Computational Science Graduate Fellowship Program Review

Mark Anderson
Director
Office of Advanced Simulation and Computing and Institutional Research and Development
NNSA is a key element in the nuclear security enterprise

- Maintain a safe, secure, and reliable US nuclear stockpile
- Develop scientific understanding necessary to assess and certify weapons without underground nuclear testing
- Support a variety of threat reduction activities that rely on the capabilities and skills developed in the nuclear weapons program.
NNSA requirements are complementary to other U.S. Government needs

**NNSA**
- Primary focus: tightly-coupled multi-physics codes for national nuclear security decisions
- Heavily optimized code-hardware integration for efficiency
- HPC leadership ensures deterrence against adversaries

**DOE/SC**
- Primary focus: codes used for scientific discovery, supports broad user community
- Adapt codes to available architecture, platforms and applications developed separately
- HPC leadership leads to scientific advances on the world stage

**NSA**
- Primary focus: data analytics and cryptography for national security
- Drives special-purpose architecture developments not necessarily efficient for NNSA and SC
- HPC leadership ensures intelligence supremacy and cyber security
Turbulence simulation is an iconic example of the need for large scale simulation.

- **Petaflops**
  - Reacting turbulence with supernova microphysics

- **Exaflops**
  - Multi-physics: exothermic reactions, shocks, variable accelerations, radiation.
  - 5000^3: “Solve” the isotropic turbulence problem?

- **Teraflops**
  - 3D hydrodynamic instability at moderate density ratio
  - High resolution geophysical flows

- **Gigaflops**
  - Buoyancy driven multi-component mixing
  - Full supernova explosions
  - Accurate hurricane prediction

- **128^3 isotropic turbulence**
- **Single mode 2D instability, ~1980.**
- **3D hydrodynamic instability at high density ratio with gravity inversion**
- **High resolution geophysical flows**

Power limitations are driving fundamental changes to architectures and programming models

- We are entering a 4th programming model era
- Industry is migrating from FLOPS-dominated to data-movement-dominated paradigm
- Two basic system approaches:
  - Homogeneous multi-core
  - Heterogeneous (GPGPUs or ??)

<table>
<thead>
<tr>
<th>Technology Challenge</th>
<th>Hardware Mitigation</th>
<th>Application Impact</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flat or decreasing processing unit (core) speeds</td>
<td>Dramatically increased CPU core count to track Moore’s Law</td>
<td>First fundamental change in programming model in decades</td>
</tr>
<tr>
<td>Memory speed and capacity improvements lag far behind compute speed improvements</td>
<td>Multiple levels/types of memory in a CPU</td>
<td>Explicit management of memory placement/motion</td>
</tr>
<tr>
<td>Complex CPU designs too power-hungry to scale to exascale</td>
<td>Heterogeneous architectures with specialized processing units</td>
<td>Must coordinate both how and where specific computations are executed</td>
</tr>
</tbody>
</table>
The future beyond CMOS and Moore’s Law holds many challenges and possibilities

- CMOS technology is reaching some fundamental physical limits
- Alternatives to the conventional von Neumann architecture are beginning to show promise
  - Neuromorphic architectures and machine learning
  - Quantum computing
Simulations are not reality, but rather potentially useful representations of reality

\[
\frac{BEM}{BAC} \notin \mathbb{R}
\]

\[
\frac{BEM}{BAC} \sim \mathbb{R}
\]

Detail from *The Parade*, Georges Seurat, 1889