Evolutionary or Revolutionary? Applied Mathematics for Exascale Computing

SIAM Annual Meeting, Chicago, IL
11 July 2014

Jeff Hittinger
If you had asked me several years ago about Exascale Computing...

meh.
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>Year</td>
<td>2000</td>
<td>2008</td>
<td>2011</td>
<td>2012</td>
<td>2023</td>
</tr>
<tr>
<td>Peak (Flops)</td>
<td>1.3e12</td>
<td>1.7e15</td>
<td>11.3e15</td>
<td>20.1e15</td>
<td>1.2e18</td>
</tr>
<tr>
<td>Linpack (Flops)</td>
<td>1.0e12</td>
<td>1.0e15</td>
<td>10.5e15</td>
<td>16.3e15</td>
<td>1.0e18</td>
</tr>
<tr>
<td>Total Cores</td>
<td>9,298</td>
<td>130,464</td>
<td>705,024</td>
<td>1,572,864</td>
<td>1e9</td>
</tr>
<tr>
<td>Processors</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>Cores/Proc</td>
<td>1</td>
<td>9(2)</td>
<td>8</td>
<td>16</td>
<td>1e3</td>
</tr>
<tr>
<td>Power (MW)</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


Using commodity hardware:
Exascale Machine: $100B
Annual Power Bill: $1B
Phenomenal science: Priceless

Hoover Dam at Night, Tex Roy Bean, CC BY-SA 3.0
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.
Exascale computing introduces several fundamental challenges

**Extreme Concurrency**
- Processing units ↑
- Bulk-synchronous will not scale
- Concurrency ↑
- Synchronization ↓
- Communication ↓
- Dynamic task parallelism

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

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

**Resilience**
- Massive number of components: hard faults ↑
- Running closer to threshold voltage: soft faults ↑
- Bulk-synchronous checkpoint restart is dead
Will Mathematics for Exascale be...

Evolutionary

OR

Revolutionary?

Mick Tsikas, Reuters
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
Problem Formulation: A dramatic potential to change the questions we ask

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!*
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
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 diagram]

[Leyffer & Mahajan]
Discretization: Partitioned algorithms will play an important role

- Partitioned algorithms in:
  - Models, equations, and operators
  - Spatial (FSI)
  - Temporal (multimethod, multirate)

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

- Stability, consistency, and accuracy

Source: J. Banks and W. Henshaw
Discretization: It is expected that high-order discretizations will become dominant

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

- Adaptivity
  - Mesh
  - Model
  - Discretization/order

- Scalable computational geometry and mesh generation

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Kolev et al.

Hornung et al.

Chen and Chacon, JCP 2012

Balanced Operational Intensity
Compute-bounded

Implicit particle mover (1D)

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Implicit particle mover (1D)
Discretization: Overcome sequential bottleneck of time integration

- **Parallel-in-time**
  - Hierarchy of representations of varying fidelity
  - Iterative time advancement

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

**Discretization:**
- Overcome sequential bottleneck of time integration

**Research Issues:**
- Optimal convergence
- Chaotic systems
- Oscillatory systems
- Hyperbolic systems

**Equation:**
- Heat equation, $129^2 \times 16,384$ space-time grid

**Figure:**
- Random initial guess
- 1 Parallel in time iteration
- 4 Parallel in time iterations

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

- Communication-avoiding
- Synchronization reduction
- Data compression
- Multiple-precision
- Randomization and sampling
- Adaptive response to load imbalance
- Scheduling and memory management
- Autotuning algorithms
- Energy-efficient algorithms

Example: Timing comparison on 100x100x100 7-point Laplacian stencil [E. Chow and A. Patel]
Data Analysis: Understanding the results

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

- Concurrent analysis frameworks
- Tight memory, comm., and I/O constraints
Data Analysis: Concurrent analysis assumes a priori knowledge of the features of interest

- Feature-Aware in situ transformations
  - Statistical
    - Principal component analysis
    - Isomap
    - Locally linear embeddings
  - Segmentation-based
    - Image recognition
    - Merge trees: topology, vorticity, etc.
  - Application-specific features

- Memory and compute-efficient
  - Sub-Linear algorithms
  - Streaming: progressive multi-resolution
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
  - Use properties of models and algorithms to detect (good) or be insensitive (better) to faults
  - Understanding how random faults alter convergence

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
Mathematics for Exascale System Software

- Autotuning as derivative-free optimization
- Adaptive runtime systems as optimal control
- Mathematically grounded scheduling
- Stochastic performance models
This afternoon, we will discuss four of these areas in more depth

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>4:00-4:25</td>
<td>Hierarchical Multilevel Methods for Exascale Uncertainty Quantification and Optimization</td>
</tr>
<tr>
<td></td>
<td>Clayton G. Webster and Stefan Wild</td>
</tr>
<tr>
<td>4:30-4:55</td>
<td>Mathematical Modeling and Discretization for Exascale Simulation</td>
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<tr>
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<td>Luis Chacon</td>
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<tr>
<td>5:00-5:25</td>
<td>Discrete Solvers at the Exascale</td>
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<tr>
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<td>Esmond G. Ng</td>
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<td>5:30-6:00</td>
<td>Resilient Algorithms and Computing Models</td>
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<tr>
<td></td>
<td>Franck Cappello</td>
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</tbody>
</table>
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

It is unlikely that we will 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](https://creativecommons.org/licenses/by-sa/3.0)
The applied mathematics community must work with others to address the challenges of exascale.
Exascale computing will allow us to compute in ways that are not feasible today

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