NATIONAL NUCLEAR SECURITY ADMINISTRATION
OFFICE OF DEFENSE PROGRAMS

# Computational Science Graduate Fellowship Program

*July 28, 2015*


*Douglas Wade*

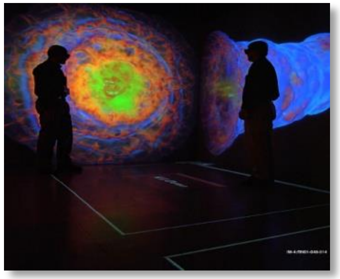
*Acting Director*

*NNSA Office of Advanced Simulation and Computing and Institutional R&D Programs, NA-114*

# Office of Advanced Simulation and Computing Overview

***Mission:*** *Provide leading edge, high-end simulation capabilities needed to meet weapons assessment and certification requirements.*

- Support the current stockpile through activities for the B61 Life Extension Program (LEP), W78 LEP study, exploring stockpile options, and support the National Ignition Campaign
- Prepare for the future stockpile through code improvements vectored toward future stockpile options and mitigating and adapting the integrated design codes (IDCs) to evolving high performance computer (HPC) architectures
- Provide computing facilities for current stockpile and prepare for increased understanding needed to support future options



***Computer Science and Visualization***

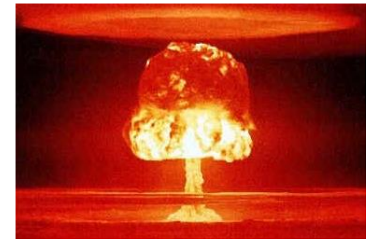
***Computing Centers***

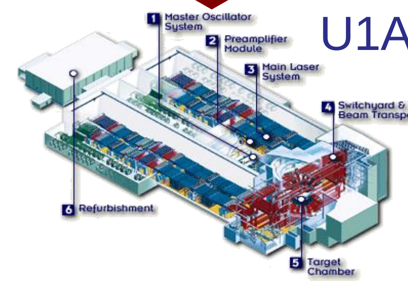
***Platforms***

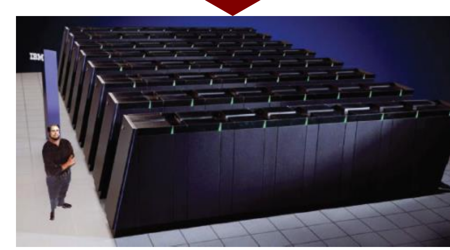

2

# Simulation is an essential element of a holistic stewardship strategy

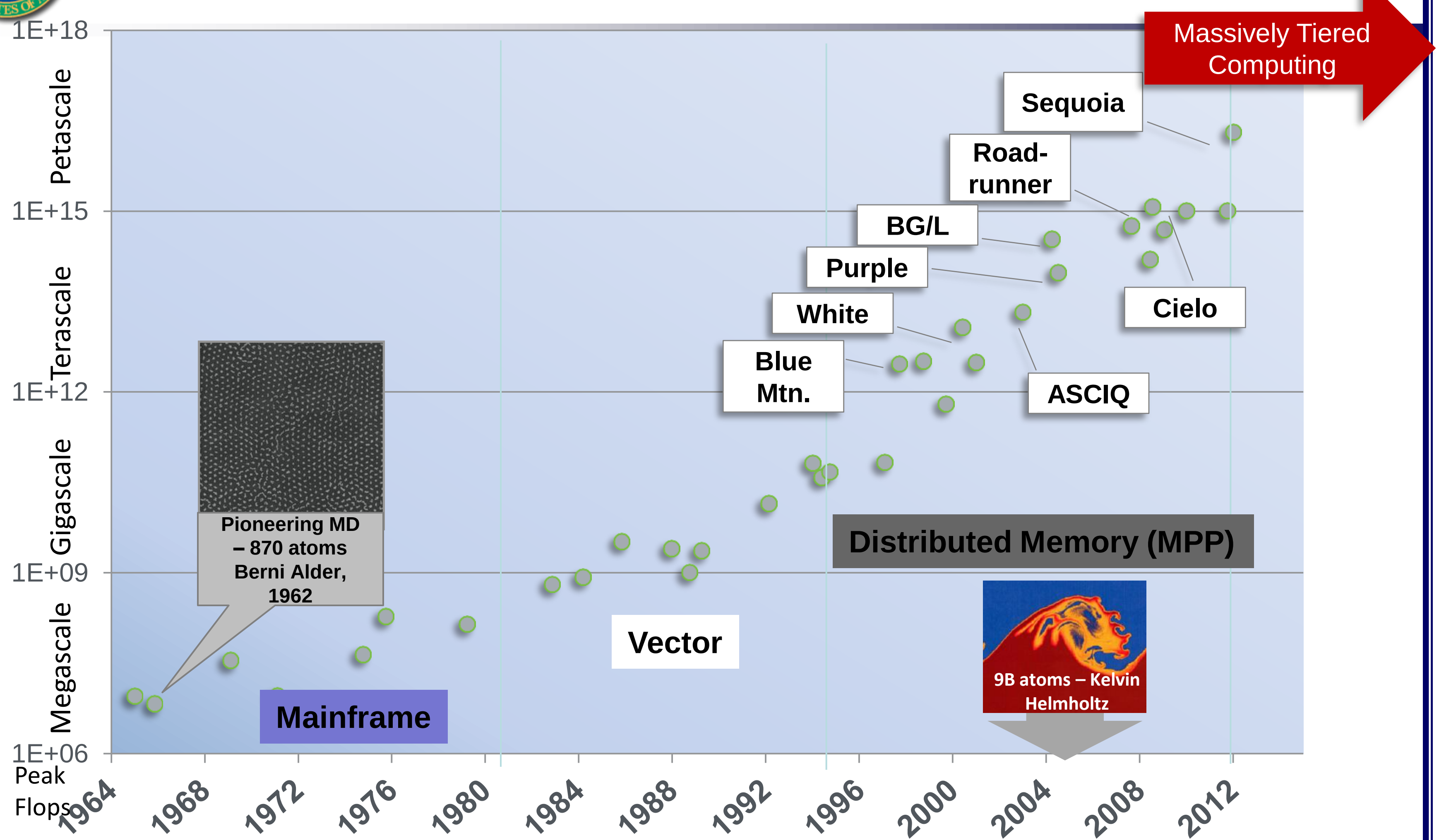
- Stockpile Stewardship assessments are based on three things
  - Simulation via the weapon codes
  - Surveillance and other supporting data
  - Designer judgment
- Simulation is the integrating element of Stockpile Stewardship
  - Combines experiment and theory to produce actionable predictions
  - Is the only credible substitute for nuclear testing in Nevada
  - Ideally, should reproduce the UGT test base without calibration
- Significant challenges lay ahead
  - Require large computations to address “details” that can be critical
  - Code performance is degrading due to industry technology changes
  - Need to adapt to changes – current capability must be maintained.





# HPC architectures drive programming models



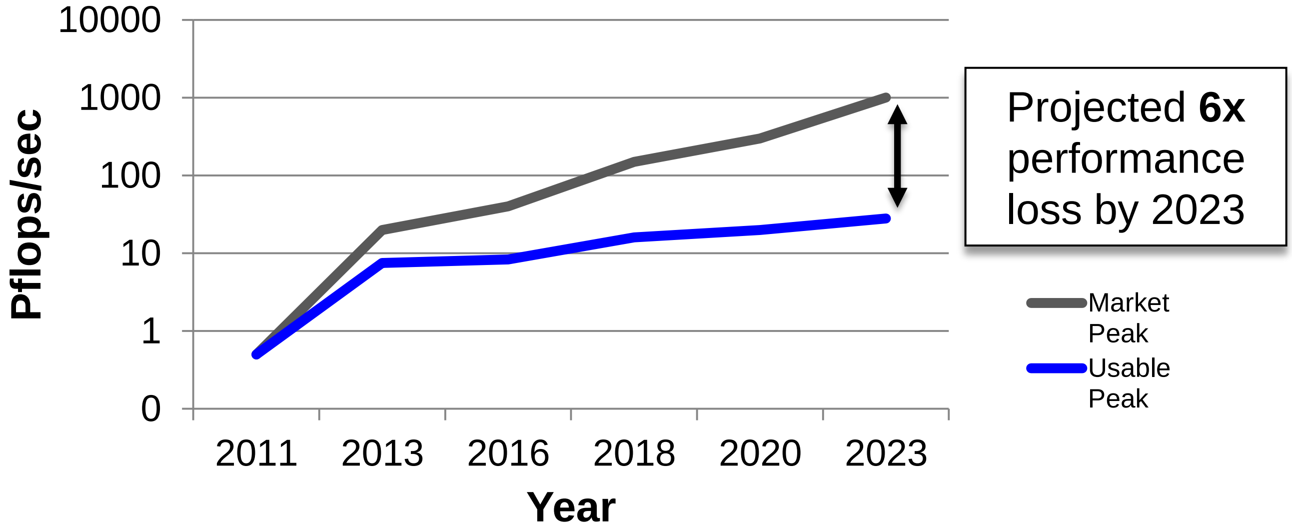

**Architectural stability has made possible remarkable advances in science. But, programming model transitions are tough…and we are approaching one now….**

# Time to solution is increasing on "faster" computers

- Changing from FLOPS-dominated to data-movement-dominated paradigm
- Problems tolerated in past must be solved
  - Processor to memory bandwidth
  - Resiliency
- Power consumption will limit the size of computer that can be built and economically operated
- New programming models and methods needed to gain promised performance

Supercomputing industry is undergoing a period of radical change: ASC's support to the stockpile *will* degrade unless aggressively addressed.

# Disruptive new technology is causing loss of stockpile code performance



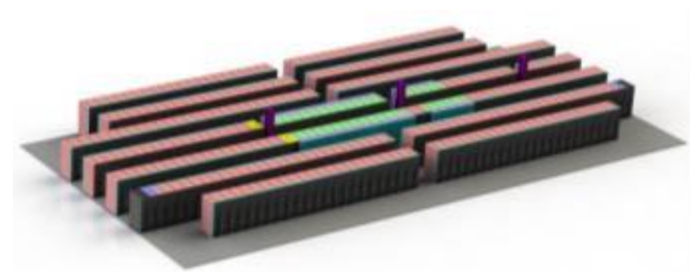

- Advanced Technology Development and Mitigation (ATDM) sub-program was created to address the highest-priority issues caused by new computing hardware
- These unavoidable issues are a subset of those on the path to exascale (they have to be tackled regardless of whether exascale computing is pursued or not)
- Development and mitigation efforts underway:
  - *Developing new software layers to help mitigate the impact of disruptive hardware changes*
  - *Creating new code teams to take fundamentally different approaches to stockpile code infrastructure and data layout than those taken for legacy codes*

# Advanced Technology System 1 (ATS 1)
# Los Alamos National Laboratory - Trinity

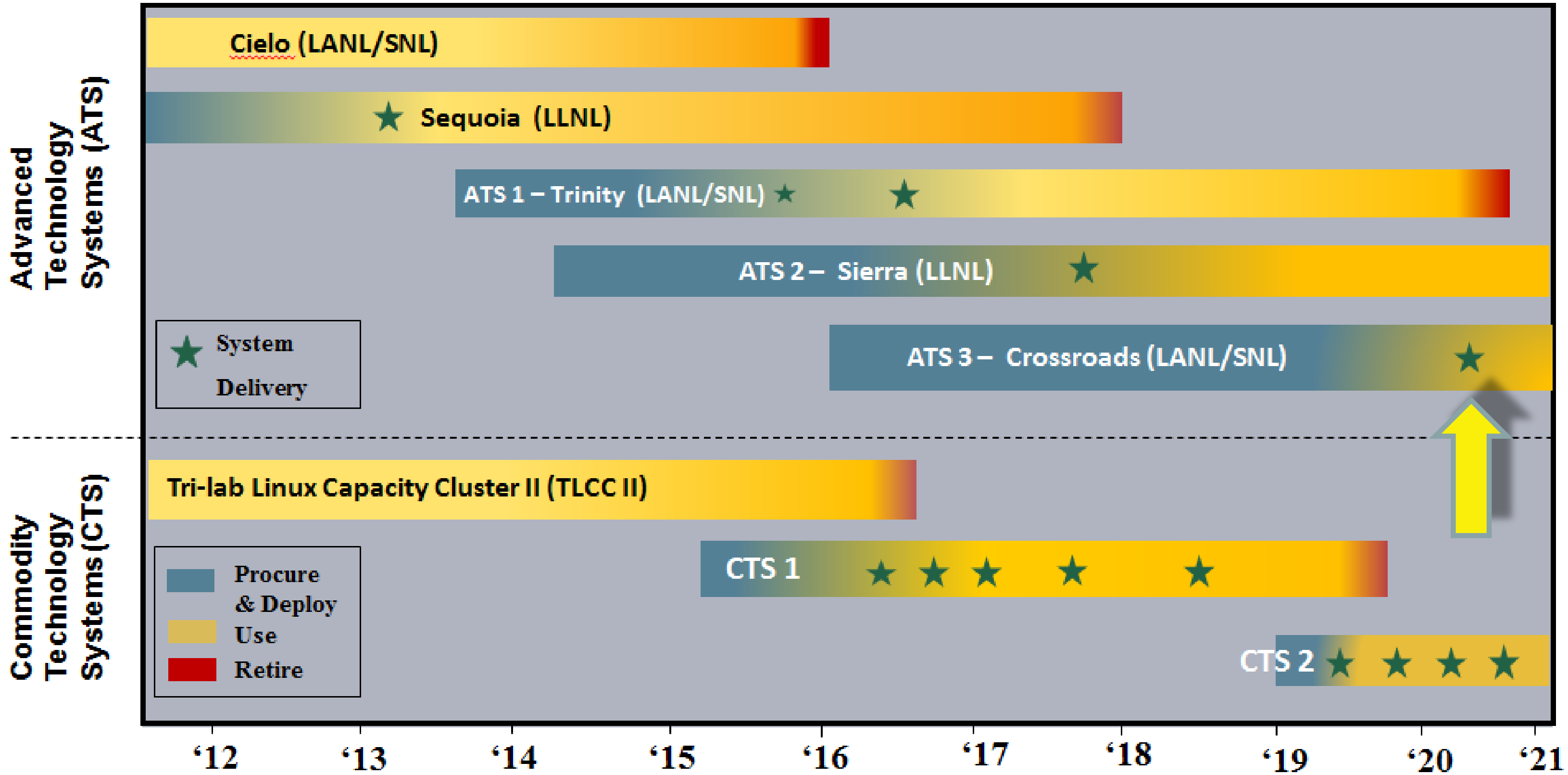
- Project Drivers:
  - Trinity is designed to support the largest, most demanding ASC applications
  - Increases in geometric and physics fidelities while satisfying analysts' time-to-solution expectations
  - Fosters a competitive environment and influence next generation architectures in the HPC industry
- Final configuration of Trinity: 42.2 PetaFLOPS; 2.11 Peta-byptes (PB) memory
- Based on mature Cray XC30 architecture but introducing <u>new architectural features</u>
  - Single system with both Intel Haswell (FY15) and Knights Landing processors (FY16)
  - Burst Buffer storage nodes
  - Advanced power management system software enhancements
- System deliveries for Phase 1 (Haswell partition) occurred in July 2015

# Advanced Technology System 2 (ATS 2)
# Lawrence Livermore National Laboratory - Sierra

- Two broad simulation classes constitute Sierra's workload
  - Assess the performance of integrated nuclear weapon systems
  - Perform weapon's science and engineering calculations
- Final configuration of Sierra: 150 PetaFLOPS; 2.7 PB memory
- Based on IBM Power processor with multiple NVIDIA Volta graphics processing units (GPUs) per node
  - 800 GB Solid state disk on each node
  - > 512 GB memory on each node
- Maximum power consumption of system and peripherals ≤ 20MW
- Architectural Diversity
- Delivery in 2017 with acceptance in 2018

# ATS 3 in 2020, and Beyond…

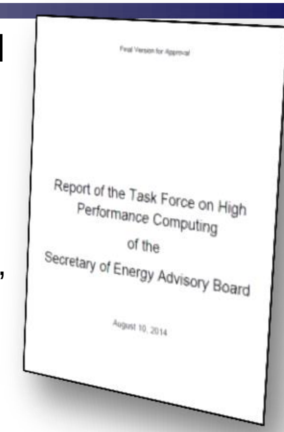



- Commodity Technology System 1 (CTS 1) deliveries to the tri-labs to occur Q2 FY16
  - Built upon scalable units of >100 TeraFLOPS each; with any single system aggregate no greater than 8 PetaFLOPS
- Crossroads (ATS 3) to be delieverd in 2020 at Los Alamos National Laboratory

**ATS 4, the first exascale machine, will follow at LLNL**

# Investments in Exascale and the "Beyond Next" Generation of HPC

Secretary of Energy Advisory Board (SEAB) Task Force reviewed the mission and national capabilities related to HPC in August 2014:


Final Version for Approval

Report of the Task Force on High Performance Computing of the Secretary of Energy Advisory Board

August 10, 2014

- **Investable needs exist for an exascale machine**:
  - NNSA mission
  - Industrial applications (e.g., oil and gas exploration, aerospace engineering, pharmaceuticals, protein structure)
  - Basic science (simulation of materials in extreme environments, combustion turbulence, photovoltaic materials, advanced reactors, climate science)
- **It is timely to invest in science, technology and human investments for "Beyond Next."**
  - With greater unreliably of integrated circuits at higher voltages/reduced transistor dimensions, current complementary metal oxide semiconductor (CMOS) technology likely provides **one last "generation" of conventional architecture**
    - Carbon nanotube transistors as a path forward: Simulations indicate these outperform scaled silicon transistors 3-5x in power/performance tradeoffs; warrants a strong government funded project to develop a carbon nanotube based post-Si CMOS microprocessor technology.
  - Longer-term technologies not yet mature enough for "next leading edge" capability at DOE, but **important**:
    - Cognitive computing (e.g. IBM's "Watson")
      - Deeper analysis of textual data with a goal of creating important new applications going beyond search and retrieval.
      - Neural network architectures: mathematical machine learning techniques and **new architectures** to process data (e.g. "neuromorphic" computation - computational theory of human cognition)
    - Quantum computing: replaces conventional bit with the "qubit" – tapping into quantum mechanics to speed computation.
- A system with 100 to 1,000x more parallelism and novel architectures requires a suite of **new software development and execution support tools**
  - Programming languages, new paradigms for communication, and performance analysis tools.

# Why does DOE invest in CSGF?

- Help ensure an adequate supply of **scientists and engineers** appropriately trained to meet national workforce needs, including those of the DOE, **in computational sciences**.
- Make national DOE laboratories available for practical work experiences for fellows ensuring **cross-disciplinary experience** in highly productive work teams.
- Strengthen collaborative ties between the national **academic** community and DOE **laboratories** so that the multidisciplinary nature of the fellowship builds the **national community of scientists**.
- Raise the visibility of careers in the computational sciences and to **encourage talented students** to pursue such careers, thus building the **next generation of leaders in computational science**.

# Conclusion

- **We are developing high confidence predictive capabilities**
  - Training the next generation scientists and engineers is more important than ever.
  - NNSA laboratories provide world-class scientific tools and multidisciplinary resources
  - Problems to tackle are urgent, challenging, and important.

- **HPC-enabled innovation is critical to the nation's security and economic competitiveness**
  - **Given the 20 year history of CSGF, you are at the bleeding edge of Computational Science at extreme scales.**
  - **You are the leaders in a race we can't afford to lose.**