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Title: Scientific Computing at Los Alamos National Laboratory

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Scientific Computing at Los Alamos National Laboratory

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June 30, 2014

Discussion Topics

- Los Alamos high performance computing strategy
  - NNSA/ASC & SC/ASCR
  - Partnerships with academia and vendors
- Perspectives on extreme-scale computing:
  Exaflop **and beyond**
- Role of Scientific Computing at Los Alamos: Open Science
  - Focus on ocean simulations for climate models

Our mission success requires computing leadership

"When we at ASCI first estimated what we would need by now in high-performance computing, we underestimated. In my view, we must continue to advance the power and resolution of our computers to do our mission; the ongoing weapon life-extension programs and our annual assessment of the deterrent depend on it."

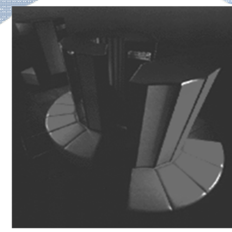
Charles McMillan, Director,
Los Alamos National Laboratory
National Security Science, April 2013

Our goal for computing is to be a recognized leader in high performance computing, especially for national security science, at the forefront of computer and computational science

Los Alamos: a pioneer of cutting edge computing for 70 years

[Small/large core memory]

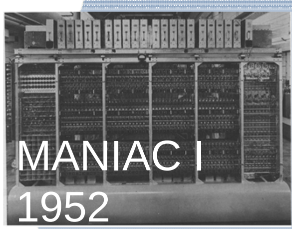
Cray 1 1976
[Vector machine]



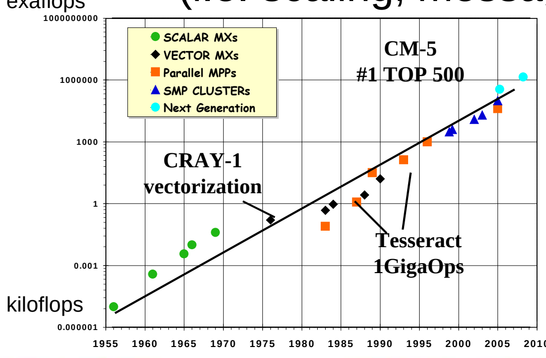
Cray X-MP 1983

TMC CM-5 1992 [hypercube]

Blue Mountain 1998
[Massively parallel]



- Core NW mission needs have been major industry driver, but that has changed.
- Significant changes in architecture have accompanied the increasing power
- Resulted in rich capability of coupling scientific algorithms to varied architectures (i.e. scaling, messaging, and vectorization)



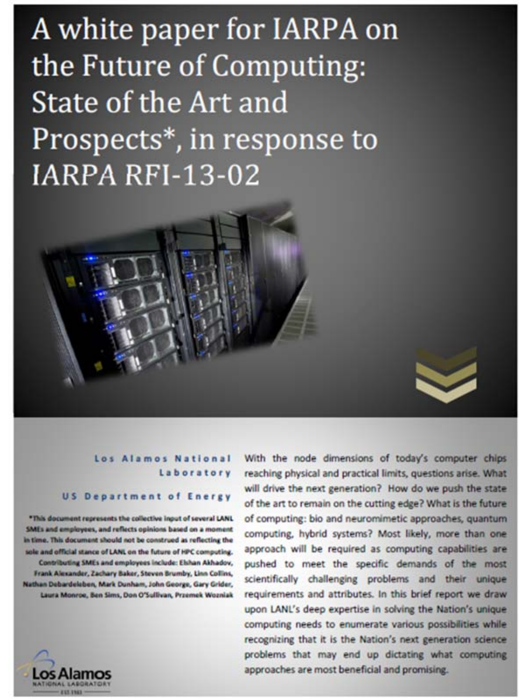
Lightning (LNXI) 2004
[commodity computing]

Roadrunner 2005-2008
[Hybrid architecture]

Our computing leadership extends beyond CMOS

Past and current quantum computing strength

Foundations of decoherence



A white paper for IARPA on the Future of Computing: State of the Art and Prospects*, in response to IARPA RFI-13-02

Los Alamos National Laboratory

US Department of Energy

*This document represents the collective input of several LANL SMEs and employees, and reflects opinions based on a moment in time. This document should not be construed as reflecting the sole and official stance of LANL on the future of HPC computing. Contributing SMEs and employees include: Elshan Akhadov, Frank Alexander, Zachary Baker, Steven Brumby, Linn Collins, Nathan Debardeleben, Mark Dunham, John George, Gary Grider, Laura Monroe, Ben Sims, Don O'Sullivan, Przemek Wozniak

With the node dimensions of today's computer chips reaching physical and practical limits, questions arise. What will drive the next generation? How do we push the state of the art to remain on the cutting edge? What is the future of computing: bio and neuromimetic approaches, quantum computing, hybrid systems? Most likely, more than one approach will be required as computing capabilities are pushed to meet the specific demands of the most scientifically challenging problems and their unique requirements and attributes. In this brief report we draw upon LANL's deep expertise in solving the Nation's unique computing needs to enumerate various possibilities while recognizing that it is the Nation's next generation science problems that may end up dictating what computing approaches are most beneficial and promising.

Los Alamos NATIONAL LABORATORY

Deployed quantum encryption technology

Vendor partnerships will become essential

The Journey to Exascale:
Mission impact, U.S. competitiveness, HPC leadership

- Petascale computing has been successful and impactful across the breadth of DOE's mission areas (including through Roadrunner & Cielo)
- Exascale computing will enable the next stage of Predictive Simulation and Analytics for scientific discovery, engineering design, and national security (and Trinity is a key step)
- Several DOE mission drivers are poised to cross the predictivity threshold
- Exascale will enhance U.S. economic competitiveness; action is needed now to ensure continued U.S. leadership

…enabling scientific discovery, new algorithms, and advanced applications at the leading edge of computational science

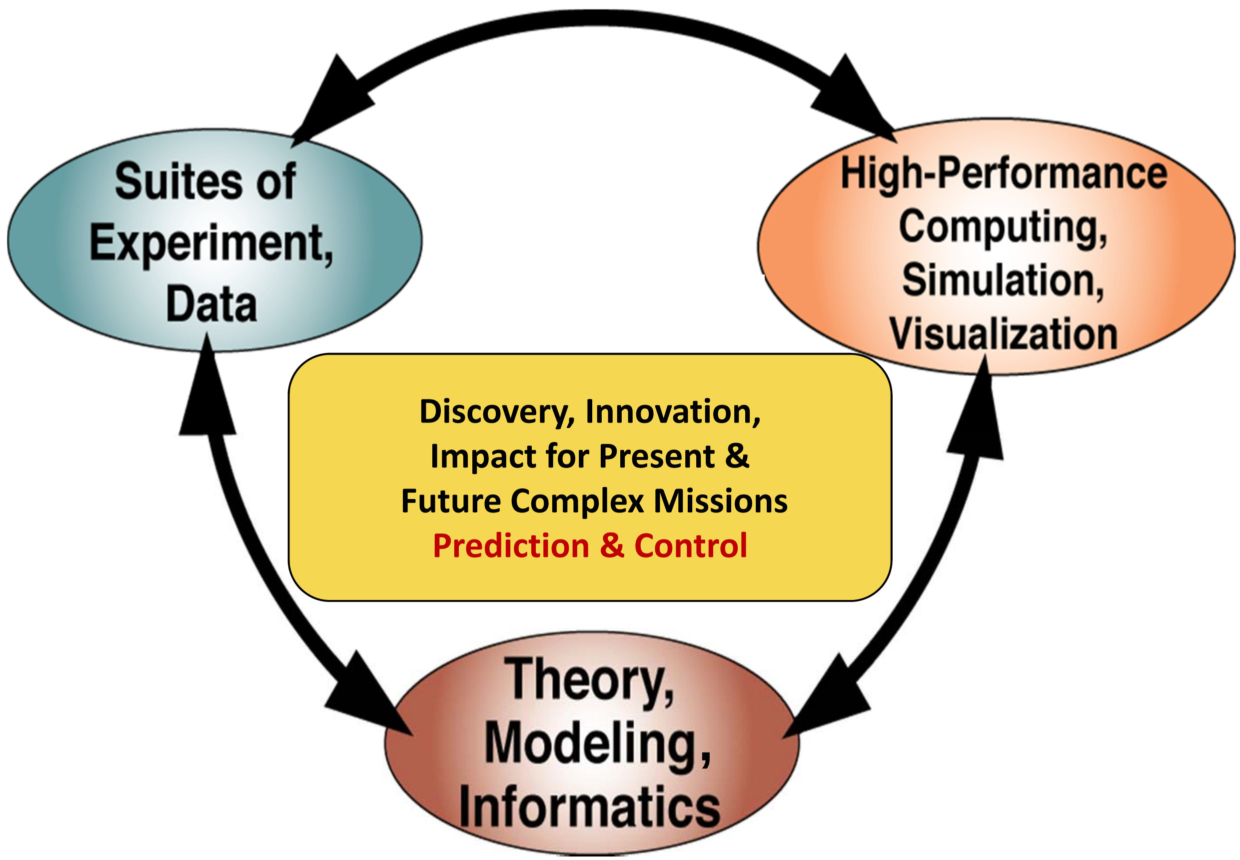
High performance computing continues to be essential for Stewardship

Strategic Objectives

- Robust Tools
  - Models, Codes, Techniques
- Prediction through Simulation
  - Verified and Validated Codes
- Balanced Operational Infrastructure
  - Platforms and Infrastructure

We are focused on Trinity acquisition ***and being ready to use it*** *(through* ***co-design*** *of infrastructure and codes)*

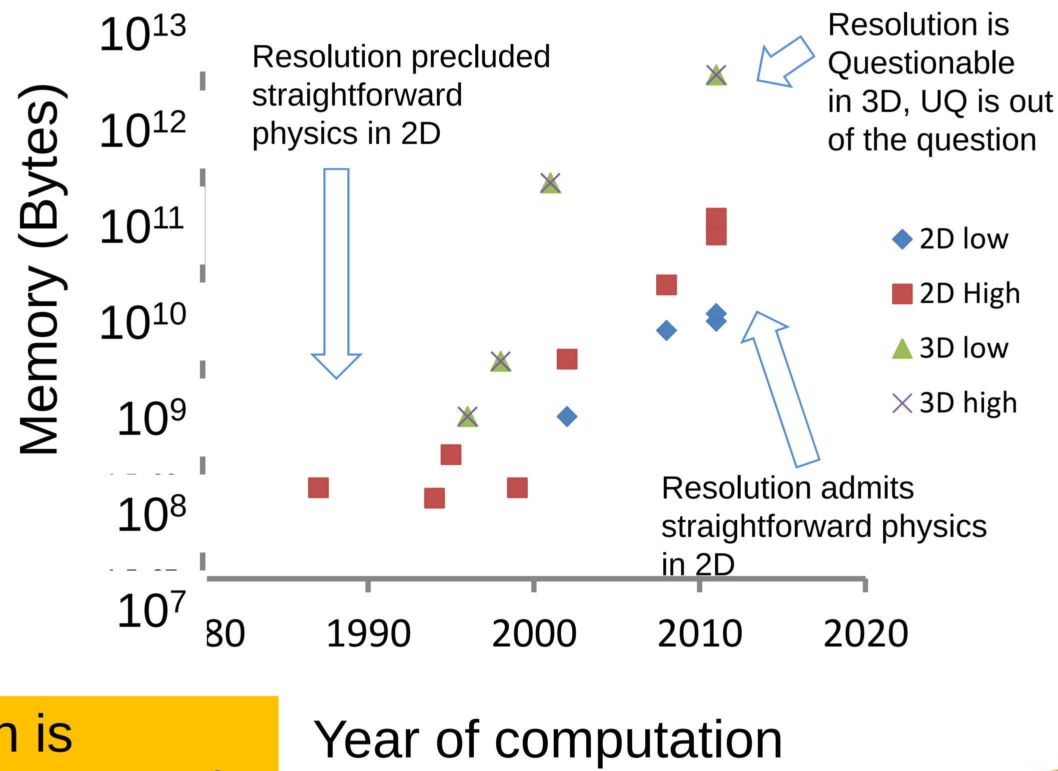
Co-Design is how we do our work



Historic trends indicate that memory requirements increase dramatically with physics fidelity

- Prediction fidelity over the last two decades is dominated by:
  - Increased resolution
  - Increased dimensionality
  - Subgrid model complexity
- Successful experimental validation of models is
  - Universal at higher resolution and full dimensionality
  - Tuned when we rely on locally valid sub-grid models

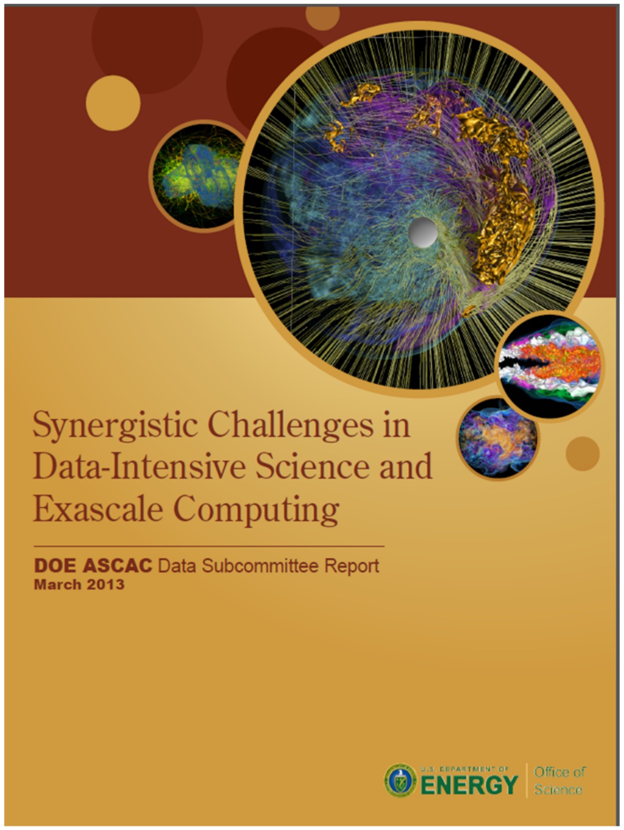
Typical Restart memory requirements



Increased resolution in simulation is changing our picture of how weapons work.

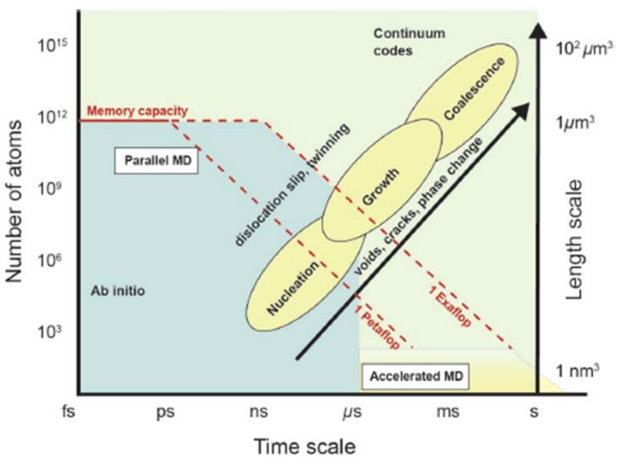
Challenges and opportunities for data-intensive computing require co-design

- ✓ The Power Challenge
- ✓ Interconnect and bandwidth
- ✓ Storage and data management hierarchies
- ✓ Scalable analytics algorithms and software



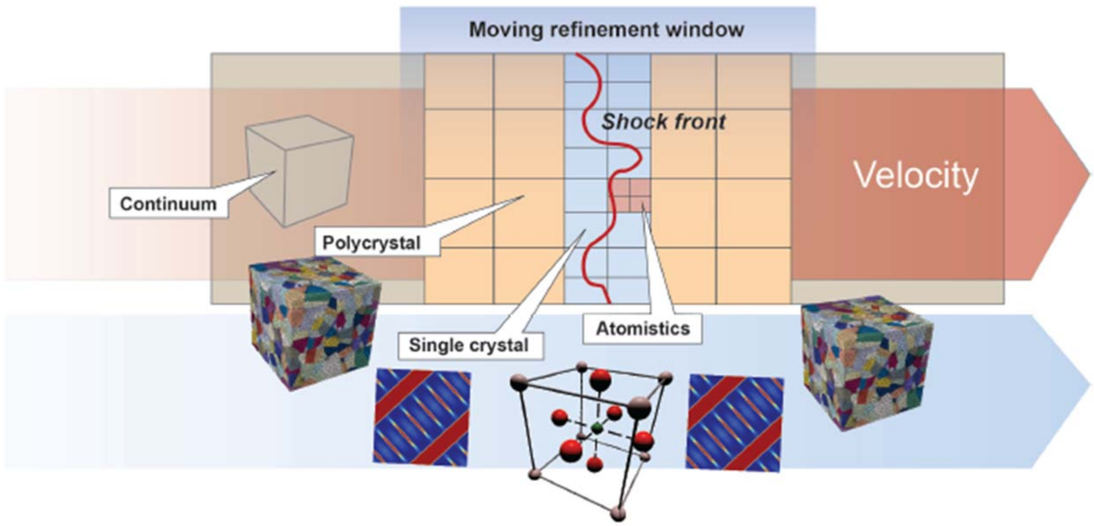
Los Alamos is making institutional investments to address these challenges

Our integrated co-design approach will couple multi-scale theory and multi-probe experiment on next-generation computing architectures for future integrated codes



Mesoscale materials phenomena need extreme-scale computing

Variable-resolution models are synergistic with multi-probe, in-situ, transient measurements



The development of validated models will reduce uncertainty in integrated codes and provide predictive descriptions of newly manufactured materials & components

Overview of climate simulations – Movies are worth 1000s of words

- "Modern" high resolution ocean models
  - comparison to vintage 2000 simulations
  - coupling biogeochemistry to ocean circulation
  - [role of resolution AND fidelity at scale]

- Regional effects are becoming resolvable (and important)
  - Arctic ice sheet variation
  - melting of Antarctic shelf
  - Tree mortality (look out the window on the bus)

We play a leadership role in national partnerships providing major modeling and simulation tools for DOE

CCSI™ Carbon Capture Simulation Initiative

CCSI: A five-Lab, multi-university, multi-industry initiative chartered by the President to accelerate carbon capture deployment. Los Alamos leads Basic Data & Models team and is a key contributor to Particle & Device Scale team and the Uncertainty Quantification team. From first review in October: "*…Progress impressive, well beyond what they might have expected at this point in the program...*"

NETL | Berkeley Lab | Lawrence Livermore National Laboratory | Los Alamos National Laboratory | Pacific Northwest National Laboratory | U.S. Department of Energy

Consortium for Advanced Simulation

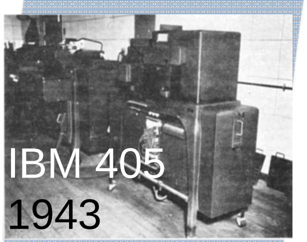
Of Light Water Reactors

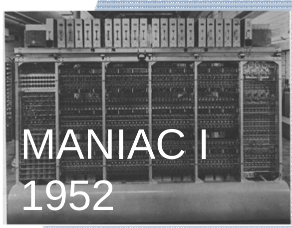
ASCEM

ASCEM (Advanced Simulation Capabilities for Environmental Management): Consortium of five Labs to develop transformational, HPC modeling to improve our ability to predict movements of underground contaminants and minimize ES&H risks across the DOE Complex.

Berkeley Lab | Los Alamos National Laboratory | Pacific Northwest National Laboratory | Oak Ridge National Laboratory | SRNL

We remain committed to leadership in extreme-scale computing

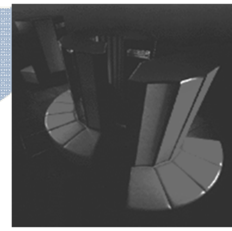

IBM 405
1943


MANIAC I
1952


MANIAC II
1957


CDC 6600
1966
[Small/large core memory]


Cray 1 1976
[Vector machine]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Exascale as well as disruptive technologies

A focus on co-design at all levels is key to our success

We welcome opportunities to contribute to and guide the national dialogue