Performance Metrics and Application Experiences on a Cray CS300-AC™ Cluster Supercomputer Equipped with Intel® Xeon Phi™ Coprocessors

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Outline

- Introduction to AACE/Beacon
- Introduction to the Intel Xeon Phi Coprocessor
- Discussion of codes ported and optimized for the Phi
  - ENZO
  - H3D
  - Boltzmann-BGK
  - Gyro
- Discussion of codes ported but not optimized for the Phi
- Conclusions
Application Acceleration Center of Excellence (AACE)

- Established by the University of Tennessee in 2011 alongside the National Institute for Computational Sciences (NICS) at Oak Ridge National Laboratory (ORNL)
- Tasked with exploring the application of emerging computing technologies to simulation in science and engineering
- An essential element of a sustainable software infrastructure for simulation in science and engineering

Managed by UT-Battelle for the U.S. Dept. of Energy
Strategic Engagement with Intel

- Multi-year agreement with Intel to jointly pursue:
  - Development of next-generation, high-performance computing solutions based on the Intel® Many Integrated Core (MIC) architecture
  - Design of scientific applications emphasizing a sustainable approach for both performance and productivity
- AACE receives early access to Intel technologies and provides application testing, performance results, and expert feedback to Intel
  - Help guide further development efforts by Intel
  - Prepare scientific community for next generation HPC technologies such as the Intel® Xeon Phi™ coprocessor
### The Beacon Project

**Beacon – Phase 1**  
Cray Xtreme-X Supercomputer

<table>
<thead>
<tr>
<th>Feature</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nodes</td>
<td>2 service, 16 compute</td>
</tr>
<tr>
<td>Interconnect</td>
<td>FDR IB Fat Tree</td>
</tr>
<tr>
<td>CPU model</td>
<td>Intel Xeon E5-2670</td>
</tr>
<tr>
<td>CPUs per node</td>
<td>2 8-core, 2.6 GHz</td>
</tr>
<tr>
<td>RAM per node</td>
<td>64 GB</td>
</tr>
<tr>
<td>SSD per node</td>
<td>80 GB</td>
</tr>
<tr>
<td>Intel® Xeon Phi™ coprocessors per node</td>
<td>2 x pre-production 50+ cores, 8 GB GDDR5 RAM</td>
</tr>
</tbody>
</table>

**Beacon – Phase 2**  
Cray Xtreme-X Supercomputer  
Peak Performance: 210.1 TFLOP/s

<table>
<thead>
<tr>
<th>Feature</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nodes</td>
<td>4 service, 6 I/O, 48 compute</td>
</tr>
<tr>
<td>Interconnect</td>
<td>FDR IB Fat Tree</td>
</tr>
<tr>
<td>CPU model</td>
<td>Intel Xeon E5-2670</td>
</tr>
<tr>
<td>CPUs per node</td>
<td>2 8-core, 2.6GHz</td>
</tr>
<tr>
<td>RAM per node</td>
<td>256 GB</td>
</tr>
<tr>
<td>SSD per node</td>
<td>2 x 480 GB (compute), 16 x 300 GB (I/O)</td>
</tr>
<tr>
<td>Intel® Xeon Phi™ Coprocessors per node</td>
<td>4 x 5110P 60-core, 1.053GHz 8 GB GDDR5 RAM</td>
</tr>
</tbody>
</table>

- Funded by NSF to port and optimize scientific codes to the Intel® Xeon Phi™ coprocessor
- State-funded expansion focuses on energy efficiency, big data applications, and industry
- Example Codes: PSC, H3D, OMEN, ENZO, MADNESS, NWCHEM, Amber, MILC, and MAGMA

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The Intel Xeon Phi Coprocessor

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Vectorization on the Intel Xeon Phi

Vector Processor: 512b SIMD Width

16 wide SP SIMD, 8 wide DP SIMD
2:1 Ratio good for circuit optimization

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Comparing Results from Intel Xeon Phi

In order to have an apples to apples comparison on the Xeon Phi, we need to consider the following:

• Compare 2 Sandybridges to 1 Xeon Phi
  • 125W x 2 vs 255 W
  • 256 bit vector x 2 vs 512 bit vector
  • Run same code on both

• Doing some quick math, this means that we have similar power and vector processing, except that the Xeon is ~2.5 times the clock speed

• So, how do we make the Xeon Phi worth our while?
  • Many more threads
  • Programming versatility
Intel Xeon Phi Programming Paradigms

- Native mode
- Offload mode
- Heterogeneous Execution
- MPI/OpenMP/Hybrid
Codes Investigated by AACE

- Atmospheric modeling – HOMME-CAM (ported)
- Astrophysics – Enzo (ported and partially optimized)
- Computational Fluid Dynamics (CFD) – BGK-Boltzmann Solver (ported and optimized)
- Earthquake modeling – AWP-ODC (ported)
- Magnetospheric Physics – H3D (ported and partially optimized) and PSC (ported)
- Tokamak Plasmas – Gyro (ported)
- Agent Based Modeling – Transims and ASCAPE (ported)
Enzo

- Community code for computational astrophysics and cosmology
- More than 1 million lines of code
- Uses powerful adaptive mesh refinement
- Highly vectorized with a hybrid MPI + OpenMP programming model
- Utilizes HDF5 and HYPRE libraries
- Multiple MPI tasks per coprocessor and many threads per MPI task

Enzo was ported and optimized for the the Intel® Xeon Phi™ Coprocessor by Dr. Robert Harkness
harkness@sdsc.edu
Preliminary Scaling Study: Native

- ENZO-C
- $128^3$ mesh (non-AMR)
- pure MPI
- native mode
- Fortran, C, C++

Results were generated on the Intel® Knights Ferry software development platform.
Multi-KNC Scaling Study: Native

- ENZO-R
- $N^3$ mesh
- Decomposed into 4x4x4 blocks
- Native mode on 16 KNC
- 4 MPI ranks per KNC
- 1,2,4,8,12,16 threads per rank

Results were generated on a Pre-Production Intel® Xeon Phi™ coprocessor Beta software, 61 cores @ 1.09 GHz and 8 GB of GDDR5 RAM @ 2.75 GHz
Hybrid3d (H3D)

- Provides breakthrough kinetic simulations of the Earth’s magnetosphere
- Models the complex solar wind-magnetosphere interaction using both electron fluid and kinetic ions
  - Unlike magnetohydrodynamics (MHD), which completely ignores ion kinetic effects
- Contains the following HPC innovations:
  1. multi-zone (asynchronous) algorithm
  2. dynamic load balancing
  3. code adaptation and optimization to large number of cores

Hybrid3d (H3D) was provided for porting to the Intel® Xeon Phi™ Coprocessor by Dr. Homa Karimabadi
hkarimabadi@ucsd.edu
Hybrid3d (H3D) Performance

Optimizations were provided by Intel senior software engineer Rob Van der Wjingaart.

Results were generated on a Pre-Production Intel® Xeon Phi™ coprocessor with B0 HW and Beta SW 61 cores @ 1.09 GHz and 8 GB of GDDR5 RAM @ 2.75 GHz.
Computational Fluid Dynamics (CFD)

Steady-state solution of a Couette flow using the Boltzmann equation with BGK collision approximation

The above CFD solvers were developed for the Intel® Xeon Phi™ Coprocessor by Ryan C. Hulguin
ryan-hulguin@tennessee.edu
Impact of Various Optimizations on the Model Boltzmann Equation Solver

- Optimized by Intel software engineer Rob Van der Wjinggaart
- Base-line solver – all loops were vectorized except for one

- Set I — Loop Vectorization
  - Stack variable pulled out of the loop
  - Class member turned into a regular structure
- Set II — Data Access
  - Arrays linearized using macros
  - Align data for more efficient access
- Set III — Parallel Overhead
  - Reduce the number of parallel sections
- Set IV — Dependency
  - Remove reduction from computational loop by saving value into a private variable
- Set V — Precision
  - Use medium precision for math function calls (-fimf-precision=medium)
- Set VI — Precision
  - Use single precision constants and intrinsics
- Set VII — Compiler Hints
  - Use #pragma SIMD instead of #pragma IVDEP
Optimization Results from the Model Boltzmann Equation Solver

Results were generated on a Pre-Production Intel® Xeon Phi™ coprocessor with B0 HW and Beta SW 61 cores @ 1.09 GHz and 8 GB of GDDR5 RAM @ 2.75 GHz
Model Boltzmann Equation Solver Performance

Relative Speedup of two 8-core 3.5 GHz Intel® Xeon E5-2670 Processors Versus an Intel® Xeon Phi™ Coprocessor

Results were generated on a Pre-Production Intel® Xeon Phi™ coprocessor with B0 HW and Beta SW
61 cores @ 1.09 GHz and 8 GB of GDDR5 RAM @ 2.75 GHz
Model Boltzmann Equation Solver Performance: Another View

Results were generated on a 5100P Intel® Xeon Phi™ coprocessor with MPSS Gold 60 cores @ 1.053 GHz and 8 GB of GDDR5 RAM @ 2.75 GHz.
GYRO is a code for the numerical simulation of fusion tokamak microturbulence

- Computes the turbulent radial transport of particles and energy in tokamak plasmas
- Solves 5-D coupled time-dependent nonlinear gyrokinetic-Maxwell equations with gyrokinetic ions and electrons
- Developed by Jeff Candy and Ron Waltz at General Atomics
- GYRO can operate as a flux-tube (local) code, or as a global code, with electrostatic or electromagnetic fluctuations.
- Propagates system forward using a second-order, implicit-explicit Runga-Kutta integrator and a fourth-order, explicit Eulerian algorithm
- Runs on a variety of machines: IBM Power, Cray XT and XE, SGI ICE and UV, Intel and Opteron Clusters
Gyro: MPI Performance

Gyro Performance on Beacon

- Xeon
- Phi
- Xeon

Timesteps/Second vs. MPI Ranks
Gyro: Threaded Performance

Gyro Performance on Beacon at Different Thread Counts

- 64 MPI Ranks
- 128 MPI Ranks

Timesteps/Second vs. Threads
Other codes ported to the Phi

<table>
<thead>
<tr>
<th>Code</th>
<th>MPI Ranks</th>
<th>Walltime</th>
<th>Speed Up</th>
<th>% Peak</th>
</tr>
</thead>
<tbody>
<tr>
<td>HOMME-CAM</td>
<td>32</td>
<td>82.65 s</td>
<td>——</td>
<td>——</td>
</tr>
<tr>
<td>HOMME-CAM</td>
<td>64</td>
<td>54.91 s</td>
<td>1.51</td>
<td>76%</td>
</tr>
<tr>
<td>PSC</td>
<td>16</td>
<td>894.41 s</td>
<td>——</td>
<td>——</td>
</tr>
<tr>
<td>PSC</td>
<td>32</td>
<td>679.58 s</td>
<td>1.32</td>
<td>66%</td>
</tr>
<tr>
<td>AWP-ODC</td>
<td>32</td>
<td>932 s</td>
<td>——</td>
<td>——</td>
</tr>
<tr>
<td>AWP-ODC</td>
<td>64</td>
<td>524 s</td>
<td>1.78</td>
<td>89%</td>
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<tr>
<td>AWP-ODC</td>
<td>128</td>
<td>287 s</td>
<td>3.25</td>
<td>81%</td>
</tr>
<tr>
<td>TRANSIMS</td>
<td>1</td>
<td>5904 s</td>
<td>serial</td>
<td>——</td>
</tr>
<tr>
<td>ASCAPE</td>
<td>1</td>
<td>30.197 s</td>
<td>serial</td>
<td>——</td>
</tr>
</tbody>
</table>
Other codes ported to the Phi

As one can see, while the Xeon Phi has a lower clock speed than the Xeon, it still exhibits speed up when running a scalable code.

However, exposing enough parallelism to beat the Xeon implementation requires some extra effort.
Conclusions

• Porting to the Intel Xeon Phi is simple

• Optimizing for the Xeon Phi takes some work, but pays dividends on all architectures

• The hybrid MPI/OpenMP model, along with vectorization, shows promise

• And....
WORLD RECORD!
“Beacon” at NICS

Intel® Xeon® + Intel Xeon Phi™ Cluster
First to Deliver
2.499 GigaFLOPS / Watt
71.4% HPL efficiency
#1 on current Green500

Other brands and names are the property of their respective owners.
Open Call for Participation

• The call for NSF-supported time on Beacon is closed, but compute time on Beacon is still available at the discretion of the director.

• Individual researchers and teams are invited to submit proposals for projects investigating the impact of the Intel® Xeon Phi™ coprocessor on areas of interest to their particular field of study. Some possible areas of interest include (but are not limited to):
  • Computational modeling and simulation
  • Data analysis and visualization
  • Novel algorithms targeting the Intel® Xeon Phi™ coprocessor
  • Programming languages and tools
  • Debugging and profiling tools
  • Performance evaluation studies and tools
  • Energy-efficient computing

• Projects involving high-performance computing (HPC) applications in fields such as biology, economics, social sciences, and other non-traditional HPC domains are especially encouraged, as are projects associated with data-intensive computing and data-driven workflows.

• See http://www.jics.tennessee.edu/aace/beacon/open-call for details.
Acknowledgements

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