Computing Challenges for the Third Decade of Stockpile Stewardship

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ASC is a key element of the nuclear security enterprise

- Defense Program’s Mission: maintain a safe, secure, and effective nuclear deterrent
- ASC is the lens through which we apply our science and nuclear test history to assess, qualify, and certify the stockpile without testing
- We also support a variety of threat reduction activities
Confidence in stockpile assessment rests on our people and tools.

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<th>Designers with test experience</th>
<th>2(^{nd}/3^{rd}) generation designers</th>
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<td>Nuclear tests</td>
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<td>Predictive science-based simulations</td>
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Our confidence, once based on nuclear tests, now must be founded on improved physics understanding incorporated into predictive simulations.
Nuclear security threats are changing

Global: Russia, China
Regional: North Korea, Iran

2018 Nuclear Posture Review directs NNSA to deliver
- Low-yield sub-launched ballistic missile
- Sea-launched cruise missile

ASC provides tools to design and certify
Computing technology is also evolving rapidly, driven by market forces broader than just HPC.

Government agencies must lead at the extreme high end, and partner with vendors to scale out and establish U.S. leadership.
Our idealized technology maturation model is modified by market forces

1. **Testbeds**
   - Small scale (node-level) R&D. Understand the potential of new technology

2. **Prototypes**
   - Built from emergent technologies. Prove rack-level production-capable systems useful for mission applications

3. **Advanced Technology Systems**
   - Leading-edge technology. Includes non-recurring engineering and early access systems

4. **Commodity Technology Systems**
   - Scalable production technology. Run mission simulation workloads

These are usually proposed by the vendors at the largest scale
Sierra, our most recent ATS system, is being deployed at Livermore.

**Component:**
- **IBM POWER9**
  - Gen2 NVLink
- **NVIDIA Volta**
  - 7 TFlop/s
  - HBM2
  - Gen2 NVLink
- **NVMe-compatible PCIe**
  - 1.6 TB SSD
  - 256 GiB DDR4
- 16 GiB Globally addressable HBM2 associated with each GPU
  - Coherent Shared Memory
- **Mellanox Interconnect**
  - Single Plane EDR InfiniBand
  - 2 to 1 Tapered Fat Tree

**Compute System**
- 4320 nodes
- 1.29 PB Memory
- 240 Compute Racks
- 125 PFLOPS (~12 MW)

**Compute Node**
- 2 IBM POWER9 CPUs
- 4 NVIDIA Volta GPUs
- NVMe-compatible PCIe
- 1.6 TB SSD
- 256 GiB DDR4
- 16 GiB Globally addressable HBM2 associated with each GPU
- Coherent Shared Memory

**Compute Rack**
- Standard 19" Width
- Warm water cooling
Coping with new hardware technologies requires new programming approaches.

Each of these eras defines a new common programming model and transitions are taking longer; NNSA is entering a fourth era.
Increasing code complexity, coupled with architecture uncertainty, is driving our labs to a new, modular approach

- Codes today are >5x larger than pre-ASCI codes
- Modular infrastructure can be reused by other codes
- Central Data Store allows individual components independently

![Source code size over time](chart.png)

Average of 60 kilo lines of code (KLOC) per year of additional code to support a representative integrated code

**Old Model**
- Graphics Edits
- Thermo-nuclear Burn
- High Explosive Modeling
- Hydro
- Magneto-hydro dynamics
- Radiation Transport
- Restarts

**New Model**
- Data Store
- Radiation Transport
- Thermo-nuclear burn
- High Explosive modeling
- Turbulence
- Magneto-hydro dynamics
- Restarts
- Graphics Edits
- Hydro
We are transforming our existing codes and developing new ones to capitalize on the hardware evolution.

Recent past applications/software designed around:

- Floating point (numerical) bottlenecks
- Coarse-grained parallelism
- Stable/predictable architecture designs

Code Transformation Process:

- Theoretical prediction of performance limiters (proactive)
- Empirically based studies on emerging hardware (responsive)

Multiple years of effort
Millions of lines of code

Future applications must design for:

- Memory and network (data motion) bottlenecks
- Fine-grained concurrency
- Multiple diverse architecture designs

Optimized software performance lags the potential offered by new hardware while architectural impacts are understood and code is transformed.

NNSA aims to minimize that lag through:

a) Co-design and Centers of Excellence (partnering with vendors)
b) Research (partnering with ASCR)
c) Early access hardware (testbeds)
d) Market incentives (large procurements)
e) Mission incentives (pressure from the users to transform)
AXOM & RAJA – Applications sharing CS software infrastructure (Livermore)

Hierarchical key-value data management

Parallel file I/O & burst buffer support

Unified cross-package message logging & parallel processing

Surface queries & spatial acceleration data structures

Mesh-aware data schema

P0

P1

P2

P3

File 0

File 1

Mesh data model

“coordsets”: {
  “coords”: {
    “type”: “explicit”
    “values”: {
      “x”: [double],
      “y”: [double]
    }
  }
},
“topologies”: {
...

AXOM: Common CS Infrastructure

Application Code

RAJA

Serial OMP3 CUDA

OMP4.5 ROCm ??

Mature Programming Models

Emerging Programming Models

RAJA allows ease of switching between backends enabling the best tools for our codes and also helping steer vendor interactions.

RAJA Performance Portability Library
Kokkos – Performance, portability and productivity (Sandia)

https://github.com/kokkos
Ristra – A software architecture for multi-physics (Los Alamos)
In addition to programming model changes, the labs now need to rethink basic algorithms. Algorithms that reduce the number of variables by increasing the computational work per variable will scale better on advanced architectures. Just as in the past, these complexities point to why the NNSA labs need to engage with the vendors (co-design) to assure NNSA codes are efficient.
Brain-inspired computing requires new approaches drawing on both simulation and data science

- Conventional machine learning (train models, optimize simulation process, etc.)
- Improving simulation workflow and optimization
- Recasting problems and algorithms to exploit new architectures designed for ML
Machine learning through the simulation cycle optimizes the simulation process

**Hypothesis generation**

Machine learning systems uncover relationships between computational models and experimental data.

**Observed molecular properties**

This “active learning” approach can be used to optimize solutions with significant reduction in compute requirements.

**Machine learning systems**

**HPC-enabled simulation**
Future large-scale simulations will be analyzed and optimized by integrated machine learning

Large state-of-the-art simulations are becoming too complex for humans to manage and control

- Failures in workflow e.g. mesh tangling
- Outputs too large for current analysis and visualization methods
- Complex parameter spaces requiring large ensembles of runs

Early results show the promise of learning systems for simulation workflow management
Recasting algorithms will let us use ML-centric architectures

\[ \frac{\partial C(x,t)}{\partial t} = D \frac{\partial^2 C(x,t)}{\partial x^2} \]
Beyond Von Neumann architectures and Moore’s Law to the next-gen computing technologies

Newer memory architectures

Neuromorphic systems

Quantum information systems

The computing landscape will continue to evolve; we must capitalize on future technologies
Balancing the simulation & computing requirements is a challenge
We also must realize that simulation and computing are tools to achieve solutions, not solutions themselves.

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

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

Detail from *The Parade*, Georges Seurat, 1889
Assessing the costs and benefits of NNSA’s investments in HPC must be mission-focused

We must remain a viable alternative to nuclear testing

How do we measure ROI for investments in HPC?

HPC systems are only a small investment in the total ASC program’s portfolio

Will the new technologies stemming from Exascale research, Cognitive Computing and BML give us our ROI?

How do we address these questions?