Extreme scalability in CAE ISV Applications

Greg Clifford
Manufacturing Segment Manager
clifford@cray.com
Introduction

- ISV codes dominate the CAE commercial workload
- Many large manufacturing companies have $\gg 10,000$ cores HPC systems
- Even for large organizations very few jobs use more than 128 MPI ranks
- There is a huge discrepancy between the scalability in production at large HPC centers and the commercial CAE environment

Can ISV applications efficiently scale to 1000’s of MPI ranks?

Spoiler alert: the answer is YES!
Often the full power available is not being leveraged
Is there a business case for scalable CAE applications?
A petaflop scale system is required to deliver the capability to move to a new level of seismic imaging.
ExxonMobil and Rosneft…could invest over $500 billion in a joint venture to explore for and produce oil in the Arctic and the Black Sea…

…recoverable hydrocarbon reserves at the three key Arctic fields are estimated at 85 billion barrels by the Associate Press.
Compute & data requirements for seismic processing are huge

- Wide demands on processing from data acquisition to seismic to res sim
- Petaflop scale systems required for state-of-the-art processing
- Petabytes of capacity and terabytes of bandwidth from I/O

The Oil & Gas industry has typically led the way on new HPC hardware technology in the commercial sector

- A single deep water well can cost >$100M…and getting deeper
- “Restating” a reserve has serious business implications

When requirements & return are huge
- the demand for “getting it right” goes up

- This is the class of simulation that drives real petascale capability computing
- You can do capacity on capability systems but not vice versa – risk mitigation
CAE trends driving HPC requirements

● “Extreme Fidelity”*
  ● Enhanced physics and models, e.g. 1 Billion cell models
  ● Large models scale better across compute cores

● Design optimization
  ● Many simulations required to explore the design space
  ● Multiple runs can require 100x compute power

● Robust design
  ● Looking for the “best solution”

“Future performance depends on highly scalable parallel software”

* ref: ANSYS CFD presentation
Compute requirements in CAE

- Robust Design
- Design Optimization
- Design Exploration
- Multiple runs
- Single run

Simulation Fidelity

“Simulation allows engineers to know, not guess – but only if IT can deliver dramatically scaled up infrastructure for mega simulations…. 1000’s of cores per mega simulation”

- Departmental cluster 100 cores
- Desktop 16 cores
- Central Compute Cluster 1000 cores
- Supercomputing Environment >2000 cores
CAE Application Workload

Basically the same ISV codes used across all industries

- **Impact/ Crash Apps**
  - ABAQUS explicit
  - LS-DYNA
  - PAM-CRASH
  - RADIOSS
- **CFD Apps**
  - CFD++
  - ANSYS Fluent
  - PowerFLOW
  - STAR-CCM+
  - “in-house”
- **Structures Apps**
  - ABAQUS implicit
  - ANSYS Mechanical
  - MSC.Nastran
- **Electromagnetic Apps**
  - “in-house” (classified)
  - ANSYS HFSS

Vast majority of large simulations are MPI parallel
Is the extreme scaling technology ready for production CAE environments?
Brief history of HPC technology in high end environments

c. 1978
Cray-1, Vector processing
1 Processor
Automated vectorization in the compiler

c. 1983
Cray X-MP, SMP parallel
8 Processors
Compiler directives for key kernels

c. 1998
Low density, slow interconnect
“Linux cluster”, MPI Parallel
100’s of “cores”
Major code restructuring

C. 2007
Extreme scalability
Proprietary interconnect
1000’s cores
Requires “end-to-end parallel”
Propagation of HPC to commercial CAE

Early adoption

- c. 1978, Cray-1, Vector processing Serial
- c. 1983, Cray X-MP, Convex
- c. 1988, Cray Y-MP, SGI

Common in Industry

- c. 2007, Extreme scalability
  Proprietary interconnect
  1000’s cores
  Requires “end-to-end parallel”
- c. 2013, Cray XE6
  driving apps: CFD, CEM, ???
- c. 2003, high density, fast interconnect
  Crash & CFD

- c. 1998, MPI Parallel
  “Linux cluster”,
  low density, slow interconnect
  ~100 MPI ranks
- c. 2013

- c. 1983, Cray X-MP, SMP
  2-4 cores
- c. 1988, Cray Y-MP, SGI
  Crash

- c. 2003, high density, fast interconnect
  Crash & CFD
- c. 1983, Cray X-MP, Convex
  MSC/NASTRAN
Do CAE algorithms scale?
WRF Results on Blue Waters (preliminary)

- WRF V3.3.1
- 1km, 1 billion cell, case 30 minute forecast, cold start
- WSM5 (mp_physics = 4) microphysics
- Results on XE6 96 cabinet system (2.3GHz IL16 sockets)

The system will scale to 10,000’s of cores

<table>
<thead>
<tr>
<th>Integer Cores</th>
<th>total nodes</th>
<th>average timestep (seconds)</th>
<th>sustained performance (GFLOPS/sec)</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>2048</td>
<td>64</td>
<td>3.995</td>
<td>2181</td>
<td>1.0</td>
</tr>
<tr>
<td>8192</td>
<td>256</td>
<td>1.065</td>
<td>8182</td>
<td>3.8</td>
</tr>
<tr>
<td>32768</td>
<td>1024</td>
<td>0.286</td>
<td>30480</td>
<td>15.6</td>
</tr>
<tr>
<td>131072</td>
<td>4096</td>
<td>0.142</td>
<td>61485</td>
<td>28.1</td>
</tr>
<tr>
<td>262144</td>
<td>8192</td>
<td>0.053</td>
<td>166332</td>
<td>75.4</td>
</tr>
</tbody>
</table>
Cavity Flow Studies using HECToR (Cray XE6)
S. Lawson, et.al. University of Liverpool

- 1.1 Billion grid point model
- Scaling to 24,000 cores
- Good agreement between experiments and CFD

Speed-up of the HMB flow solver using (a) 105 million point mesh with 24576 blocks and (b) 1100 million point mesh with 196608 blocks.

* Ref: [http://www.hector.ac.uk/casestudies/ucav.php](http://www.hector.ac.uk/casestudies/ucav.php)
CTH Shock Physics

CTH is a multi-material, large deformation, strong shock wave, solid mechanics code and is one of the most heavily used computational structural mechanics codes on DoD HPC platforms.

“For large models CTH will show linear scaling to over 10,000 cores. We have not seen a limit to the scalability of the CTH application”

“A single parametric study can easily consume all of the Jaguar resources”

CTH developer
Large Cray systems running ISV applications

- Several of the largest Cray systems are running CAE applications
  - CAE codes scaling to over 10,000 cores
- Both In-house and ISV applications
- Commercial companies are using Cray systems at the HPC centers
Are scalable systems applicable to commercial environments?
Two Cray Commercial Customers

- **GE Global Research**
  - Became aware of the capability of Cray systems through a grant at ORNL
  - Using Jaguar and their in-house code, modeled the “time-resolved unsteady flows in the moving blades”
    - Ref. Digital Manufacturing Report, June 2012

- **Major Oil Company**
  - Recently installed and accepted a Cray XE6 system
  - System used to scale key in-house code

*The common thread here is that both of these organizations had important codes that would not scale on their internal clusters*
Are ISV applications extremely scalable?

For many simulation areas...YES!
ANSYS Fluent scaling to >3000 cores on XE6
Aeroelastic Simulation, “Supercritical Wing”
In support of AIAA Aeroelastic Prediction Workshop

Fluent simulation, 13.7 million cells
CRAY XE6, AMD Interlagos 2.1GHz IL16, Cray MPI

![Graph showing scaling to >3000 cores on XE6](image)

Number of Cores

Rating for 100 iterations

Number of nodes
Performance testing of Fluent has shown scalability to over 3000 cores even with this modest size model.
Cray XE6: Extreme Scalability with EXA PowerFLOW

- Cray XE6: “Scaling to a larger number of cores than any other platform”
- Scaling to over 3000 cores
- 3X the total performance of any other systems

* ref: EXA press release Oct 2011
## STAR-CCM+ benchmark
100M cell automotive aerodynamics

<table>
<thead>
<tr>
<th>Cores/MPI Ranks</th>
<th>Cray XE6, “Interlagos“ 8 “core pairs”, 2.1 GHz Star-CCM+</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>72</td>
<td>24.0</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>4.5 nodes</td>
<td></td>
</tr>
<tr>
<td>144</td>
<td>12.1</td>
<td>2.0</td>
</tr>
<tr>
<td></td>
<td>9 nodes</td>
<td></td>
</tr>
<tr>
<td>288</td>
<td>6.0</td>
<td>4.0</td>
</tr>
<tr>
<td></td>
<td>18 nodes</td>
<td></td>
</tr>
<tr>
<td>576</td>
<td>3.3</td>
<td>7.3</td>
</tr>
<tr>
<td></td>
<td>36 nodes</td>
<td></td>
</tr>
<tr>
<td>1152</td>
<td>2.0</td>
<td>12.0</td>
</tr>
<tr>
<td></td>
<td>72 nodes</td>
<td></td>
</tr>
<tr>
<td>2304</td>
<td>1.1</td>
<td>21.2</td>
</tr>
<tr>
<td></td>
<td>144 nodes</td>
<td></td>
</tr>
</tbody>
</table>

Performance: Seconds per iteration

Number of Nodes used in that run
## LS-DYNA benchmark

Two car crash simulation, 2.4M elements
Hybrid parallel

<table>
<thead>
<tr>
<th>Total number of cores</th>
<th>Cray XE6 MC-12, 2.1 GHz Hybrid parallel</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>144</td>
<td>21,193</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>6 nodes</td>
<td></td>
</tr>
<tr>
<td>288</td>
<td>12,274</td>
<td>1.7</td>
</tr>
<tr>
<td></td>
<td>12 nodes</td>
<td></td>
</tr>
<tr>
<td>576</td>
<td>7,643</td>
<td>2.8</td>
</tr>
<tr>
<td></td>
<td>24 nodes</td>
<td></td>
</tr>
<tr>
<td>1152</td>
<td>5,258</td>
<td>4.0</td>
</tr>
<tr>
<td></td>
<td>48 nodes</td>
<td></td>
</tr>
</tbody>
</table>

Performance: Elapsed time (sec)

Number of Nodes used in that run
## Status of select ISV applications

<table>
<thead>
<tr>
<th>ISV Application</th>
<th>Primary segment</th>
<th>Demonstrated scalability *</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANSYS Fluent</td>
<td>Commercial CFD</td>
<td>&gt;4000 cores</td>
</tr>
<tr>
<td>LS-DYNA**</td>
<td>Impact/crash analysis</td>
<td>&gt;4000 cores</td>
</tr>
<tr>
<td>CFD++</td>
<td>Aero CFD</td>
<td>&gt;2000 cores</td>
</tr>
<tr>
<td>STAR-CCM+</td>
<td>Commercial CFD</td>
<td>&gt;3000 cores</td>
</tr>
<tr>
<td>PowerFLOW</td>
<td>External CFD</td>
<td>&gt;4000 cores</td>
</tr>
<tr>
<td>RADIOSS</td>
<td>Impact/Crash analysis</td>
<td>&gt;1000 cores</td>
</tr>
<tr>
<td>Abaqus</td>
<td>Structural analysis</td>
<td>&gt;64 cores</td>
</tr>
</tbody>
</table>

* Demonstrated scalability typically limited by the simulation model available

** Currently working on a 10M element crash simulation model which should scale much higher
If a model scales to 1000 cores will a similar size model also scale that high?

Not necessarily
Obstacles to extreme scalability using ISV CAE codes

1. Most CAE environments are configured for capacity computing
   - Difficult to schedule 1000’s of cores
   - Simulation size and complexity driven by available compute
   - This will change as compute environments evolve

2. Applications must deliver “end-to-end” scalability
   - “Amdahl’s Law” requires vast majority of the code to be parallel
   - This includes all of the features in a general purpose
   - This is an active area of development for CAE ISVs

3. Application license fees are an issue
   - Application cost can be 2-5 times the hardware costs
   - ISVs are encouraging scalable computing and are adjusting their licensing models
External Aerodynamics

118M cells
unsteady solution, 1350 time steps
moving mesh, rotating boundary condition (tires)

384 cores
350 Hours of elapsed time

Terabytes of data
Cray XE6 with Lustre file system
Pressure based, coupled solver
Compressible, LES

Scaling to 4096 cores with 91% efficiency

- Something happens at about 4500 cores but this will be addressed as the project to improve scaling progresses

- It is this type of cooperative work between application users, ISVs and Cray, that will lead to extreme scaling for the vast majority of simulations.
ANSYS presentation at 2012 Cray User Group (CUG)

ANSYS HPC Licensing options

Scalable licensing
- ANSYS HPC (per-process)
- ANSYS HPC Pack
  - Each simulation consumes one or more Packs
  - Parallel enabled increases quickly with added Packs
- ANSYS HPC Workgroup
  - 128 to 2048 parallel shared across any number of simulations on a single server
- ANSYS HPC Enterprise
  - Similar to HPC Workgroup but deploy and use anywhere in the world

Single solution for multiphysics and any level of fidelity
Summary: Well-balanced Scalable Supercomputer

- Compilers, Performance Tools and Libraries
- O/S Technology
- Packaging & ECOpHex Liquid Cooling
- Throughput: Scalable Storage Solution
- Gemini Interconnector
- State-of-the-art Processor

Scalable Supercomputer “Beyond Commodity” areas
Summary: Well-balanced Scalable Applications Infrastructure

- Scalable analysis tools: e.g. visualization
- Large models
- End-to-end simulation scalability
- Scalable Compute Power
- Clear ROI for scalability: e.g. application costs

Extreme scalability for CAE simulation
Backup Slides
A Comparison of the Performance Characteristics of Capability and Capacity Class HPC Systems
By Douglas Doerfler, Mahesh Rajan, Marcus Epperson, Courtenay Vaughan, Kevin Pedretti, Richard Barrett, Brian Barrett, Sandia National Laboratories