High Performance Computing in Science and Engineering: the Tree and the Fruit

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Simulation: third pillar of scientific discovery

- Theory
- Experiment
- Simulation

"theoretical experiments"

Computational simulation:

"a means of scientific discovery that employs a computer system to simulate a physical system according to laws derived from theory and experiment"

not an “other” but a hybrid and a platform for integration of both
Simulation driven by price and capability

By the Gordon Bell Prize, simulation cost per performance has improved by nearly a million times in two decades. Performance on real applications (e.g., mechanics, materials, petroleum reservoirs, gravitation) has improved more than a million times.

<table>
<thead>
<tr>
<th>Year</th>
<th>Cost per delivered Gigaflop/s</th>
<th>Gigaflop/s delivered to applications</th>
</tr>
</thead>
<tbody>
<tr>
<td>1989</td>
<td>$2,500,000</td>
<td>1</td>
</tr>
<tr>
<td>1999</td>
<td>$6,900</td>
<td>1,020</td>
</tr>
<tr>
<td>2009</td>
<td>$8</td>
<td>1,350,000</td>
</tr>
</tbody>
</table>
Whimsical remarks on simulation progress measured by Bell Prizes, since 1988

- If similar improvements in speed ($10^6$) had been realized in the airline industry, a 15-hour flight (e.g., JFK-NRT) would require one-twentieth of a second today.

- If similar improvements in storage ($10^4$) had been realized in the publishing industry, our office bookcases could hold the book portion of the collection of the U.S. Library of Congress (~22M volumes).

- If similar reductions in cost ($>10^5$) had been realized in the higher education industry, tuition room and board (at a college in the USA) would cost about $0.20 per year.
Thought experiment:
How to use peanuts as price per ton falls?

- In 2012, at $1,150./ton:
  - make sandwiches
- By 2015, at $115./ton:
  - make recipe substitutions
- By 2018, at $11.50/ton:
  - use as feedstock for plastics, etc.
- By 2021, at $1.15/ton:
  - heat homes
- By 2024, at $0.115/ton:
  - pave roads 😊

The cost of computing has been on a curve like this for two decades and promises to continue. Like everyone else, scientists and engineers plan increasing uses for it…
1979: Computational Fluid Dynamics for B767

- Much CFD penetration
  Opportunities exist for higher accuracy and expanded complexity

- Some CFD penetration
  Opportunities exist for large increases in design process speed and application

- CFD penetration opportunity

Diagram items:
- Cab Design
- Inlet Design
- Nacelle Design
- High-Speed Wing Design
- Wing-Body Fairing Design
- Engine/Airframe Integration

C/o Douglas Ball, Boeing
2005: Computational Fluid Dynamics for B787

Much CFD penetration.
Opportunities exist for higher accuracy and expanded complexity

Some CFD penetration.
Opportunities exist for large increases in design process speed and application

CFD penetration opportunity

Wind Tunnel Corrections
Cabin Noise
Cab Design
Air Data System Location
Design for FOD Prevention
Interior Air Quality
Connexion Antenna
Inlet Design
Inlet Certification
Nacelle Design
Engine Bay Thermal Analysis
Reynolds Number Corrections for Loads and S&C
Thrust Reverser Design
Planform Design
Aerodynamics

High-Speed Wing Design
High-Lift Wing Design
ECS Inlet Design
Icing
Exhaust System Design

Wing Tip Design
Control Failure Analysis
Vertical Tail and Aft Body Design
Buffet Boundary
Wing Controls

Wing-Body Fairing Design
APU Inlet and Ducting
Avionics Cooling
Design For Loads

APU and Propulsion Fire Suppression
Vortex Generator Placement
Flutter
Wake Vortex Alleviation

Engine/Airframe Integration
Aeroelastics

Community Noise
Nacelle Design
Inlet Certification
Engine Bay Thermal Analysis

c/o Douglas Ball, Boeing

NITRD Symposium, 16 Feb 2012
## 2011 buyer driving factors in HPC

### Top Reasons for Acquiring HPC Systems

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Ranking</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ability to do new/ better science</td>
<td>8.18</td>
</tr>
<tr>
<td>Ability to run larger problems</td>
<td>7.69</td>
</tr>
<tr>
<td>Performance on OUR applications</td>
<td>7.38</td>
</tr>
<tr>
<td>Throughput</td>
<td>7.17</td>
</tr>
<tr>
<td>Price/ Performance</td>
<td>6.99</td>
</tr>
<tr>
<td>To improve our competitiveness</td>
<td>6.06</td>
</tr>
<tr>
<td>Total cost of ownership</td>
<td>6.03</td>
</tr>
<tr>
<td>Capacity mgmt</td>
<td>5.29</td>
</tr>
<tr>
<td>Regulations/ certification</td>
<td>3.08</td>
</tr>
</tbody>
</table>

Source: IDC, 2011
The imperative of simulation

In these, and many other areas, simulation is an important complement to experiment.
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Balance shift in modality of scientific discovery

- **Discover**
- **Experimentation & Observation**
- **Simulation**
- **Typical research organization**
- **Computationally aware organization**
- **Los Alamos**
- **SciDAC**
- **Understand**
- **Confirm**
- **Predict**

1950 to 2050: Shift in balance from discover to predict.
Moore’s Law: exponential growth in time

Attributed to Gordon Moore of Intel from a paper in 1965 projecting CMOS transistor density, the term is applied today throughout science and technology.
“Moore’s Law” for fusion energy simulations

Magnetic Fusion Energy: “Effective speed” increases came from both faster hardware and improved algorithms

- Full Earth Simulator (Japan)
- 1000 NERSC SP3 processors (typical)
- 16 processor Cray C90
- Cray YMP

Effective sustained speed in equiv. gigaflops

10^6
10^5
10^4
10^3
10^2
10^1
10^0


Calendar Year

- Improved linear solvers
- High-order elements
- Semi-implicit
- Partially-implicit
- Gyro-kinetics
- Delta-f, magnetic coordinates
- Improved electron models

Effective speed from hardware improvements alone

Figure from DOE “SCaLeS report” Volume 2 (Keyes et al., 2004)
"Moore’s Law" for clean combustion simulations

Combustion: “Effective speed” increases came from both faster hardware and improved algorithms.

Figure from DOE “SCaLeS report” Volume 2 (Keyes et al., 2004)
Moore’s Law and numerical algorithms

- First popularized in the 1992 NITRD bluebook: apply successive generations of algorithms to a fixed problem (“Poisson equation”)
- In 24 “doubling times” (1.5 years) for Moore’s Law for transistor density, better algorithms (software) contributed as much as better hardware
- $2^{24} \approx 16$ million $\Rightarrow$ 6 months of computing now takes 1 second on fixed hardware*
- Two factors of 16 million each if the best algorithm runs on the best hardware!

*algorithmic factor of improvement increases with problem size
These “Moore’s Laws” get to the “bottom line”

Increased computational capability & accuracy

CFD Tools
- Boeing Tools
- A300
- A388
- Cartesian Grid Tech
- TRANAIR
- CARTAIR Optimization
- TUNS3D-MB
- ZEUS
- CFL3D/ZEUS CFD++
- Unstructured adaptive grid 3D-NS

Boeing Products
- 767
- 757
- 737-300
- 777
- 737NG
- 787

Wind Tunnel vs. CFD
- 77 wings tested
- 38 nacelle installation
- 18 CFD runs base
- 11 CFD runs

Less testing, lower cost, better products

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c/o Paul Johnson and Mark Goldhammer, Boeing

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These “Moore’s Laws” keep the country safe

Stockpile stewardship

Complex multi-material, unstructured electromagnetics

1.2 billion unknowns

2,000 processors

6 minutes – interactive timescale for engineers!

Not previously tractable at any turnaround
An exciting knowledge fusion for simulation

科学模型

数值算法

计算机架构

科学软件工程

“Computational science is undergoing a phase transition.”
Ecosystem: industry, national labs, academia

- Mission-oriented and idea-oriented organizations make great partners for scientific discovery and technological advance
- No country does it better than the USA

- basic/applied
- short-term/long-term
- incubate/curate
- feedcorn/seedcorn

In most countries, the barriers between basic and applied are much higher – even within academia!

Reward structures discourage exchanges, internships, cross-pollinations critical to innovation.
Basic research deposits into “treasury of ideas”

- “Treasury” opened as scientists adapt to opportunities and constraints
  - driven by limiting resource (processing, storage, bandwidth, etc.), which is cyclical
- Algorithms arise to fill the gap
  - between architectures that are available and applications that must be executed
- Many algorithms are mined from the literature, rather than invented
  - underlining the importance of basic research
- Many algorithmic advances are driven by particular physical problems outside of the academic sandbox
  - underlining the importance of applied research

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Born</th>
<th>Why?</th>
<th>Reborn</th>
<th>Why?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conjugate gradients</td>
<td>1952</td>
<td>direct solver</td>
<td>1970s</td>
<td>iterative solver</td>
</tr>
<tr>
<td>Schwarz Alternating procedure</td>
<td>1869</td>
<td>existence proof</td>
<td>1980s</td>
<td>parallel solver</td>
</tr>
<tr>
<td>Space-filling curves</td>
<td>1890</td>
<td>topological curiosity</td>
<td>1990s</td>
<td>memory mapping function</td>
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NITRD agency success story: PETSc (1992- )

- The Portable Extensible Toolkit for Scientific Computing (PETSc)
  - used in thousands of scientific and engineering codes
  - software structure has inspired countless other library developers
- Suite of distributed data structures and routines for the scalable solution of large systems of equations
- Has won R&D 100 award, been part of multiple Gordon Bell prizes, Best Paper prizes; its developers won DOE’s E. O. Lawrence award in 2011
- Funded by Argonne National Laboratory, DOE, and NSF

The “SciDAC” model of leveraging

Many applications drive

Math

CS

Applications

PETSc

MPI

Enabling technologies respond to all

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On to: the fourth pillar of scientific discovery

- **Data-enabled science**

  “... Authors in this volume ... refine an understanding of this new paradigm from a variety of disciplinary perspectives.”
  — Gordon Bell, Microsoft Research

Third and fourth paradigms belong together!

- **Future for simulation will embrace data culture**
  - Inverse problems
  - Data assimilation
  - Uncertainty quantification
  - Immersive visualization and computational steering

- **Future for data will embrace simulation culture**
  - Simulation has mature culture of “optimal algorithms”
  - Complexity of solution or representation grows slowly in problem size or difficulty, *e.g.*, multigrid, multipole, FFT, sparse grids, spectral, interior point, solution-based adaptivity, importance sampling, etc.
  - Data analysis is at the beginning of optimality results
  - Complexity of solution or representation typically grows rapidly; but see recent breakthroughs, *e.g.*, wavelets, compressed sensing

- **See Alex Szalay’s talk for fourth paradigm**
The Tree and the Fruit

High performance computing is a phenomenally productive tree in the pursuit of scientific knowledge and technological advance.

High performance computing is also itself a fruit – an exciting fusion of computer science and mathematics that grows extraordinarily well in the USA.

NITRD rightfully enjoys the credit for envisioning and provisioning HPC for over twenty exhilarating years. May they stretch forward to the unimaginable.