Why Exascale Computing will be slightly less disruptive than the comet that killed the dinosaurs

Numerical Methods for Large-Scale Nonlinear Problems and Their Applications

ICERM, Providence, RI

Jeffrey A. F. Hittinger
Center for Applied Scientific Computing

August 4, 2015
What are things one can find in museums...
Our exascale “comet” approaches...

National Strategic Computing Initiative
Executive Order 13702 (July 29, 2015)

Create systems that can apply exaflops of computing power to exabytes of data
We lack the computing power to tackle Grand Challenge Science problems

Combustion
- High-pressure, turbulent reacting flow
- Complex moving geometry
- Multiphase: fuel injection and soot
- Stochasticity
- Optimal engine design

Climate
- Coupling atmosphere, oceans, ice sheets, land mass, biosphere
- Global to microscopic
- Catastrophic rare events
- Extreme weather patterns
- Assessments for policy

Materials
- Transient mesoscale behavior of new materials
- Search for novel, optimal materials
- Model from nanometers to microns, femtoseconds to minutes

Need (at least) exascale computing resources
## What is an exascale-class machine?

<table>
<thead>
<tr>
<th></th>
<th>ASCI Red</th>
<th>Road Runner</th>
<th>K Computer</th>
<th>Sequoia</th>
<th>Exascale</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Year</strong></td>
<td>2000</td>
<td>2008</td>
<td>2011</td>
<td>2012</td>
<td>2023</td>
</tr>
<tr>
<td><strong>Peak (Flops)</strong></td>
<td>1.3e12</td>
<td>1.7e15</td>
<td>11.3e15</td>
<td>20.1e15</td>
<td>1.2e18</td>
</tr>
<tr>
<td><strong>Linpack (Flops)</strong></td>
<td>1.0e12</td>
<td>1.0e15</td>
<td>10.5e15</td>
<td>16.3e15</td>
<td>1.0e18</td>
</tr>
<tr>
<td><strong>Total Cores</strong></td>
<td>9,298</td>
<td>130,464</td>
<td>705,024</td>
<td>1,572,864</td>
<td>1e9</td>
</tr>
<tr>
<td><strong>Processors</strong></td>
<td>9,298</td>
<td>12,960(6,912)</td>
<td>88,128</td>
<td>98,304</td>
<td>1e6</td>
</tr>
<tr>
<td><strong>Cores/Proc</strong></td>
<td>1</td>
<td>9(2)</td>
<td>8</td>
<td>16</td>
<td>1e3</td>
</tr>
<tr>
<td><strong>Power (MW)</strong></td>
<td>0.85</td>
<td>2.35</td>
<td>9.89</td>
<td>7.9</td>
<td>~20</td>
</tr>
</tbody>
</table>

Adapted from B. Harrod, “DOE Exascale Computing Initiative Update,” Aug 15, 2012
Power has become the dominant constraint

Based on current technology, scaling today’s systems to an exaflop level would consume more than a gigawatt of power, roughly the output of Hoover Dam

Power is also driving architecture changes

- Power densities limit clock speeds
- More cores and specialized accelerators
- Data motion costs on-chip and off-chip
- Volatile memory (DRAM) is power-hungry

Original data collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond and C. Batten.
Future Node Architectures will have many cores and deep memory hierarchies

Memory Stacks on Package
Low Capacity, High Bandwidth

Lightweight Cores
(tiny, simple, massively parallel)
Throughput-Optimized

Integrated NIC

Bulk Cores
Latency Optimized

NVRAM: Burst Buffers / rack-local storage

Based on slide from J. Shalf
Exascale computing introduces several fundamental challenges

**Extreme Concurrency**
- Processing units $\uparrow$
- Bulk-synchronous will not scale
- Concurrency $\uparrow$
- Synchronization $\downarrow$
- Communication $\downarrow$
- Dynamic task parallelism

**Limited Memory**
- Memory gains less than processing
- Memory/core $\downarrow$
- Minimize memory usage
- Deeper, heterogeneous memory hierarchies

**Data Locality**
- Transfer gains less than processing
- Bandwidth/core $\downarrow$
- Energy and time penalties for data motion
- Greater need for data locality
- Reduce data transfers

**Resilience**
- Massive number of components: hard faults $\uparrow$
- Running closer to threshold voltage: soft faults $\uparrow$
- Bulk-synchronous checkpoint restart is dead
Hardware improvements are not enough

\[ O(N^p) \]

**Machine improvements tend to improve base or coefficient**

**Model and algorithm improvements can improve exponent**
Will Algorithms for Exascale be...

OR

Evolutionary

Mick Tsikas, Reuters

Revolutionary?
DOE ASCR chartered an Exascale Applied Mathematics Working Group

Identify:
- gaps in thinking about exascale
- new algorithmic approaches
- new scientific questions
- a more holistic approach

Team
- Jack Dongarra*
- John Bell
- Luis Chacon
- Rob Falgout
- Mike Heroux
- Jeff Hittinger*
- Paul Hovland
- Esmond Ng
- Clayton Webster
- Stefan Wild

*co-chairs

Process
- Community Workshop (Aug 2013)
- Fact-finding teleconferences
- Grand Challenge reports
An organizing principle we used was the concept of the *Mathematics Stack*

Areas outside of this conceptual organization:
- Optimization and optimal control for system management
- Discrete mathematics and graph analysis
- Finite state machines and discrete event simulation
Mathematical Modeling: Uncertainty quantification plays a larger role at exascale

We must be clever in combating the curse of dimensionality

- Adaptive hierarchical methods
- Advanced multilevel methods
  - Model hierarchies
  - Stochastic hierarchies
- Architecture-aware UQ
- Adaptive and robust methods for fusing computation and experimental data

Performance Increase 3D FEM Nonlinear Diffusion
Phipps, Edwards, Hu, Webster, Equinox project, ASCR XUQ

Blue Gene/Q
1 MPI Rank/Node, 64 Threads/Rank
(~ 64x64x64 Mesh/Node)

- PCG Solve
  - Ensemble = 16
  - Ensemble = 32
- AMG Setup
  - Ensemble = 16
  - Ensemble = 32

Ensemble Speed-Up

Nodes

1 2 4 8 16 32 64 128
1.0 1.5 2.0 2.5 3.0 3.5 4.0 4.5
Mathematical Modeling: Exascale will enable the solution of new optimization problems

- Concurrent-point methods
- Mixed-integer, simulation-based, and global optimization
- Multi-fidelity hierarchies
- Robust optimization and optimization under UQ
- Optimal design and coupling of experiments

Branch and Bound Tree for MIPDECO

- MIPDECOs generate huge search trees
- Each node is PDE-constrained optimization

[Branch and Bound Tree for MIPDECO diagram]

[Branch and Bound Tree for MIPDECO diagram] [Leyffer & Mahajan]
Mathematical Modeling: In forward simulation, we must consider new models

- Can we model additional physics?
- How else can we model the problem?
- Do some models expose more concurrency?
- Scale-bridging models
  - Hierarchical representations
  - Coarse-graining
- Particle vs. continuum

*We must respect the physics!*
Discretization: High-order, partitioning, and adaptivity will play important roles

- **High-order discretizations**
  - High arithmetic intensity
  - Maximize on-node performance
  - Robustness? BCs?

- **Partitioned algorithms**
  - Models, equations, and operators
  - Spatial (FSI)
  - Temporal (multimethod)

- **Need better coupling strategies**
  - High-order
  - Splittings based on strength of coupling
  - Compatible interface treatments
  - Nonlinearly converged strategies

- **Adaptivity in mesh, model, discretization and order**

- **Scalable computational geometry and mesh generation**

![Diagram](image)
Parallel-in-time
- More concurrency, not faster clock speeds
- Hierarchy of representations of varying fidelity
- Iterative time advancement
- Compressible Navier-Stokes:
  - Vortex shedding problem
  - 8x speedup at 4K cores
  - Crossover at 80 cores

Research issues:
- Optimal convergence
- Chaotic systems
- Oscillatory systems
- Hyperbolic systems

J. Schroder et al., XBRAID project
Scalable Solvers: In solving the discrete system, numerous topics must be addressed

- Communication-avoiding
- Synchronization reduction
- Data compression
- Mixed-precision
- Randomization and sampling
- Adaptive load balancing
- Scheduling and memory management
- Autotuning algorithms
- Energy-efficient algorithms

Example: Timings on $100^3$ 7-point Laplacian stencil [E. Chow and A. Patel]

$$l_{ij} = u_{jj}^{-1} a_{ij} - u_{jj}^{-1} \sum_{k=1}^{j-1} l_{ik} u_{kj} \quad i > j$$

$$u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj} \quad i \leq j$$
Data Analysis: Understanding the results

- Compute power increasing faster than I/O
- Data movement is too expensive

- Feature-Aware in situ transformations
- Memory and compute-efficient
Resilience and Correctness: Trusting the results in the presence of faults

- **Resilient programming models**
  - Skeptical
  - Relaxed bulk synchronous
  - Local failure, local recovery
  - Selective reliability

- **Algorithm-Based Fault Tolerance**
  - Protect from *silent data corruption*
  - Use properties of models and algorithms to detect (good) or be insensitive (better) to faults
  - Understanding how random faults alter solutions / convergence

**What is the right approach for stochastic or chaotic models?**

Data from M. Heroux, M. Hoemmen, K. Teranishi
Resilience and Correctness: Dynamic adaptation impairs determinism

- Reproducibility and verification techniques rely on determinism
- Can we justify cost of enforcing determinism?
- Should we interpret reproducibility and verification statistically?
- Analysis to understand the variability of deterministic algorithms
Evolutionary or revolutionary? A Punctuated Equilibrium perspective for HPC evolution

**Punctuated Equilibrium:** Long periods of slow change disrupted by short periods of rapid change

**Transitions may be rapid, but continuity with the past is maintained**
Math is the DNA of computing that provides the common thread for (r)evolution

Some approaches may become extinct

Some approaches will adjust and continue

Some disfavored approaches will gain importance

Some dominant approaches will lose importance

Some new approaches will be created

We will not discard the 400+ year legacy of the scientific revolution and begin anew in only a decade
It’s the end of the world as we know it... and I feel fine

It’s an opportunity to solve challenging problems

What will emerge?

Don Davis, [http://www.donaldedavis.com/BIGPUB/BIGIMPCT.jpg](http://www.donaldedavis.com/BIGPUB/BIGIMPCT.jpg), CC0

Wolpertinger, Rainer Zenz, [CC BY-SA 3.0](http://creativecommons.org/licenses/by-sa/3.0/)
Exascale computing will allow us to compute in ways that are not feasible today.

- Transition poses numerous scientific and technological challenges.
- Advances in applied mathematics will be essential.
- Success will require close interdisciplinary collaboration.
- It will result in significant scientific breakthroughs.
Many additional resources are available

**Exascale Mathematics Report**
http://science.energy.gov/ascr/news-and-resources/program-documents

**Exascale Mathematics Working Group Website**
- White Papers
- Workshop presentations
- Background information

https://collab.mcs.anl.gov/display/examath/Exascale+Mathematics+Home

**DOE Grand Challenge Science Reports**

http://science.energy.gov/ascr/news-and-resources/workshops-and-conferences/grand-challenges