Accelerating Simulation & Analysis with Hybrid GPU Parallelization and Cloud Computing

Devin Jensen
August 2012
Altair Knows HPC

*Altair is the only company that:*

**makes** HPC tools…

**develops** HPC applications…

…and **uses** these to solve real HPC problems

500 Altair engineers worldwide **use HPC every day** for real-world modeling & simulation
Innovation Intelligence®

26+
Years of Innovation

40+
Offices in 18 Countries

1500+
Employees Worldwide
## Customers

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<tr>
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<th>Government</th>
<th>Life/Earth Sciences</th>
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Hardware Trends and Software Evolution

- Multi Level Parallelism
- Hybrid MPI/OpenMP & Heterogeneous CPU/GPU
- SMP Parallelization
- MPI Clusterization
- Single Threaded & Vectorization

Source: Intel Corp.
Motivations to use GPU for Solvers

- Cost effective solution
- Power efficient solution

How much of the peak can we get?
- Which part of the code is best suited?
- How much coding effort is required?
- What will be the speedup for my application?
• **Ecosystem based on CUDA (+ OpenACC with CRAY, PGI and CAPS)**
  
  • Any NVIDIA graphic card supports CUDA
  
  • Strong market presence

• **Products**
  
  • Tesla and Quadro GPUs based on the Fermi Architecture
  
  • Announcement of Kepler Architecture, ~2X faster than Fermi, HyperQ, virtualization,…
AcuSolve GPU Porting on NVIDIA CUDA

- High performance computational fluid dynamics software (CFD)
- The leading finite element based CFD technology
- High accuracy and scalability on massively parallel architectures

S-duct
80K Degrees of Freedom
Hybrid MPI/OpenMP for Multi-GPU test

8 core CPU 1 core + 1 GPU

Lower is better

*Performance gain versus 4 core CPU
RADIOSS Porting on GPU

- Assess the potential of GPU for RADIOSS
- Focus on Implicit
  - Direct Solver
    - Highly optimized compute intensive solver
    - Limited scalability on multicores and cluster
  - Iterative Solver
    - Ability to solve huge problems with low memory requirement
    - Efficient parallelization
    - High cost on CPU due to large number of iterations for convergence
- Double Precision required
- Integrate GPU parallelization into our Hybrid parallelization technology
RADIOSS Porting on GPU & Accelerators

• **CUDA official version planned for HW12**
  • RADIOSS implicit direct solver and iterative solver available under Linux
  • Support for NVIDIA Fermi and Kepler (K20 Q1’13)
  • Altair RADIOSS presentation at GTC2012

• **OpenCL Beta version**
  • Only RADIOSS Implicit Iterative Solver available under Linux and Windows
  • Support for AMD FirePro
  • Altair RADIOSS presentation at AFDS2011
RADIOSS Direct Solver GPU Porting

- **CUBLAS (DGEMM)** – perfect candidate to speed up update module
  - Frontal matrix could be too huge to fit in GPU memory
  - Frontal matrix could be too small and thus inefficient w/ GPU
  - Data transfer is not trivial
  - Only the lower triangular matrix is interesting

\[
A = \begin{pmatrix}
B & V^t \\
V & C
\end{pmatrix}
\]

- **Pivoting is required in real applications**
  - Pivot searching is a sequential operation
  - Factor module has limited parallel potential
  - It could be as expensive as “update” module in extreme case

- **Asynchronous computing**
  - Overlap the computation
  - Overlap the communication
RADIOSS Direct Solver – Non Pivoting Case

<table>
<thead>
<tr>
<th>Linear static – Non Pivoting Case</th>
<th>Benchmark</th>
<th>2.8 Millions of Degrees of Freedom</th>
</tr>
</thead>
<tbody>
<tr>
<td>Platform</td>
<td>Intel Xeon X5550, 4 Core, 48GB RAM NVIDIA C2070, CUDA 4.0 MKL 10.3, RHEL 5.1</td>
<td></td>
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</table>

GPU speedup - non-pivoting case

- **Solver**
- **elapsed**

Lower is better

- 3.9X
- 2.9X

**update**

**profile** (%)

- base(BCSLIB-EXT)
- improved

**total**
RADIOSS Iterative Solver (Implicit)

- Preconditioned Conjugate Gradient (PCG) solves iteratively $M^{-1} \cdot (Ax - b) = 0$
  - Convergence speed depends on preconditioner M
  - Low memory consumption
  - Efficient parallelization: SMP, MPI

- Porting under CUDA
  - Few kernels to write in Cuda ⇒ Sparse Matrix Vector
  - Use of CUBLAS ⇒ DAXPY & DDOT

- Extend Hybrid to multi GPUs programming
  - MPI to manage communication between GPU
  - Portions of code not GPU enabled benefit from OpenMP parallelization
  - Programming model expandable to multi nodes with multiple GPUs
**RADIOSS PCG – Linear Benchmark #2**

**Linear Problem #2**
Hood of a car with pressure loads
Refined model
Compute displacements and stresses

<table>
<thead>
<tr>
<th>Benchmark</th>
<th>2.2 Millions of Degrees of Freedom</th>
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<tbody>
<tr>
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<td>62 Millions of non zero</td>
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<td>380000 Shells + 13000 Solids + 1100</td>
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<td>RBE3</td>
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<td>5300 iterations</td>
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<tr>
<th>Platform</th>
<th>NVIDIA PSG Cluster – 2 nodes with:</th>
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<tr>
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<td>Dual NVIDIA M2090 GPUs</td>
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<tr>
<td></td>
<td>CUDA v3.2</td>
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<tr>
<td></td>
<td>Intel Westmere 2x6 X5670@2,93Ghz</td>
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<td>Linux RHEL 5.4 with Intel MPI 4.0</td>
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| Performance     | Elapsed time decreased by up to 13X|

Multi GPUs performance is better for bigger models

*Performance gain versus SMP 6-core*
GPU For Explicit?

- **Explicit is very difficult to port on GPU**
  - Data movement between CPU and GPU current bottleneck
  - Require full memory allocated on GPU and therefore full code ported
    ✓ Huge development cost
    ✓ Challenge of multiple code bases
  - Potential gain remains small with current technology approach
    ✓ Data locality and cache reuse is not possible on GPU
    ✓ Memory size limitation

- **Follow hardware evolution**
  - AMD APU (CPU+GPU)
  - Intel Xeon Phi
  - NVIDIA through OpenACC initiative
Altair Solvers on NVIDIA GPUs

- RADIOSS implicit direct & iterative solvers have been successfully ported on NVIDIA GPU using CUDA
- Adding GPU improves performance of Altair solvers significantly
- For iterative solver, Hybrid MPP allows to run on multi GPU card workstation and GPU cluster with good scalability and enhanced performance
- GPU support for implicit solvers is planned for HyperWorks 12
HyperWorks 3D display

- OpenGL stereoscopic display in HyperMesh & HyperView
- Supported by NVIDIA graphics cards
- Compatible with NVIDIA 3D Vision glasses
- Available in HyperWorks 12.0
HyperView Performance Gains From Shaders

Gains in graphics performance – **2x to 6x** improvement in animation frame rate, model rotation, & pan
Licensing Model for Solvers

- Licensing has been set to encourage GPU testing
- One GPU is considered as one additional core only
Where does PBS Professional manage NVIDIA GPUs?

Tokyo Institute of Technology – TSUBAME 2.0

- Reliability
- Robust advance reservations
- GPU support
- Mixed architecture support (Linux, Windows)

~100,000 simultaneous jobs

~2,000 users

2.4 Petaflops
17,984 cores
4,200 GPUs
80 TB mem
174 TB SSD
7 PB disk

PBS Professional offers THE best scalability in the industry...

- NEC

Decreed as one of the “Greenest Production Supercomputer in the World” on the June 2012 Green 500 List, for achieving a high level of energy-efficiency.

HP’s biggest Top500 machine
Purpose-Built for High Performance Computing

IDC study (published 2009) on job scheduling ranked PBS Professional #1

5 Strategic Pillars

- Easy to Use
- Hard to Break
- Do More (with Less)
- Keep Track and Plan
- Open Architecture
Accelerating Your Gateway to HPC Cloud Computing

Structure our Thoughts

- High Performance [N/W & H/W]
- Dynamic Provisioning [Self Service]
- Elasticity / Scale On Demand / Pay as you go
- Large Data Handling
- Ease of access and use / Abstract
Accelerating your Gateway to HPC Cloud Computing

End Users Needs

Focus on My Task / Project → Deliver Results!

**Does have**

- Workstations
- "Limited" Access to Software
- Ideas, Innovation, Agility

**Does NOT have**

- Expertise in IT Infrastructure
- Sufficient compute resources
- Financial / Abundance of Money
Accelerating your Gateway to HPC Cloud Computing

End Users Needs

**Ease of Access:** All you need is just a Browser to access HPC & Domain specific resources

**Ease of Use:** All you need is a browser based application hiding the complexity

**Handle Big Data:** All you need is a way to visualize the managed big data again through a browser based application

User Interface → Portals
Accelerating your Gateway to HPC Cloud Computing

Altair Enterprise Portals

Ease of Use
Ease of Access
Handle Big Data

HyperWorks Enterprise Applications

Compute Manager
Display Manager
Simulation Manager
Process Manager
Performance Manager
COMPUTE MANAGER

Ease of Use | Ease of Access | Handle Big Data
Accelerating your Gateway to HPC Cloud Computing

Compute Manager

Let’s See

Ease of Use  |  Ease of Access  |  Handle Big Data
Accelerating your Gateway to HPC Cloud Computing

Compute Manager

Let’s See

Ease of Use  Ease of Access  Handle Big Data
Accelerating your Gateway to HPC Cloud Computing

HyperWorks Enterprise

Complete Simulation Lifecycle Management

HyperWorks Units

Compute Manager

Display Manager

Simulation Manager

Process Manager

Performance Manager

HyperWorks Units

HyperWorks Enterprise

HyperWorks

PBS Professional

It is “HyperWorks in the Cloud”
Accelerating your Gateway to HPC Cloud Computing

Implementation Models

HyperWorks Enterprise
PBS Works

Private Cloud

Hybrid Cloud
PBS Professional

HyperWorks
On-Demand

Public Cloud
# Accelerating your Gateway to HPC Cloud Computing

## HyperWorks On-Demand: The Basics

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<tr>
<td>Scalable up to 10,000 cores QDR Non-blocking InfiniBand Physical and cyber security</td>
<td>Powered by PBS Professional &amp; HyperWorks Enterprise</td>
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<table>
<thead>
<tr>
<th>HyperWorks Solvers HyperWorks Desktop(^1) Altair Partner Alliance(^1)</th>
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<td>1: coming soon</td>
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</table>

\(^1\): coming soon

IaaS + PaaS + SaaS = HWaaS
Accelerating your Gateway to HPC Cloud Computing

The High-Powered Altair Data Center

- Scalable, modular facility located in Troy, MI
- Can be easily extended to support up to more than 10,000 cores
- Incorporates extensive physical and cyber security measures
- Extremely high compute-power density
- A state-of-the-art facility for HPC simulation computing
Accelerating your Gateway to HPC Cloud Computing

HyperWorks On-Demand

HyperWorks On-Demand™
High Performance Innovation in the Cloud

HyperWorks On-Demand is a High Performance Computing solution for design innovation "in the Cloud". It leverages the patented Altair licensing system and provides access to best-in-class HyperWorks software through a modern, secure, and efficient web-based platform.

Customer ID: customer_name
Username: johndoe
Password: ****

Login

Altair’s user portals is the gateway to HyperWorks On-Demand
Altair Knows HPC

Altair is the only company that:

**makes** HPC tools…

[Image of PBS Works]

**develops** HPC applications…

[Image of HyperWorks]

…and **uses** these to solve real HPC problems

[Image of Altair Product Design]

500 Altair engineers worldwide **use HPC every day** for real-world modeling & simulation
For More Information

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• Visit Us Online
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  • www.altairhyperworks.com
  • wwwpbsworks.com

Thanks, NVIDIA
Thank YOU!