SOS-14 Future Directions in GPU HW Panel

John Morrison
Los Alamos National Laboratory
March 9, 2010
A Roadrunner Petaflop in a Quadchart!

Accelerated Node Concept

Cell-accelerated compute node

Add Cells to each individual node

Multi-socket multi-cores Opteron cluster nodes

I/O gateway nodes

(100’s of such cluster nodes)

“Connected Unit” Cluster Interconnect Switch/Fabric

Triblade Node with PCIe-connected Cells

Cell with 8 Specialized vector cores

Two QS22’s (2 Cells each)

Expansion blade

LS21 with 2 Opterons

Design objective: One Cell processor for every Opteron core, plus the same memory footprint for each (4GB each), with the fastest feasible interconnects

Connected Unit cluster
180 compute nodes w/ Cells + 12 I/O nodes

12,240 PowerXCell 8i chips ⇒ 1.33 PF, 49 TB
6,120 dual-core Opterons ⇒ 44 TF, 49 TB

17 CUs
3264 nodes

12 links per CU to each of 8 switches
Eight 2nd-stage 288-port IB 4X DDR switches

Three programs work together

SPE Program

PPE Program

x86 Program

Cell

SPE (8)

SPE compiler

Posix Threads
DMA
IBM ALF
LANL CML

PPE

PowerPC compiler

IBM DaCS
IBM ALF
LANL CML

x86 compiler

Opteron

MPi (cluster)

IB (one per node)
Roadrunner Open Science is the 3rd of 5 Waves of Application Code Efforts

1. Assessment Codes (summer & fall 2007)
   - Proof of Cell & Hybrid programming capability: 4 codes
   - Prototype hardware: old Cell/QS20 blades & very first PowerXCell 8i chip

2. Full-System Pre-Acceptance Testing (fall 2008)
   - High Performance LINPACK
   - Gordon Bell finalists: VPIC & SPaSM
   - PetaVision (sustained 1+ single-precision-PF!)
   - PPM (Paul Woodward, Univ. of Minnesota)

3. Roadrunner Open Science (spring & summer 2009)
   - 10 projects using 8 codes

4. Institutional Computing on Cerrillos
   - 19 new projects started May 2009

5. Classified ASC Use (starting Dec. 2009)
The 10 Roadrunner Open Science projects

<table>
<thead>
<tr>
<th>Science (code)</th>
<th>Description</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Laser Plasma Instabilities (VPIC)</strong></td>
<td>Study the nonlinear physics of laser backscatter energy transfer and plasma instabilities related to the National Ignition Facility (NIF).</td>
<td><strong>Completed</strong></td>
</tr>
<tr>
<td><strong>Magnetic Reconnection (VPIC)</strong></td>
<td>Study the continuous breaking and rearrangement of magnetic field lines in plasmas relevant to both space and laboratory applications.</td>
<td><strong>Completed</strong></td>
</tr>
<tr>
<td><strong>Thermonuclear Burn Kinetics (VPIC)</strong></td>
<td>Study how the TN burn process impacts the velocity distributions of the reacting particle populations and the impact that has on sustaining the burn. (ASC effort)</td>
<td><strong>Code complete</strong></td>
</tr>
<tr>
<td><strong>Spall and Ejecta (SPaSM)</strong></td>
<td>Study how materials break up internally, Spall, and how pieces fly off, Ejecta, as shock waves force the material to break apart at the atomic scale. (ASC effort)</td>
<td><strong>Mostly completed</strong></td>
</tr>
<tr>
<td><strong>HIV Phylogenetics (ML)</strong></td>
<td>Determine “best” evolutionary relationship trees from a large set of actual genetic HIV genetic sequences (phylogenetic tree) for HIV vaccine targeting.</td>
<td><strong>Completed</strong></td>
</tr>
<tr>
<td><strong>Properties of Metallic Nanowires (ParRep)</strong></td>
<td>Apply the parallel-replica approach at the atomistic scale for simulating material properties of nanowires crucial for switches in future nanodevices.</td>
<td><strong>Completed</strong></td>
</tr>
<tr>
<td><strong>DNS of Reacting Turbulence (CFDNS)</strong></td>
<td>Study thermonuclear burning in turbulent conditions in Type Ia supernovae using Direct Numerical Simulations (DNS) with full rad-hydro.</td>
<td><strong>Completed</strong></td>
</tr>
<tr>
<td><strong>The Roadrunner Universe (RRU)</strong></td>
<td>Create a repository of particle simulations of the distribution of matter in the universe to look at galaxy-scale concentrations and structures (dark matter halos).</td>
<td><strong>Partially completed</strong></td>
</tr>
<tr>
<td><strong>Supernovae Light-Curves (Cassio)</strong></td>
<td>Study the impact of 2D asymmetries on the radiative light output in core collapse supernovae. Coupled RAGE on Opteron-only with Jayenne-Milagro IMC (accelerated).</td>
<td><strong>Code complete</strong></td>
</tr>
<tr>
<td><strong>Cellulosomes (Gromacs)</strong></td>
<td>Study the effectiveness of the decomposition of cellulose sheets of plant fiber by cellusome bacteria related to biofuels (cellulosic alcohol) production due to performance issues &amp; manpower.</td>
<td><strong>Code work stopped</strong></td>
</tr>
</tbody>
</table>

*UNCLASSIFIED*
Roadrunner Open Science is a grand success.

- The goals of Open Science were attained:
  - We broadened the applicability of the Roadrunner architecture to new applications areas.
  - We increased the pool of knowledgeable programmers for Cell & Roadrunner, but also for similar expected future Exascale architectures.
  - 7 of 10 Open Science projects were clear successes.
  - Significant scientific accomplishments were achieved.
  - The Roadrunner machine is now more stable and better tested.

This effort has set the stage to take on Classified nuclear weapons work.
ASC Milestone work is underway

- Precursors to current work:
  - Deployment of development cluster in LANL classified environment
  - FY2009 classified code release milestone

- Calculations for 2010 ASC milestones are being performed on Roadrunner

- Speedup vs Opteron for accelerated code portions
  - ~20x for idealized problem
  - 5-10^x for actual problems reported by milestone users