Theoretical & Basic Research

Phase 0
Concept/Vision

Phase 1
Feasibility

Phase 2
Design/Development

Phase 3
Prototyping

Phase 4
Production/Deployment

NCSA
Bridges the Gap BETWEEN Basic Research & Commercialization

Product Life Cycle

Phase 0
Concept/Vision

Phase 1
Feasibility

Phase 2
Design/Development

Phase 3
Prototyping

Phase 4
Production/Deployment

Over the horizon development ...

Theoretical & Basic Research

Applied Prototyping & Development

Optimization & Robustification

Commercialization & Production (.com or .org)

UNIVERSITIES & LABS

APPLICATION/ECONOMIC DEVELOPMENT

PRIVATE INDUSTRY

BLUE WATERS IBM-NCSA-UIUC
One-Third of FORTUNE 50®
HPC ≠ SUPERCOMPUTING

BIG COMPUTING

BIG SCIENCE

BIG DATA
INDUSTRY INNOVATION

National Center for Supercomputing Applications
University of Illinois at Urbana-Champaign

BLUE WATERS IBM-NCSA-UIUC
Competitive Advantage

Winning globally requires HPC-driven solutions.

Suzy Tichenor, Council on Competitiveness, March 2008
Thanks to HPC, virtual prototyping was used to develop the 787 Dreamliner. Boeing conducted tens of thousands of virtual wing prototypes, yet only 11 physical wind tunnel tests.

*Image courtesy The Boeing Company.*
GM Takes Data Sharing to the Next Level

“The movement of data between the CAD and PLM systems can be daunting and time consuming, resulting in unnecessary delays and launch issues.”

Source: Kevin Kelly, Sr. Editor, AutoFieldGuide.com
www.autofieldguide.com/articles/080709.html
High Performance Computing: Enabling Next-Gen Energy & Propulsion

Physics Modeling / Diagnostics  ➔  Design Technologies  ➔  Energy Efficient, Green Systems

HPC + Fluid Dynamics = Improved Efficiency, Emissions, Noise, Durability ... American Competitiveness in Aerospace, Manufacturing

- High-performance Compressors
- Low-emission Combustors
- Durable Turbines
- Quieter, more efficient Jet Engines

HPC + Simulation Science:
- Physics in detail, scale not feasible (technical, cost) via testing
- Rapid Optimization for Differentiating Products

Enable cost-effective development of game-changing technology

- Open Rotor Engines for double-digit fuel-burn advantage over today’s engines
- Revolutionary Pulse-Detonation Technology

HPC + Multi-physics = Enable US Energy Security & Renewable Goals

- Designing high-yield, quiet Wind Turbines
- Reduce cost, improve performance of Gasification Systems
- Next-gen Boiling Water Reactors

Other areas impacted by HPC @ GE: Materials Design, Manufacturing Process Efficiency, Healthcare and Life-Sciences, Strategic Materials
NSF STRATEGY FOR HIGH-END COMPUTING

Science and Engineering Capability (logarithmic scale)

Track 1 System
- UIUC/NCSA (>1 PF sustained) $208M

Track 2 Systems
- PSC (?) $30M
- UT/ORNL (~1PF) $30M
- TACC (500+TF) $30M

Track 3 Systems
- Leading University HPC Centers

FY’07 FY’08 FY’09 FY’10 FY’11

BLUE WATERS IBM-NCSA-UIUC
Giga- 

Tera-

Peta-

Exa-

Zetta-

Yotta-

(Bytes, Flop/s)
## Sustained Petaflop/s

<table>
<thead>
<tr>
<th>SYSTEM ATTRIBUTE</th>
<th>ABE</th>
<th>BLUE WATERS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vendor</td>
<td>Dell</td>
<td>IBM</td>
</tr>
<tr>
<td>Processor</td>
<td>Intel Xeon 5300</td>
<td>IBM Power7</td>
</tr>
<tr>
<td>Peak Performance (Petaflop/s)</td>
<td>0.088</td>
<td>NDA</td>
</tr>
<tr>
<td>Sustained Performance (Petaflop/s)</td>
<td>0.005</td>
<td>≥1</td>
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<tr>
<td>Number of Cores/Chip</td>
<td>4</td>
<td>NDA</td>
</tr>
<tr>
<td>Number of Processor Cores</td>
<td>9600</td>
<td>&gt;200,000</td>
</tr>
<tr>
<td>Amount of Memory (TB)</td>
<td>14.4</td>
<td>&gt;800</td>
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<tr>
<td>Amount of Disk Storage (TB)</td>
<td>100</td>
<td>&gt;10,000</td>
</tr>
<tr>
<td>Amount of Archival Storage (PB)</td>
<td>5</td>
<td>&gt;500</td>
</tr>
<tr>
<td>External Bandwidth (Gbps)</td>
<td>40</td>
<td>100-400</td>
</tr>
</tbody>
</table>
TOP500® PEAK PERFORMANCE (COMBINED)
Petascale Application Collaboration Teams

MILC (lattice QCD)

NAMD (molecular dynamics)

Pseudospectral Method (turbulence)

NSF Challenge: >=1 Sustained petaflop/s

Photos courtesy of NERSC, UIUC, IBM
Dr. Klaus Schulten’s UIUC team can see things in simulation through computational microscopes that cannot be seen in experimentation.

His NAMD code is one of the benchmarks for sustainable petascale computing.

- Protein misfolding causes disease. Why?
- When does a molecule break, not bend?
- Why are blood clots stiffer than normal blood?

Today’s simulations are <1 millisecond.

Need to get to 1 millisecond, then simulate teams of proteins.
Dr. Carlos A Pantano-Rubino’s UIUC team has barely enough research capability to simulate 1in³ of combustion.

What coordinated basic/applied research is needed for new breakthroughs?

How can greater understanding of turbulence affect fuel efficiency?

Boeing’s Dr. Forrester Johnson says that a 1% improvement in airline fuel efficiency is worth $350B.
Industry Path to Petascale

**USERS**
- Aerospace
- Automotive
- Bio/Chemical
- Oil & Gas
- Pharma
- Energy
- Distribution
- Finance
- Tech

**DEVELOPERS**
- In-house
- Commercial
- Proprietary
- Open Source
- ISV

**WORKFORCE**
- Corporate
- University
- HPC experts
- Domain experts
- Industry Labs
Largest FORTUNE 100® Industry Sectors

25
Finance/Insurance

Bank of America
CITI
JPMorganChase
AIG
Morgan Stanley
Merrill Lynch
Goldman Sachs
State Farm Insurance
MetLife

17
Manufacturing

GM
Ford
GE
Boeing
United Technologies
CAT
Lockheed Martin

17
Retail/Wholesale

Walmart
Home Depot
Kroger
Costco
Target
Sears
Lowe’s

BLUE WATERS IBM-NCSA-UIUC
U.S. FORTUNE 100® Manufacturing Companies

Range: $20B - $200B
GLOBAL 100® Manufacturing Companies

Range: $65B - $230B (4 US; 6 ASIA; 7 EU)
Petascale Computing Facility
Cell Processor

- GFLOPS: 200
- Bandwidth between host memory and PE memory (GB/s): 25.6
- Local memory to PE bandwidth (GB/s): 
- Frequency (GHz): 3.2
- # of processing elements: 8

Diagram:
- Memory Interface Controller
- I/O Interface
- PowerPC Processor Unit (PPU)
- PowerPC Processor Storage Subsystem (PPSS)
- L2 cache
- L1 instruction cache
- L1 data cache
- Memory Flow Controller (MFC)
- DMA Controller
- Local Store (LS)
- Synergistic Processor Element (SPE)
- Synergistic Processor Element (SPE)0
- SPE7

BLUE WATERS IBM-NCSA-UIUC
FPGA SRC-6 MAP-E

GFLOPS: 24
Bandwidth: 1.4 GB/s between host memory and PE memory
Local memory to PE bandwidth: 4.8 GB/s
Frequency (GHz): 0.1
Number of processing elements: 

---

**Control FPGA**

- **OBM A**: 64
- **OBM B**: 64
- **OBM C**: 64
- **OBM D**: 64
- **OBM E**: 64
- **OBM F**: 64

**User FPGA 0**

- **Dual-ported Memory**: 192
- **User FPGA 1**: 192

2400 MB/s each

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BLUE WATERS IBM-NCSA-UIUC
NVIDIA 8800 GTX GPU

GFLOPS 345.6
Bandwidth between host memory and PE memory (GB/s) 2.0
Local memory to PE bandwidth (GB/s) 86.4
Frequency (GHz) 1.35
# of processing elements 128
Cosmology Codes

Fig 1. Execution time vs. dataset size

- Cell SP speedup: 59.1X
- Quadro SP speedup 88.2X
- GeForce SP speedup 154.1X

Fig 2. Speedup vs. dataset size

- H101 DP speedup: 6.8X
- PowerXCell DP speedup 88.2X
- GeForce DP speedup 54.5X

Volodymyr Kindratenko, Dylan Roeh, Guochun Shi (NCSA), Robert Brunner (UIUC Dept of Astronomy)

BLUE WATERS IBM-NCSA-UIUC
Results

• **FPGA**
  - Great on specific applications (e.g. Black-Scholes)
  - Low power
  - Cannot re-port – must instead rebuild circuitry
  - Must constantly think of hardware engineering

• **CELL**
  - Improved performance over FPGA
  - Doesn’t scale well

• **GPU**
  - Overall best performance
  - Larger community of users keeps costs low
  - Already has college-level mind share
  - Code needs to be redesigned
  - 800X improvement for quantum chemistry

• **90/10 RULE**
  - 90% of execution time in 10% of lines of code
  - Need small kernels – compact with well-defined data sets
NCSA’s Abe Lincoln

• Abe
  • 1200 blades; 2.33 GHz Intel Xeon Clovertown
  • Dual-socket, quad-core (9,600 cores)
  • Infiniband & GigE
  • 9.6 TB total memory

• Lincoln
  • 96 nVidia Tesla units
  • 192 nodes
  • 2 GPUs, 8 traditional cores, 1 PCI bus per node

• Abe Lincoln
  • Cluster with NVIDIA Tesla GPUs
  • Mix of MPI, file system and GPUs
  • Tesla is designed for HPC, not gaming
  • Could use hardware rendering to speed up viz

• Results
  • Need better balance and higher memory
  • Perhaps 4/4/2
The only way to discover the limits of the possible is to go beyond them into the impossible.

Arthur C. Clarke
"Technology and the Future" (Clarke’s second law)

See new possibilities... and achieve them!