The Continuing NNSA Commitment to State of the Art Modeling and Computation

Petascale to Exascale Workshop
San Francisco, CA

Presented by:
Dr. Allan Hauer
Chief Scientist, Office of Stockpile Stewardship

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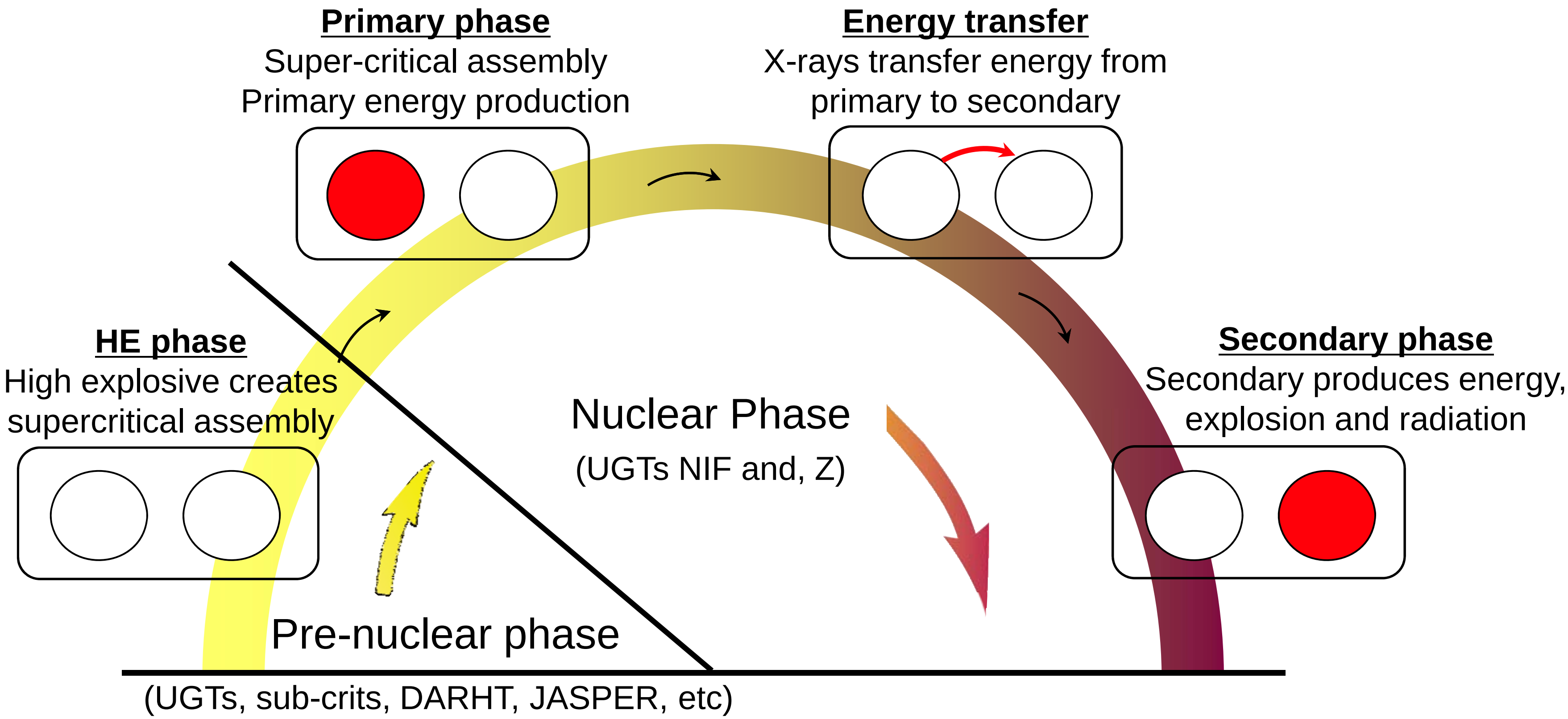
NNSA has a continuing need for advanced computation

- **Aging of the nuclear stockpile presents growing challenges**
- **NNSA sponsored computational research has produced outstanding accomplishments.**
- **There are specific National Security requirements for extension of computational capability to the exascale regime.**
- **NNSA will maintain a continuing commitment to state of the art modeling and computation.**

Nuclear weapons span an enormous range of physical parameters –from condensed matter to HED to plasma conditions

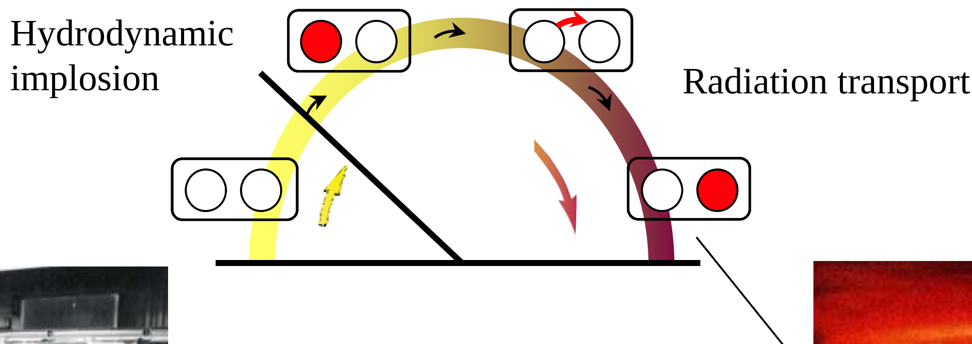
Computational and experimental advances must deal with a huge span of physical states

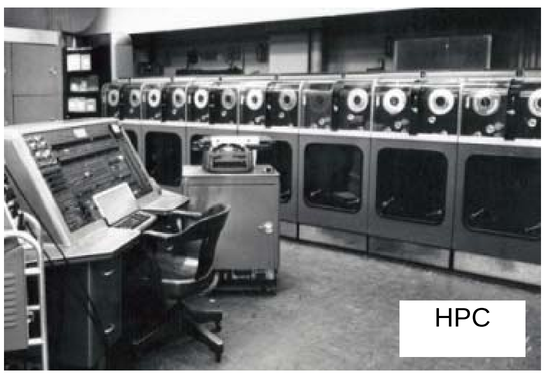


Weapons operation proceeds *through the conditions of planetary, to stellar interiors*

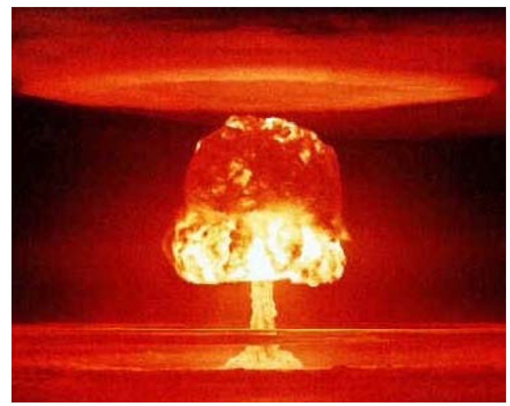
In the nuclear test era, incomplete physical models were benchmarked to integrated tests

In the nuclear test era incomplete physical models were calibrated to test results





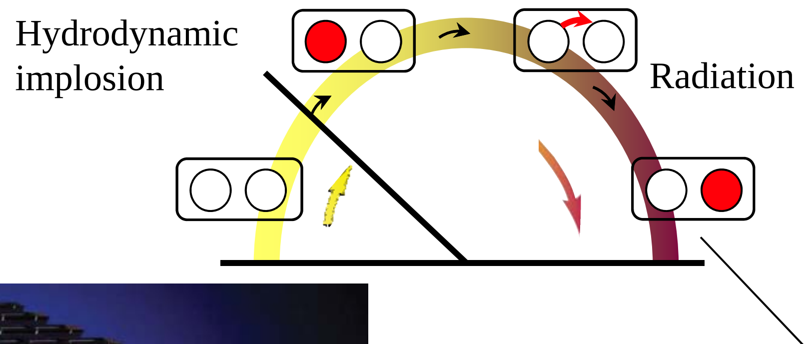
Codes with much empiricism

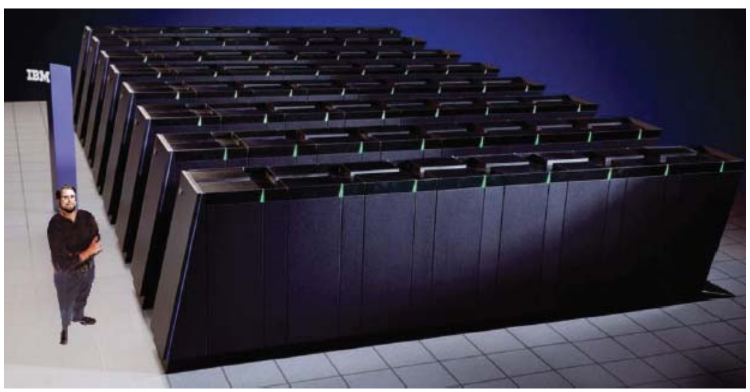


This methodology lacked the generality needed in today's environment

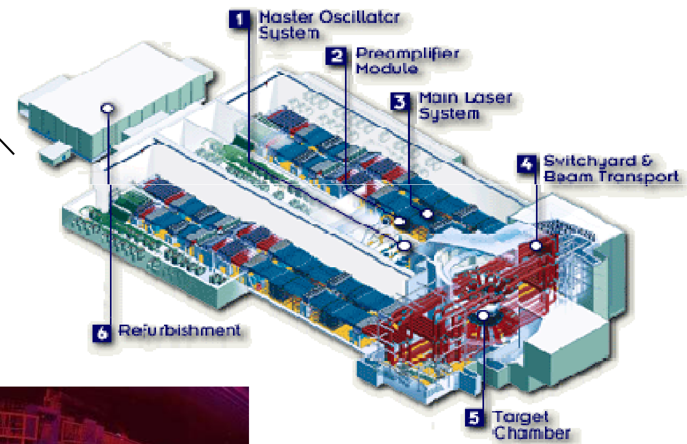
Without nuclear test, stewardship must rely on advanced simulation and sophisticated new experiments

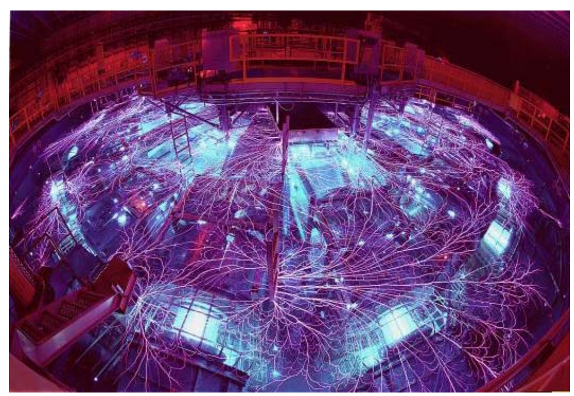
Without nuclear test data, much more complete modeling validated by quantitative experiments is required





National Ignition Facility





Z Machine

Some universal issues drive the need for more advanced, validated modeling

- Significant aging of the stockpile introduces many issues
  - **Transformation of key materials**
  - **Need to replace or refurbish important subsystems**
- Obsolescence of manufacturing or fabrication methods
- Insertion of modern safety and security features
- Analysis of potential sources of proliferation
  - **simulation assessment within Nuclear Counter-Terrorism & Global Security**
- With reduced stockpile size – a greater emphasis on uncertainty reduction
  - Uncertainty Quantification (UQ) will be a major thrust

An impressive array of computational and experimental tools are being developed to respond to these issues

- Advanced molecular dynamic methods have made important contributions in many key areas
  - Materials modeling – from atomistic to macroscopic behavior
  - Fluid and plasma modeling including turbulence
- 3D modeling across a wide range of material states
- Advanced Radiation hydrodynamic modeling
  - Turbulence modeling

Complete application of these methods to National Security problems of interest will require **considerable increase in computational power**

The Stockpile Stewardship Program demands a wide range of ASC simulation tools

- **Integrated Design and Analysis Codes (IDCs)**
- **Main workhorses of the designers and analysts**
  - **Typically very large, complex, multi-physics codes**
  - **Used for performance, safety, surety, weapon system response & survivability**

- **Material Property Codes (MPCs)**
  - **Develop the material property libraries essential for utilizing the IDCs**
    - **(e.g. opacity, equation of state, high explosive detonation)**
  - **Typically complex, multi-scale, state-of-the-art, single physics codes**
  - **Multi-scale overlap, from atomistic to continuum**

- **Specialist Codes**
  - **Enhance future IDC and MPC development by exploring physical phenomena, or numerical algorithms, and identifying the future paths forward**
    - **e.g. Linear solvers, Turbulence codes, UQ frameworks, Visualization,…**

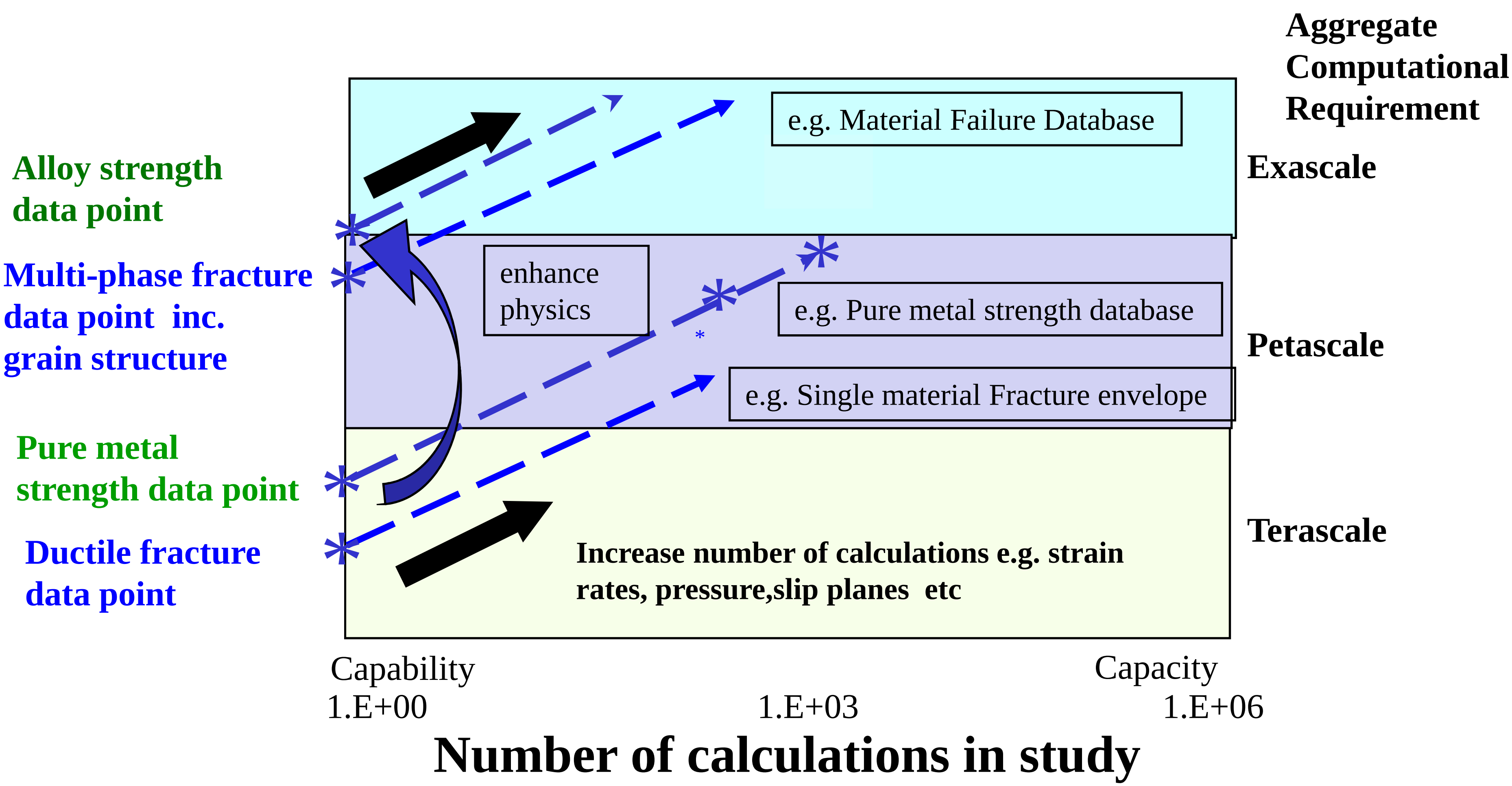
Current terascale and petascale computing has enabled the initial exploitation of these tools and established the scaling laws for future SSP requirements

Simulation capabilities have advanced significantly but significant advancement is required for our future mission

We can do …	We can't currently do …
• Simulate in 3D	• high resolution or complete problems in 3D
• Interpolate	• Extrapolate
• Simulations to support today's certification	• Predict when aging, damage, etc will happen and require action
• Assess some new options	• Assess other desired options
• Some broader national security	• Other broader national security

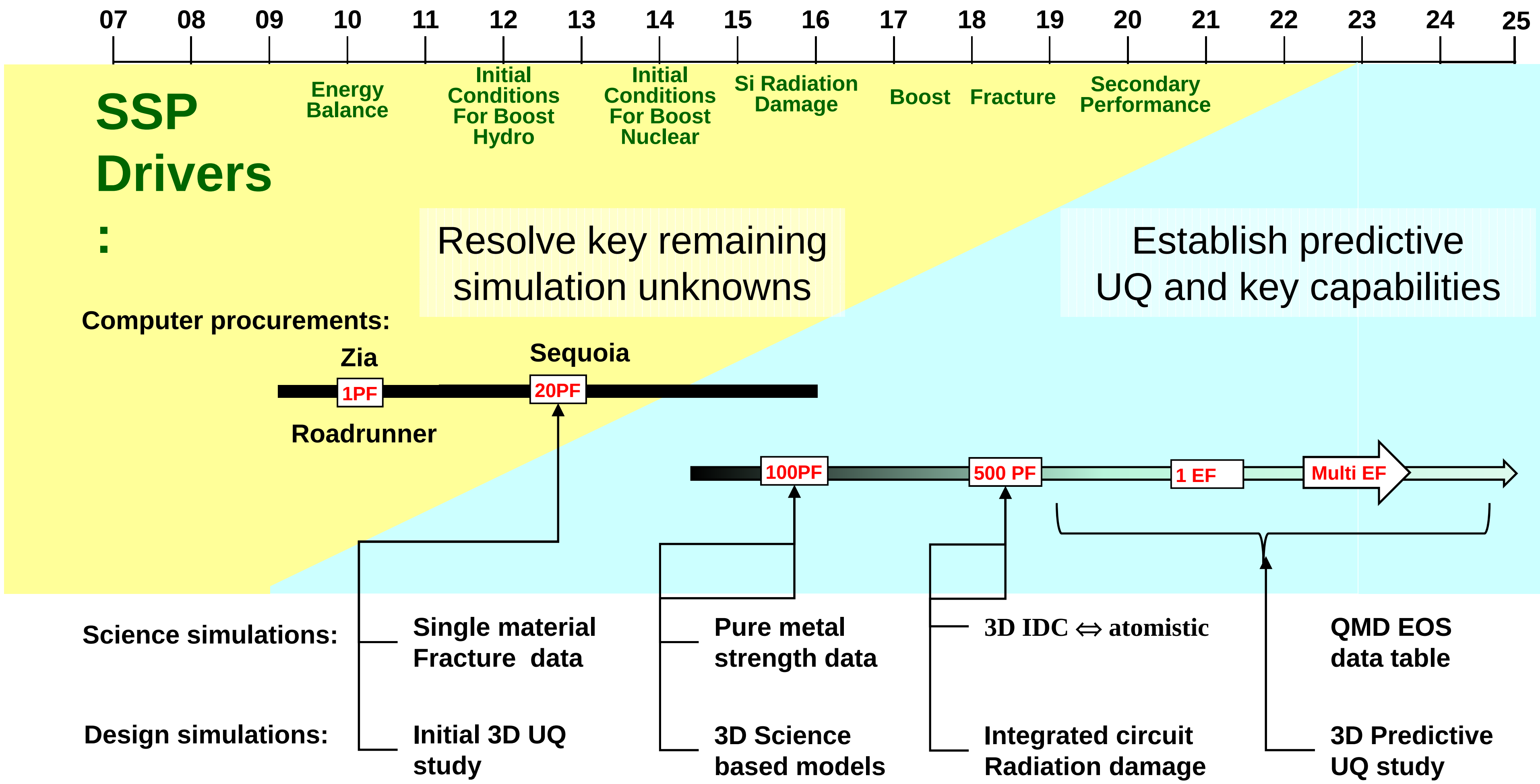
Unclassified

Modeling of key materials problems has been used as one key test of exascale requirements



Simulation of microstructure needed for multi-scale strength models development. Inclusion of more features pushes the calculations into the Exaflop regime

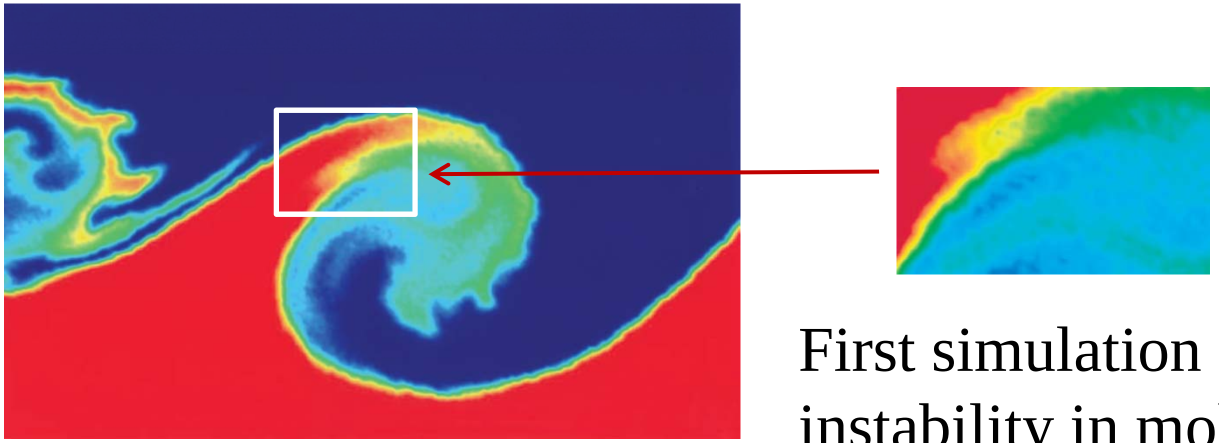
SSP requirements are driving advanced physical understanding, which will require Exascale to establish predictive 3D UQ



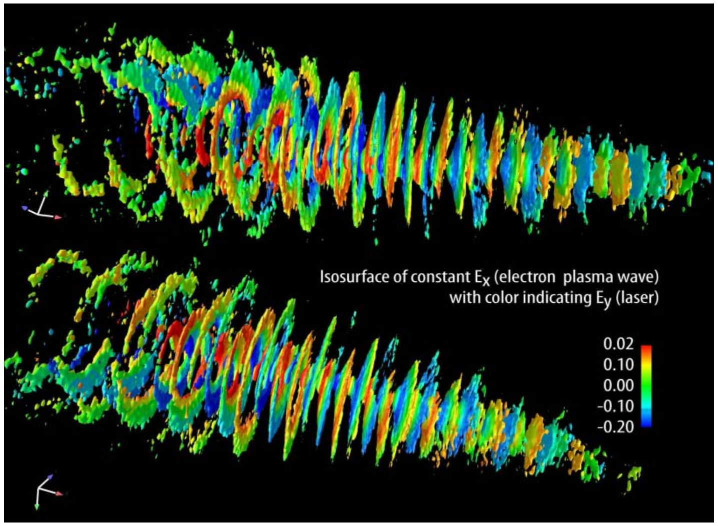
By 2022, ASC should provide a simulation capability for the SSP to support the Stockpile with confidence using QMU methodologies exploiting predictive UQ capabilities

NNSA sponsored simulations have received wide recognition

Gordon Bell Award winners



First simulation of Kelvin-Helmholtz instability in molten metals



VPIC simulation of high intensity Laser-matter interaction

ASC Academic Alliances continue to sponsor highly successful research

University of Michigan

Center for Radiative Shock Hydrodynamics (CRASH)
(PI: Paul Drake)

Problem: **To simulate the structure of radiative shocks produced in specific experiments on the Omega laser and to quantify the accuracy with which predictions of a given measured output from a particular experiment can be made.**

Science: **Radiation hydrodynamics, numerical methods for fluids, plasma, radiation transport, HED, radiation shock.**

Partner:

- **Texas A&M (UQ & rad transport).**

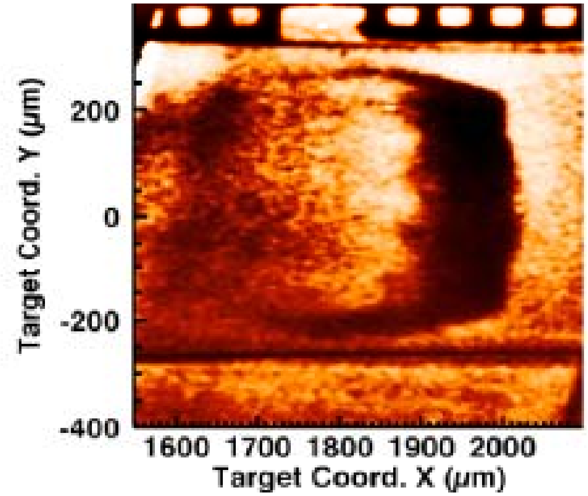


Fig. 7. Radiograph of a radiative shock in Xe gas.

ASC Academic Alliances continue to sponsor highly successful research

University of Texas at Austin

Center for Predictive Engineering and Computational Sciences (PECOS) (PI: Robert Moser)

Problem: **To simulate the multi-scale, multi-physics phenomena associated with vehicle re-entry into the atmosphere specifically, predict the ablation rate of the thermal protection system.**

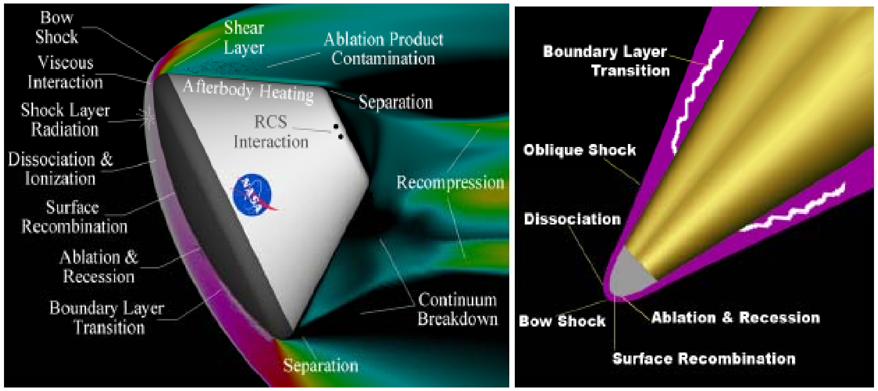


Figure 1: Illustration of dominant physical phenomena in both capsule and missile reentry

Science: **EOS and constitutive properties, fluid dynamics and turbulence, computational materials and chemistry, radiative transport and heating, advanced materials, molecular modeling, plasmas.**

Partner:

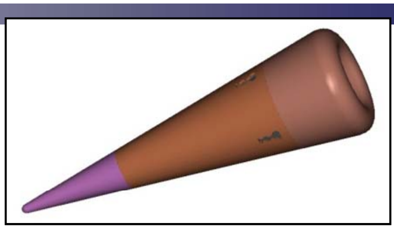
- **Texas A&M (radiation transport).**

The credibility of the country's national security capabilities will depend on continued leadership and dominance in simulation in the 21'st Century

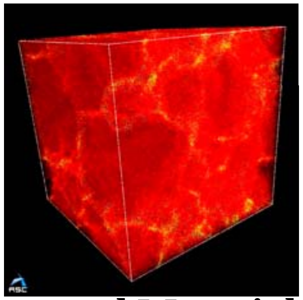
- **The sheer complexity of the exascale challenge is an opportunity for continued American leadership**
  - **Lead in determining future architectures and programming models,**

- **The START (and possibly CTBT) era will require certification without reliance on calibration**
  - **Response is a drive to a predictive capability with quantified uncertainties**

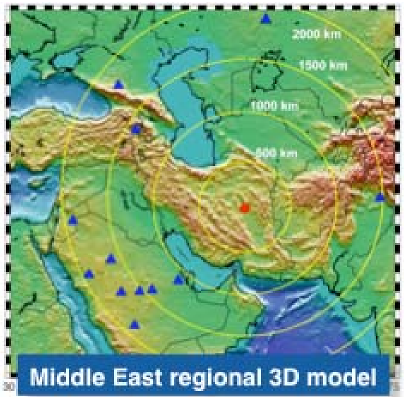
- **Broader application of exascale computing can provide tremendous advantages in Global Security**



Predictive Simulation of Physical Systems



Advanced Materials Models and Databases



Rapid differentiation between geologic or nuclear events

Conclusions

- NNSA will continue to support advanced modeling and high performance computation
- National Security based requirements for exascale computational capability are compelling
- NNSA will continue to support strong interaction with the broad scientific community in the development of high performance computing
  - It is recognized that careful consideration of application specific architecture choices will require careful consideration