Industrial Computational Breakthroughs on Blue Waters

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Think Big !

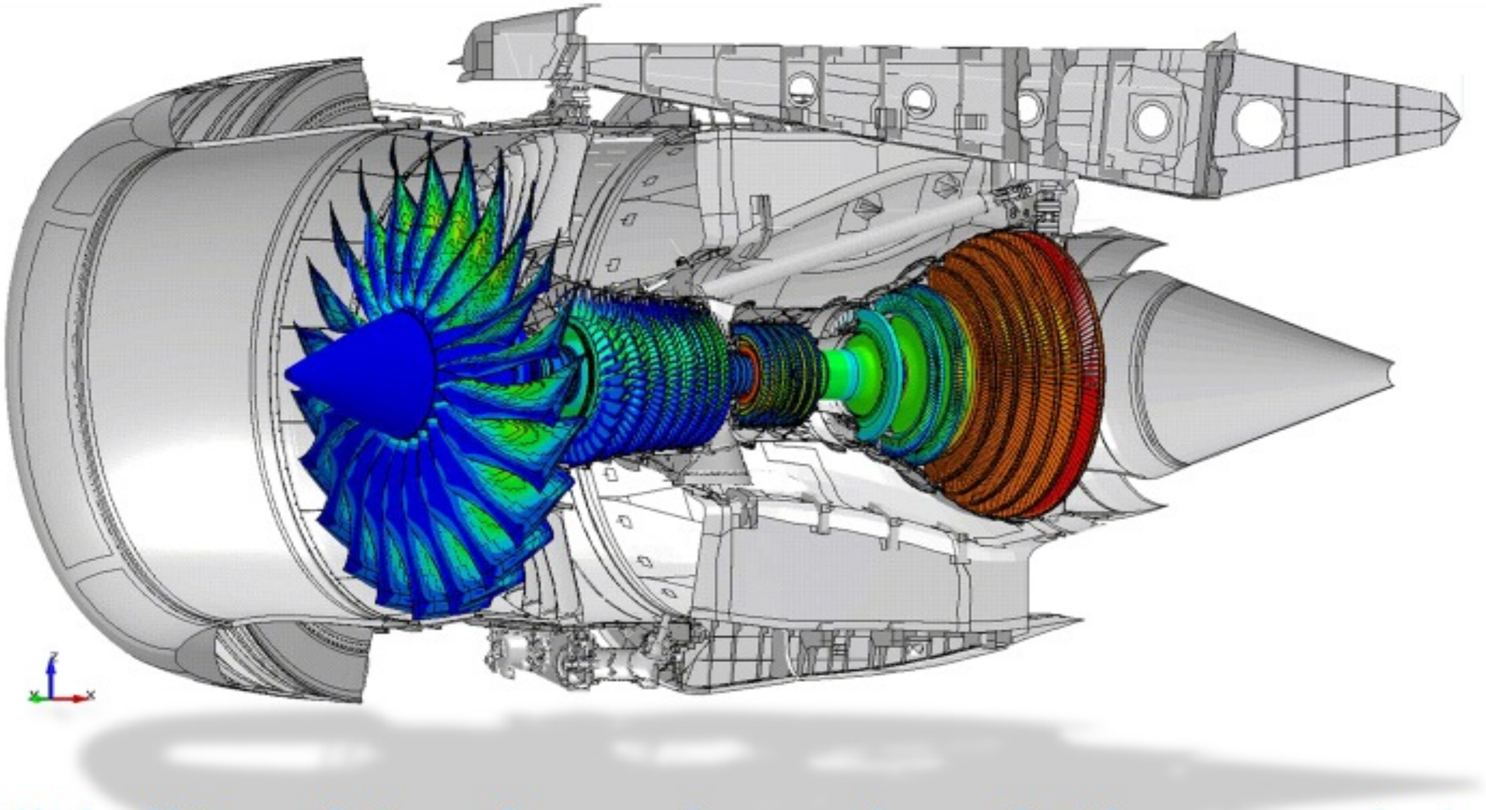
Supercomputing in Engineering ?
A view from 2003

“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

A vision from our Industrial Partner

Dr. Yoon Ho, Rolls Royce, ISC14

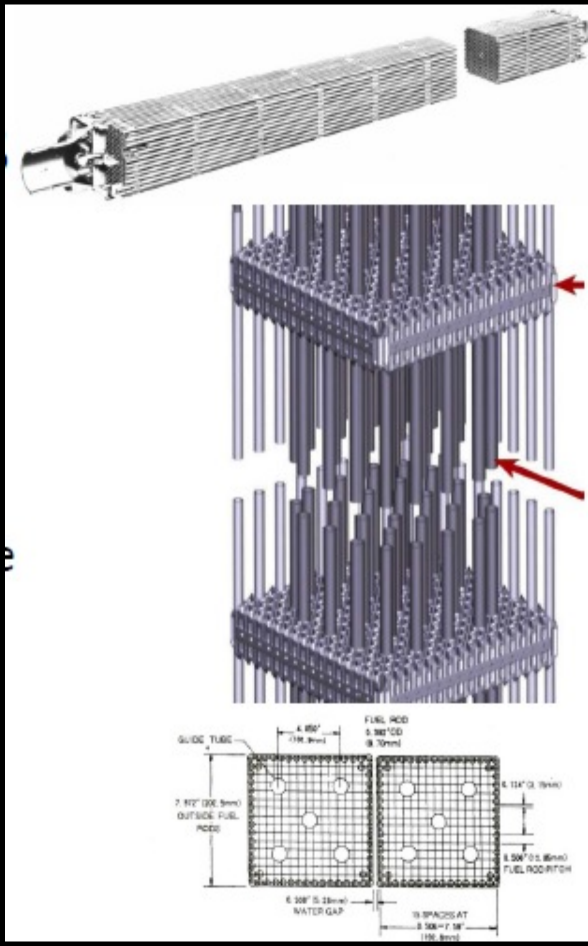


High fidelity virtual engine simulation and design

- > 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

Manufacturing

Rolls-Royce
Dow
CAT
P&G
GE
John Deere

Energy

ExxonMobil Upstream Research
bp
bhpbilliton

Technology

DataDirect Networks
HDF
CRAY
intel
allinea
Charmworks
Adaptive Computing
DELL
QuesTek Innovations LLC
Illinois Rocstar

Life Sciences

Mayo Clinic
Agrible
syngenta

Institutes

Prairie Research Institute
ARI Illinois Applied Research Institute
The Dark Energy Survey
Milwaukee Institute

University of Illinois NCSA Private Sector Program Partners, May 2015

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)

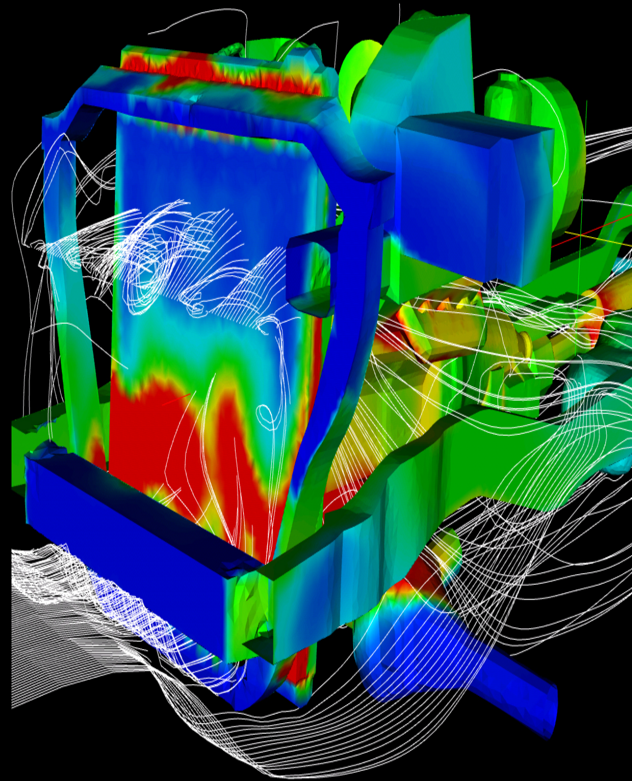
36,000+cores **Ansys-Fluent** (Ansys Inc., Cray, Dell, NCSA)

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

NCSA

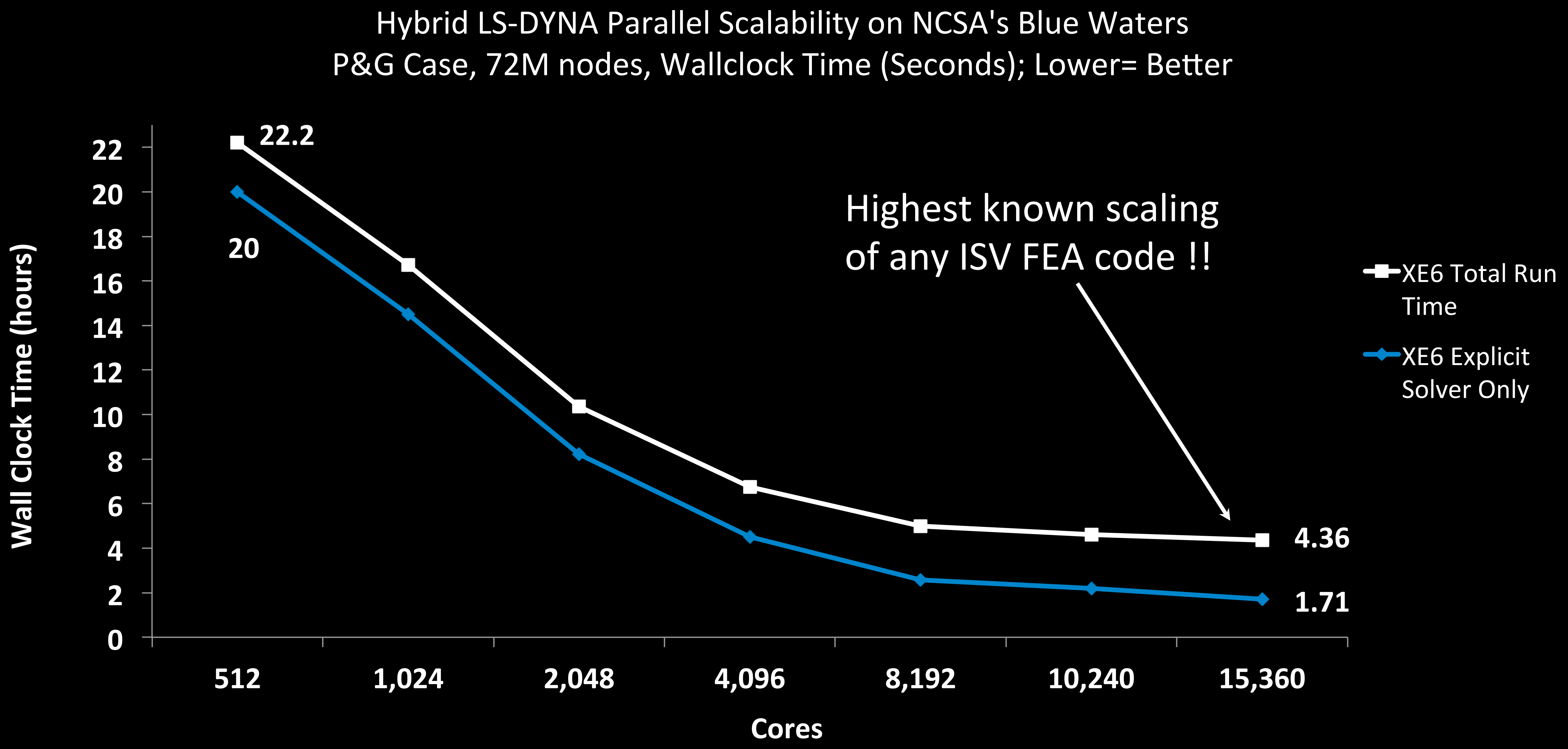
P&G

Livermore Software Technology Corporation

CRAY

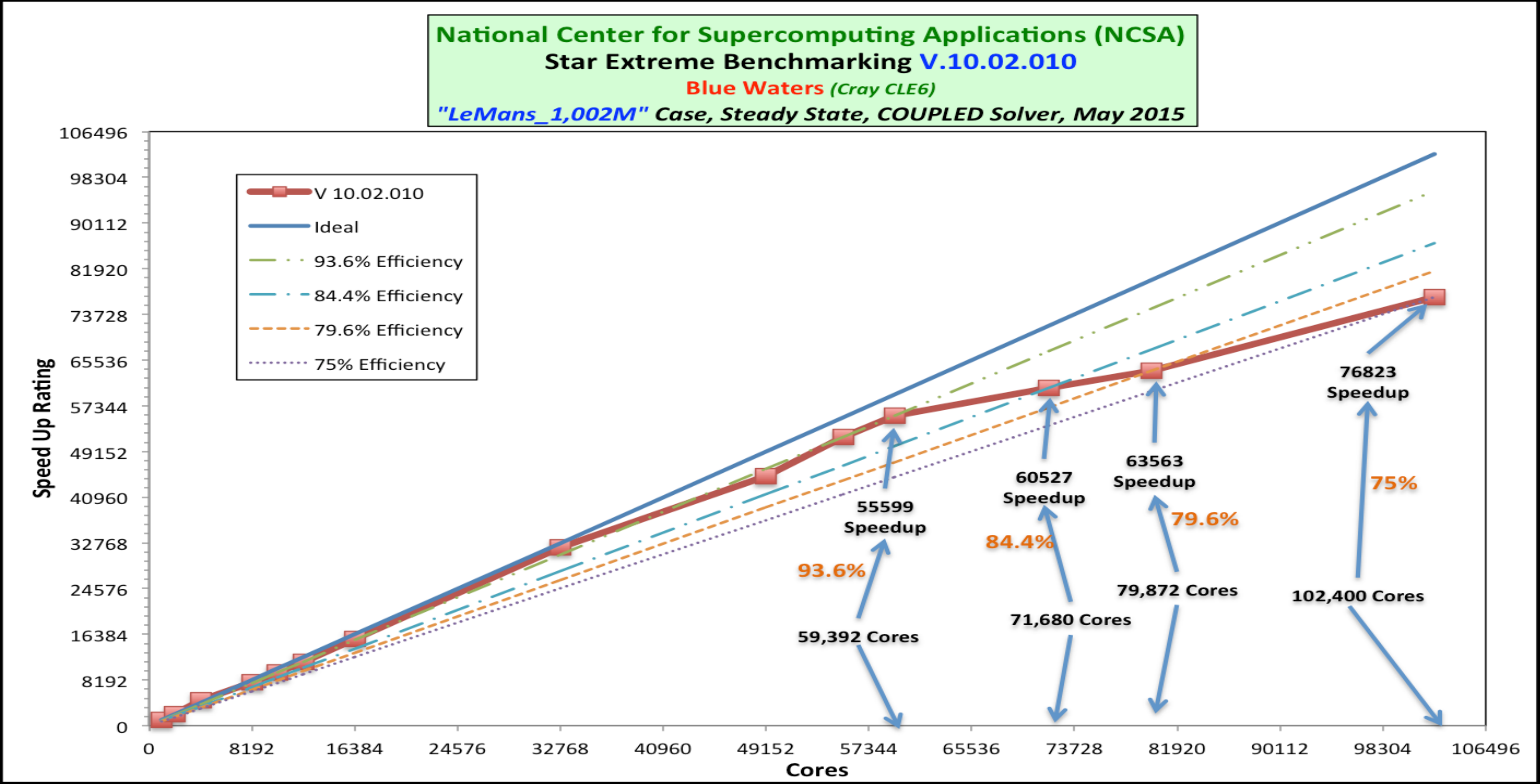
LS-DYNA Scalability

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



ISV CFD Scaling Breakthrough

Dr. Ahmed A. Taha, NCSA



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

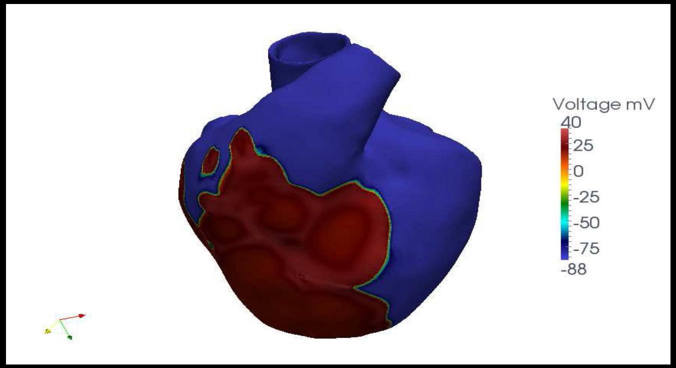
Ported to Blue Waters in 2014

Top Supercomputing Achievement Hpcwire Readers Choice at SC 2014 !

2 Real-World Cases Solved with Alya on Blue Waters

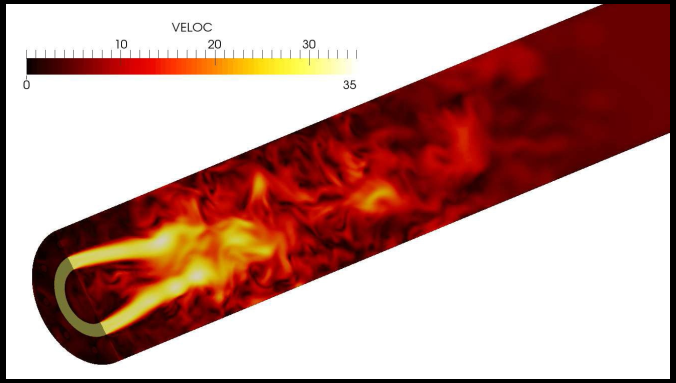
Human Heart

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



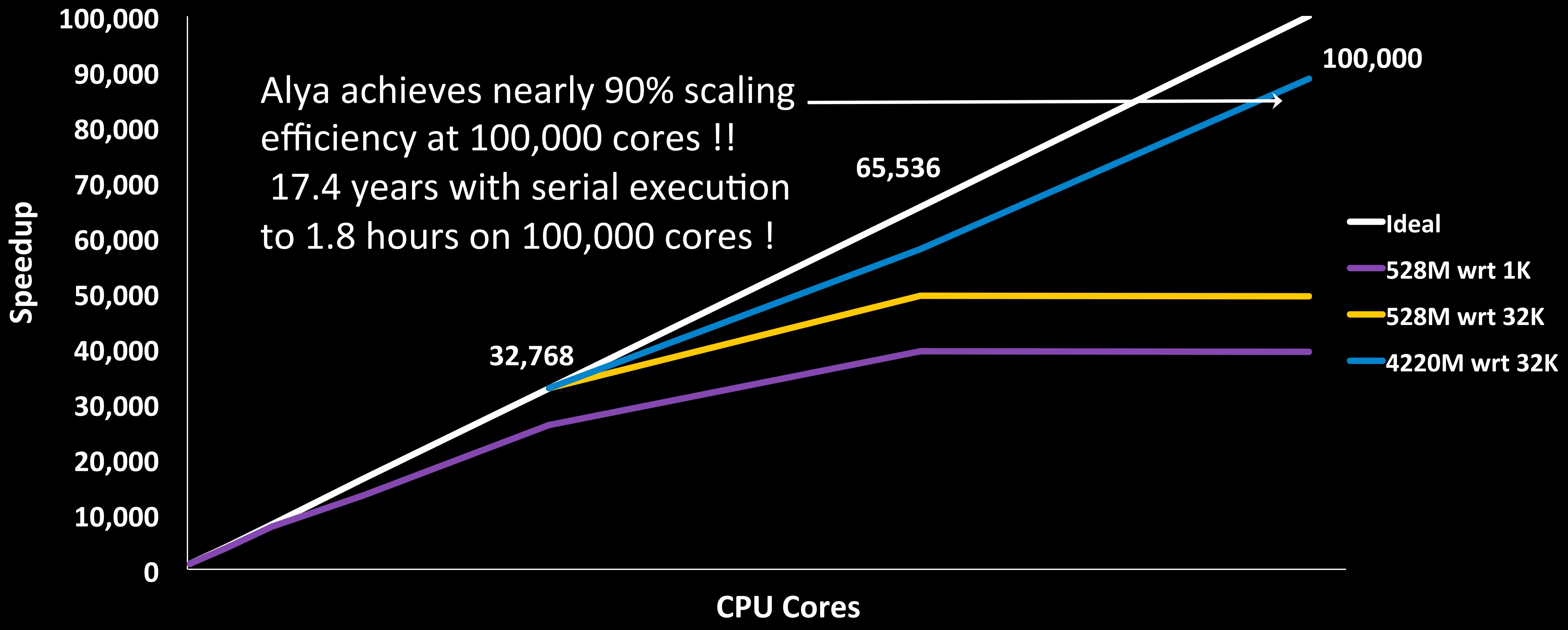
Kiln Furnace

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



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

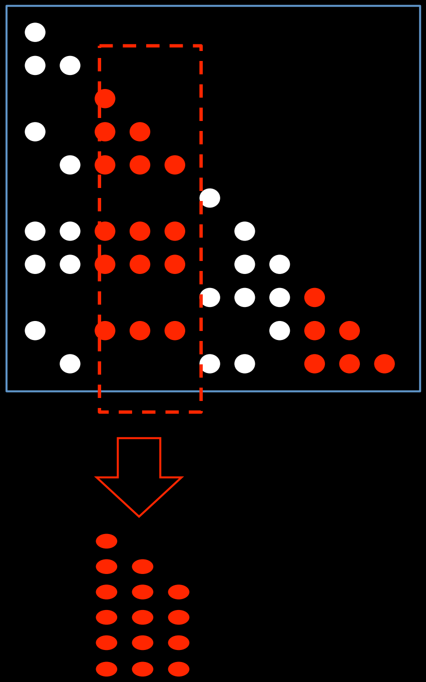
- A wide range of applications: finite element solid mechanics, computational fluid dynamics, geo-physics, circuit design, linear programming etc.

- Used for nonlinear problems in every NR iteration

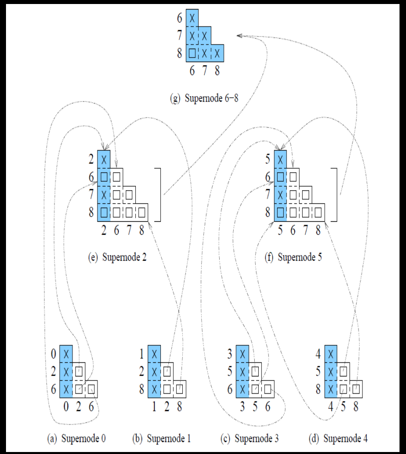
$$\left[K_{i-1}^{t+\Delta t}\right]\left\{\Delta U_{i-1}\right\} = \left\{P^{t+\Delta t}\right\} - \left\{S_{i-1}^{t+\Delta t}\right\}$$

$$\left\{U_{i}^{t+\Delta t}\right\} = \left\{U_{i-1}^{t+\Delta t}\right\} + \left\{\Delta U_{i-1}\right\}$$

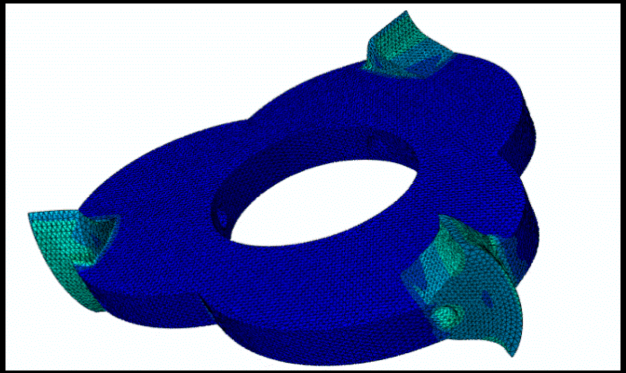
Sparse Direct Multifrontal Algorithm in Watson Sparse Matrix Package -WSMP

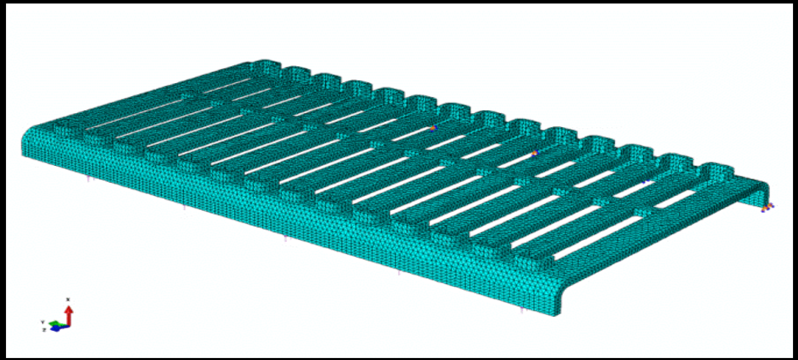


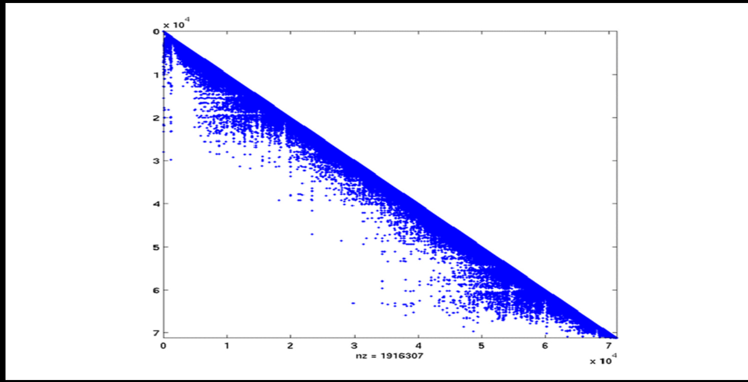
- Highly robust but memory expensive, often the only choice for ill-conditioned problems, but often more efficient then iterative solver for less ill-conditioned problems
- LU Decomposition introduces new non-zeros “fill-ins”
- Reordering of columns and rows is used to minimize “fill-ins”
- Collections 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

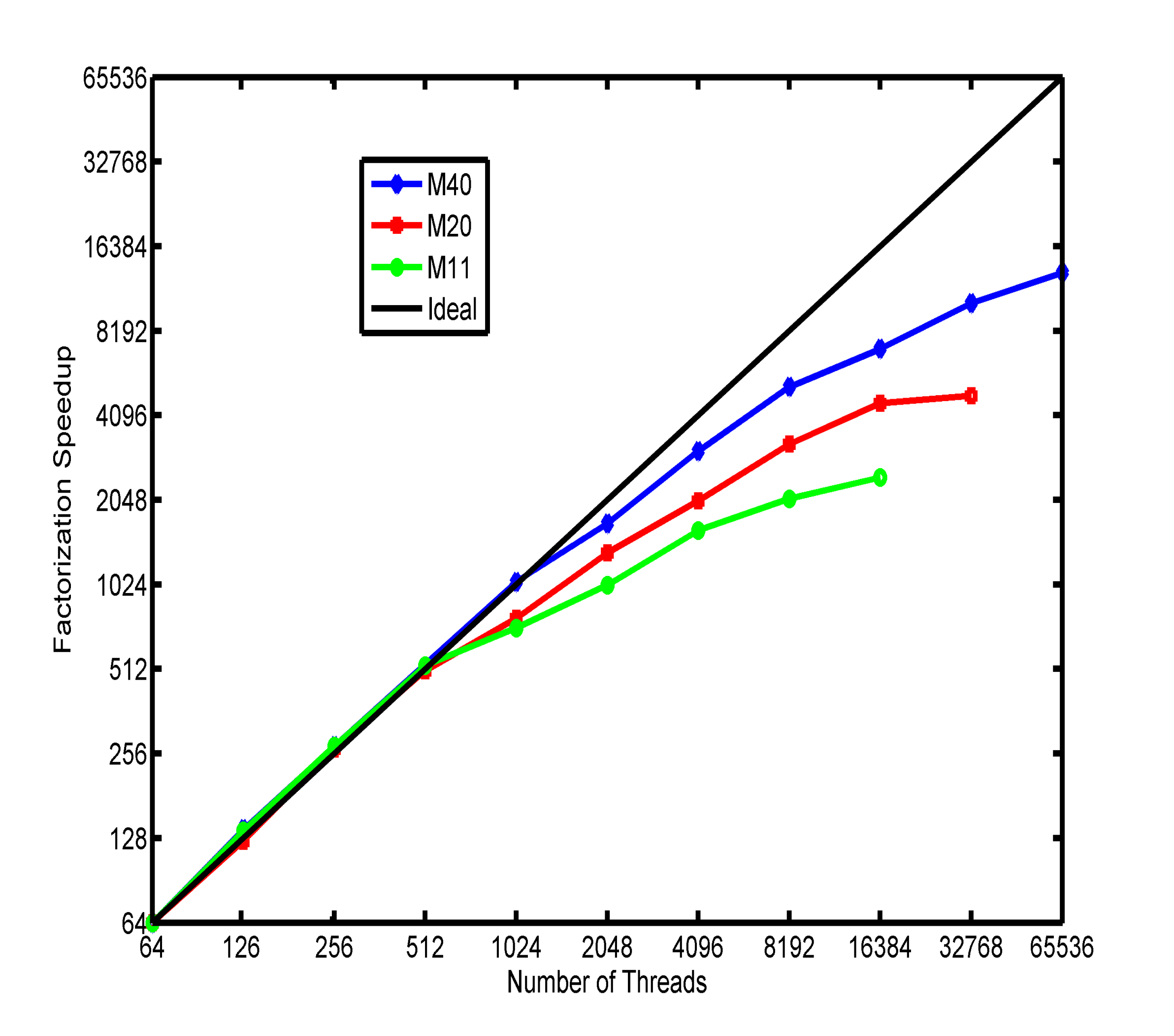


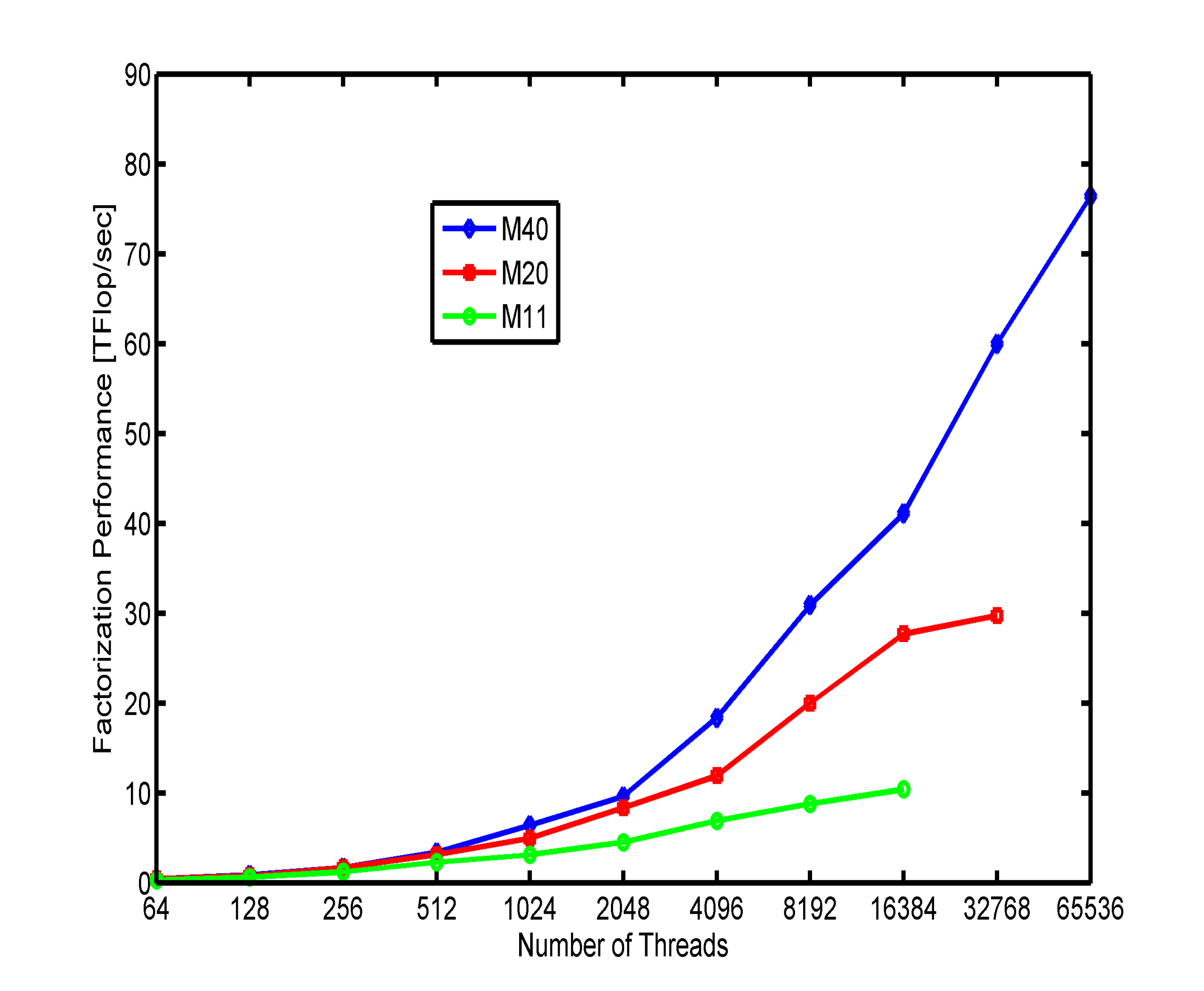




	MODEL	N	NNZ	COND
M2	rrc	2246022	175360626	5.9E+06
M11	ndemc-cac	11562627	937454416	6.8E+09
M20	rrc	20056050	1634926088	2.7E+07
M40	rrc	39979380	3290344248	5.8E+07

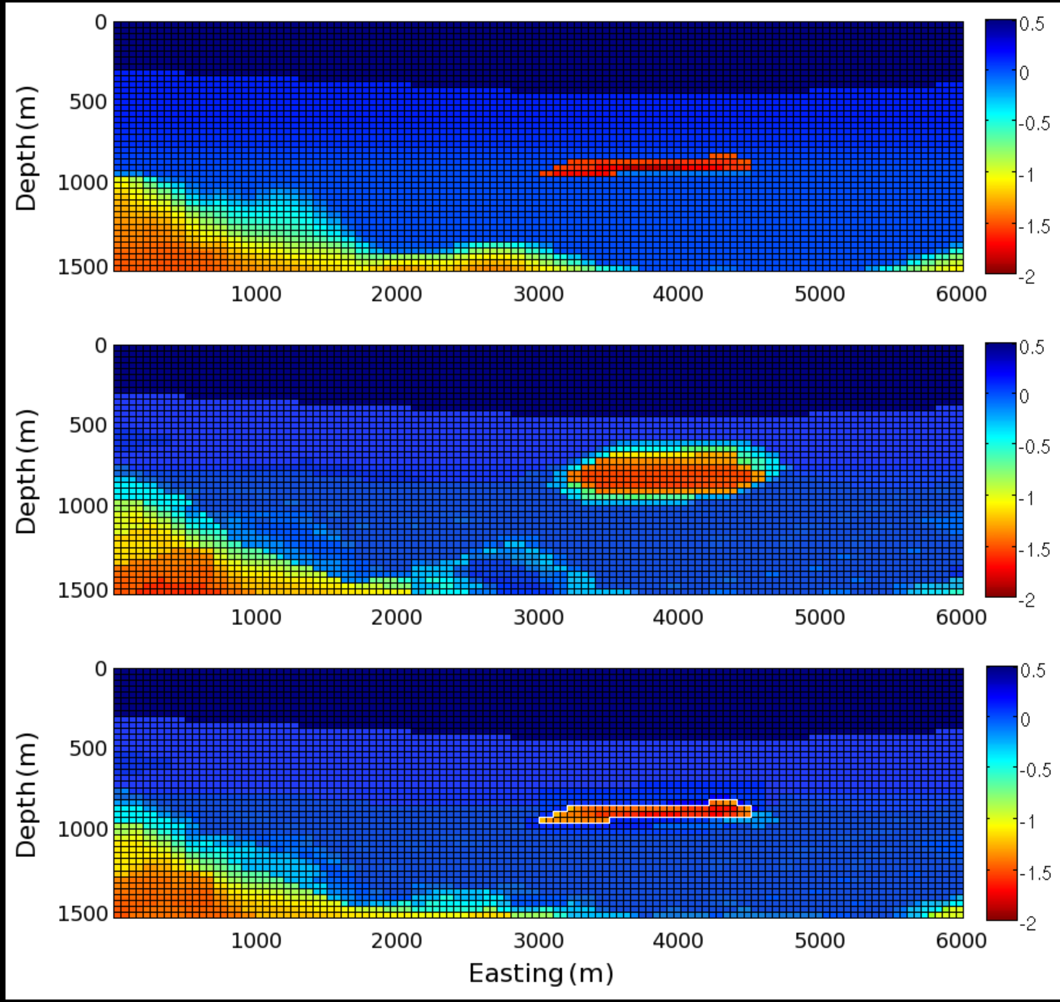
WSMP Factorization Speedup and Performance with FEA Tests



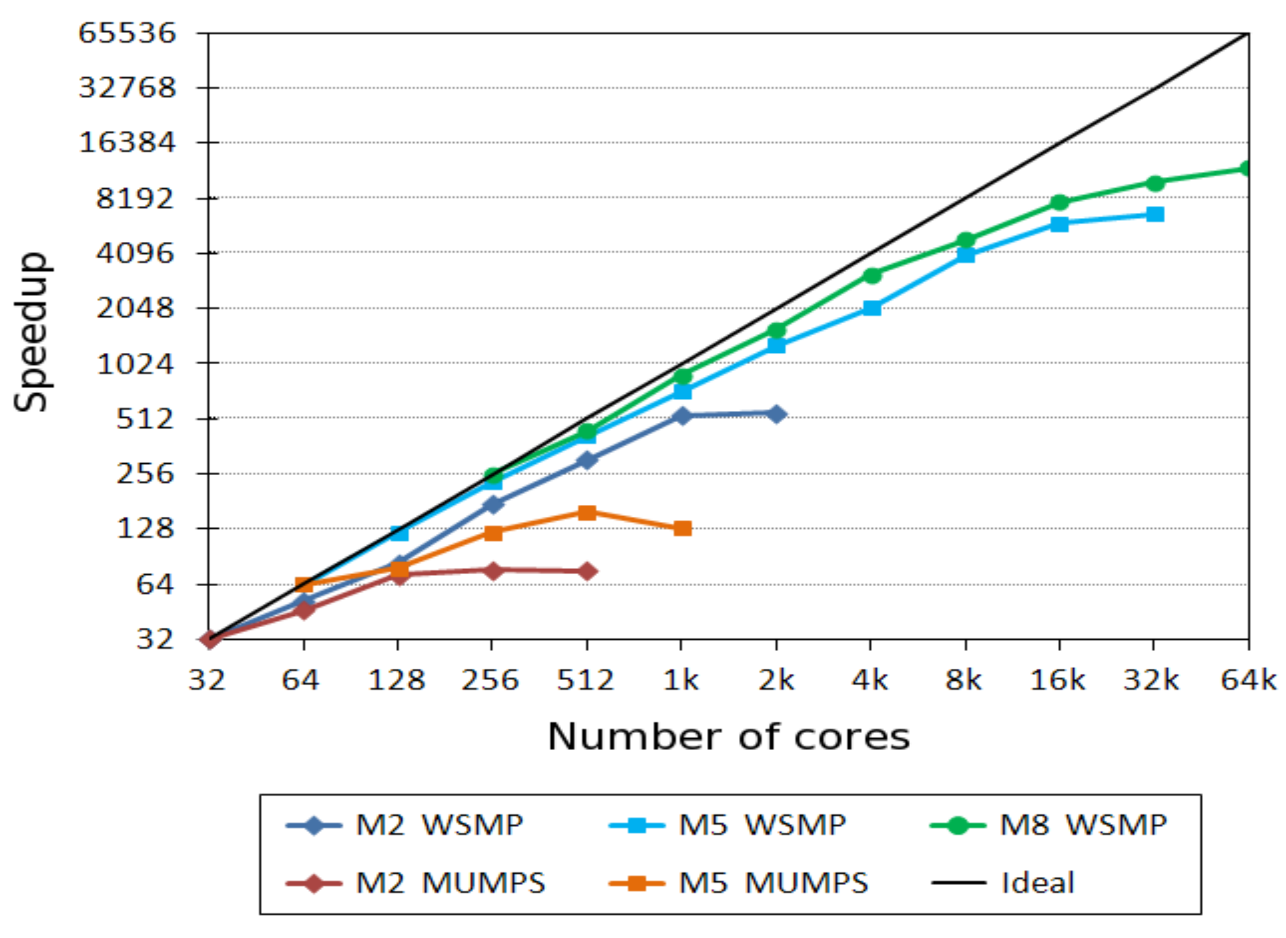


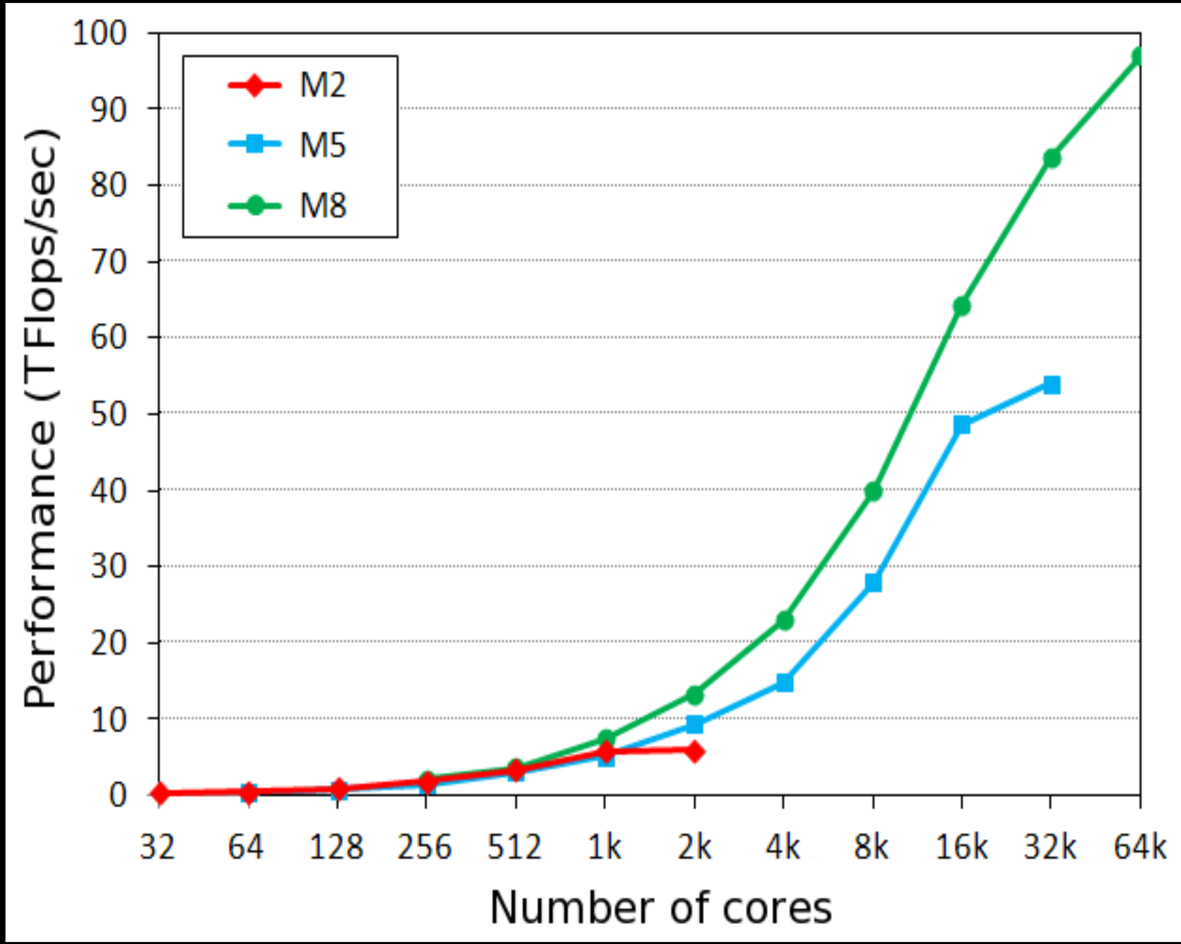
Direct Sparse Solvers in Geophysical Applications

- 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



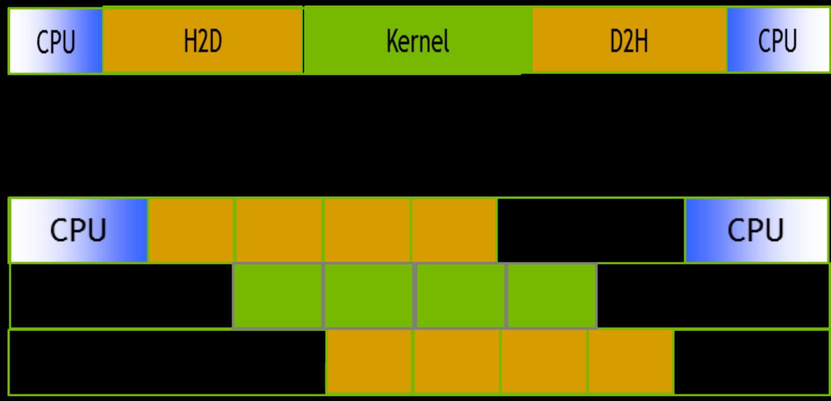
Factorization Speedup and Performance and with Geophysical Tests





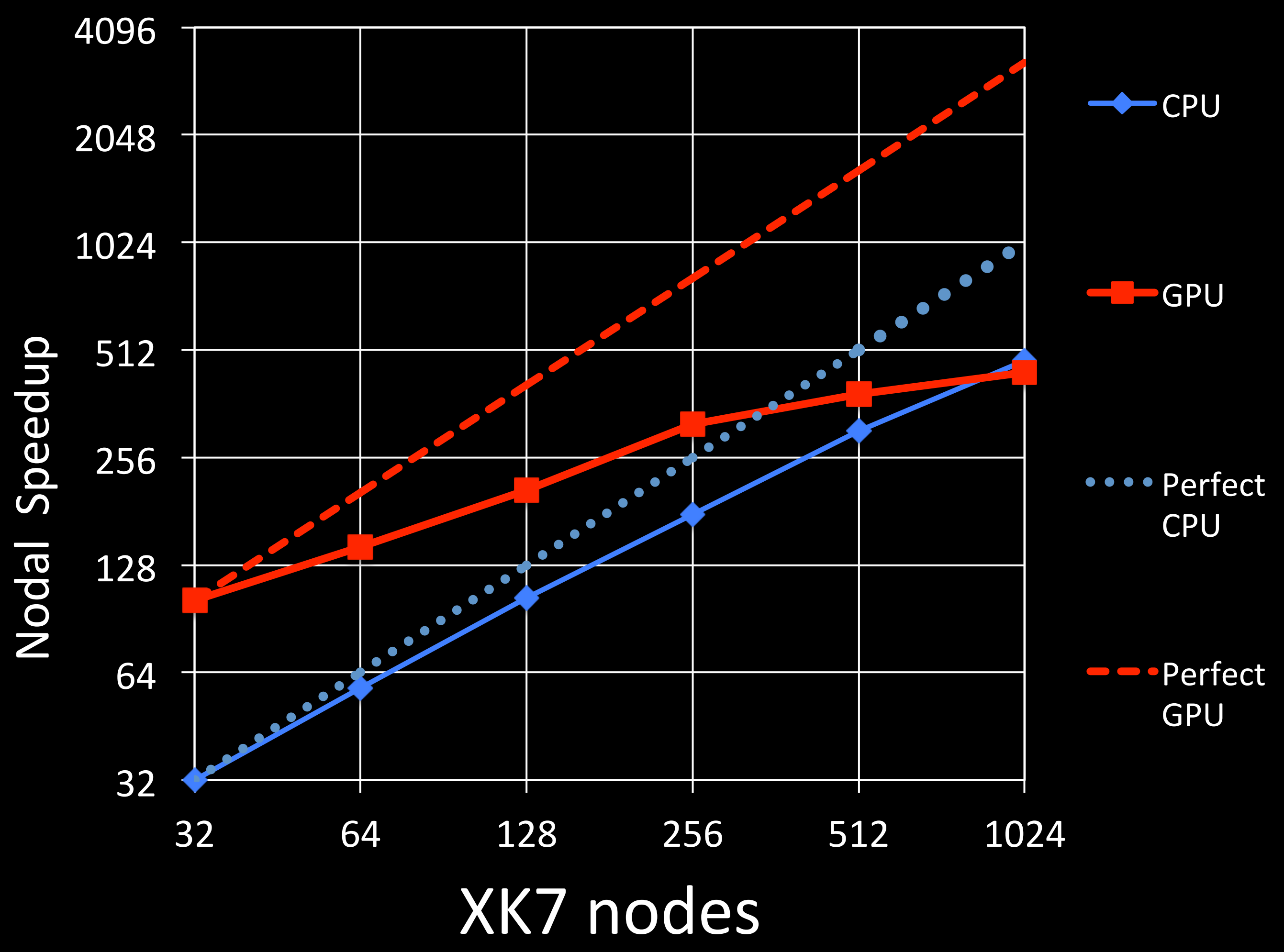
GPU Accelerated WSMP -ACCEL_WSMP
Minimally invasive approach
Nvidia, IBM-Watson and NCSA

- 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



Speedup of GPU Accelerated 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

Special THANKS goes to NSF, The Blue Waters Project Team, Cray, Rolls Royce, Procter and Gamble, Caterpillar, Ansys Inc., LSTC, IBM-Watson, Nvidia, Barcelona Supercomputing Center and other partners (NDA)

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