x Peta | Exa-flop year sustained
Stellar Astrophysics provides a target-rich environment for these architectures

- Large number of DOF at each grid point
- Lots of opportunities to hide latency via multiphysics
Strong scaling with improved local physical fidelity is good, but not the whole answer.

- Many problems (e.g. Type Ia SNe) are woefully underresolved
- Diminishing bytes/FLOP will limit spatial resolution (distributed memory)
- AMR will become even more essential
  - Data locality becomes a problem
- Task-based AMR systems
  - cf. Uintah, MADNESS
Summary

• We are not in the advent of exascale-like architectures, we are *in medias res*.

• Tools, compilers, etc. are becoming available to help make the transition.

• The specific details of the platforms matter much less than the overarching theme of hierarchical parallelism.

• Multiphysics simulations have unrealized parallelism to tap.
  
  – Applications relying on, e.g., solution to large linear systems could also benefit from a task based approach.