Industrial Computational Breakthroughs on Blue Waters

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Think Big!

Supercomputing in Engineering? A view from 2003

“It is amazing what one can do these days on a dual-core laptop computer. Nevertheless, the appetite for more speed and memory, if anything is increasing. There always seems to be some calculations that ones wants to do that exceeds available resources. It makes one think that computers have and will always come in one size and one speed: “Too small and too slow”. This will be the case despite supercomputers becoming the size of football fields!”

Prof. Tom Hughes, 2003, President of International Association for Computing Mechanics-IACM
High fidelity virtual engine simulation and design

- > 1 trillion degrees of freedom (DOF)
- > 1 billion core hours per calculation
Direct Numerical Simulation of the Multiphase Flow in Nuclear Reactor Core (year 2060 ?)
Prof. Igor Bolotnov, NCSU, HPC-User Forum 9/2014

• About 160 fuel Assemblies (17x17 each, 4m long)
• Reynolds Number of 5,000 (typical reactor condition)
• Mesh Size 40,000T elements
• Should run up to 320B cores at 128K elements/core
• Would resolve 13.6B bubbles at average 1% void fraction
• Remember: Number of Grid Points ~ Re^{9/4}
Private Sector Program at NCSA

Solve industry’s most demanding HPC challenges

Aerospace, agriculture, consumer goods, energy, life sciences, health care, and technology sectors

Largest HPC industry engagement program in the World
Industrial Application Breakthroughs on Blue Waters!

15,000+ cores  **LS-DYNA** (Cray, LSTC, Rolls Royce, P&G, NCSA)

100,000+ cores  **Star-CCM+** (CD-Adapco, Cray, NCSA)

36,000+ cores  **Ansys-Fluent** (Ansys Inc., Cray, Dell, NCSA)

65,000+ cores  **WSMP** (IBM-Watson, NCSA, BSC)

512 XK7 nodes  **ACCEL_WSMP** (Nvidia, IBM-Watson, NCSA)

100,000+ cores  **Alya** (BSC and NCSA)

**Abaqus over CLE and Gemini** (Simulia DS, Cray, NCSA, NDA)
Explicit FEA LS-DYNA

NCSA Private Sector Program, Procter & Gamble, LSTC, and Cray

Real geometry, loads, boundary conditions, highly non-linear transient dynamic problem with difficult (eroding) contact conditions

MPP and Hybrid DYNA solvers ported and optimized for Cray Linux and “Gemini” interconnect
LS-DYNA Scalability

From 400 days with serial execution to 4.3 hours on 15,000 cores!

Hybrid LS-DYNA Parallel Scalability on NCSA's Blue Waters
P&G Case, 72M nodes, Wallclock Time (Seconds); Lower = Better

Highest known scaling of any ISV FEA code!!
ISV CFD Scaling Breakthrough

Dr. Ahmed A. Taha, NCSA

National Center for Supercomputing Applications (NCSA)
Star Extreme Benchmarking V.10.02.010
Blue Waters (Cray CLE6)
"LeMans_1.002M" Case, Steady State, COUPLED Solver, May 2015

Graph showing speedup rating vs. cores for different efficiencies and a specific case scenario.
Alya-Power of Multiphysics on the Extreme HPC Scale

Designed by the Barcelona Supercomputer Center as a multiphysics parallel FEA code

Unstructured spatial discretization, explicit and implicit integration in time

Staggered schemes (with iterations) for coupled physics on a single mesh

Mesh partitioning and hybrid parallel implementation

Uses built-in iterative CG solver with various preconditioning techniques

Highly modular, with each module representing a different physics; easy to combine them at job launch

Ported to Blue Waters in 2014

Top Supercomputing Achievement  Hpcwire Readers Choice at SC 2014 !
2 Real-World Cases Solved with Alya on Blue Waters

**Human Heart**
- Non-linear solid mechanics
- Coupled with electrical propagation
- 3.4 billion elements, scaled to 100,000 cores

**Kiln Furnace**
- Transient incompressible turbulent flow
- Coupled with energy and combustion
- 4.22 billion elements, scaled to 100,000 cores
Alya – Kiln Furnace

BSC “Alya” on NCSA Blue Waters; 4.22 Billion Elements
Transient incompressible turbulent flow coupled with energy and combustion

Alya achieves nearly 90% scaling efficiency at 100,000 cores!!
17.4 years with serial execution to 1.8 hours on 100,000 cores!
Massively Parallel Linear Solvers in Implicit Codes

• Implicit code spends 70-80% of time solving large systems of linear equations, \( Ax=b \), where \( A \) is sparse i.e., most coefficients are zero

• A wide range of applications: finite element solid mechanics, computational fluid dynamics, geo-physics, circuit design, linear programming etc.

• Used for nonlinear problems in every NR iteration

\[
\begin{align*}
\mathbf{K}_{i-1}^{t+\Delta t} & \quad \{\Delta U_{i-1}\} = \{P_{i-1}^{t+\Delta t}\} - \{S_{i-1}^{t+\Delta t}\} \\
\{U_i^{t+\Delta t}\} & = \{U_{i-1}^{t+\Delta t}\} + \{\Delta U_{i-1}\}
\end{align*}
\]
Sparse Direct Multifrontal Algorithm in Watson Sparse Matrix Package - WSMP

• Highly robust but memory expensive, often the only choice for ill-conditioned problems, but often more efficient than iterative solver for less ill-conditioned problems

• LU Decomposition introduces new non-zeros “fill-ins”

• Reordering of columns and rows is used to minimize “fill-ins”

• Collections of columns with similar non-zero pattern- Supernodes are detected during symbolic factorization

• Operations on Supernodes provide opportunity for dense matrix math operations with BLAS operations

• Hybrid Implementation (MPI and p-threads)
# FEA Test Problems

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WSMP Factorization Speedup and Performance with FEA Tests

![Graph 1: Factorization Speedup](image1)

- M40
- M20
- M11
- Ideal

![Graph 2: Factorization Performance](image2)

- M40
- M20
- M11

Number of Threads:
- 64
- 128
- 256
- 512
- 1024
- 2048
- 4096
- 8192
- 16384
- 32768
- 65536
Direct Sparse Solvers in Geophysical Applications

- A single failed drilling effort can cost the oil/gas company many millions of dollars!
- The goal of the inversion is to recover the conductivity given measurements of the electric and/or magnetic fields and characterize the geological structure.
- The modeling and inversion of the three-dimensional EM data in the frequency domain requires considering many sources and frequencies.
- The computational cost is enormous and the use of HPC mandatory.
- The inversion code spent 80-90% time solving thousands of large often ill-conditioned Ax=b.
- Direct sparse solver methods are efficient for multisource problems with multiple RHS.
Factorization Speedup and Performance and with Geophysical Tests
GPU Accelerated WSMP - ACCEL_WSMP
Minimally invasive approach
Nvidia, IBM-Watson and NCSA

• Intercepting BLAS level 3 calls with large dimensions perform tiling and send them to GPU

• Use host pinned buffers to increase copy-up/copy-down speed and enable asynchronous memory copies

• Send small BLAS calls to the CPU

• Can be used with ANY application, not just WSMP
The GPU acceleration can beneficially scale to more than 512 nodes of Blue Waters (relevant scale for majority of GPU clusters in production)

Wider scale acceleration on GPUs is hampered by work imbalance due to larger block size on GPU and limited PCIe communication between the GPU and CPU

Working on improvements: block size adjustments to improve work balance, hiding MPI + PCIe latencies, applying GPU-aware MPI, etc.
• The NCSA Private Sector Program’s core mission is to help its partner community gain a competitive edge through expert use of cutting edge, high-performance digital and human resources.

• Blue Waters can tackle a very wide range of challenging tasks from industry demonstrating the feasibility of efficiently solving large size real world multi-physics or geophysics problems with high fidelity both with commercial and in-house codes.

• This is increasingly important work for the US industry and economy, since the scale of computing used in the cutting edge HPC systems, such as Blue Waters, is approximately 5 years ahead of that used by the leading industrial adopter.

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