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The FY05 ASC Level 1 Milestone Report: Requirements to Move to Petaflop Platform

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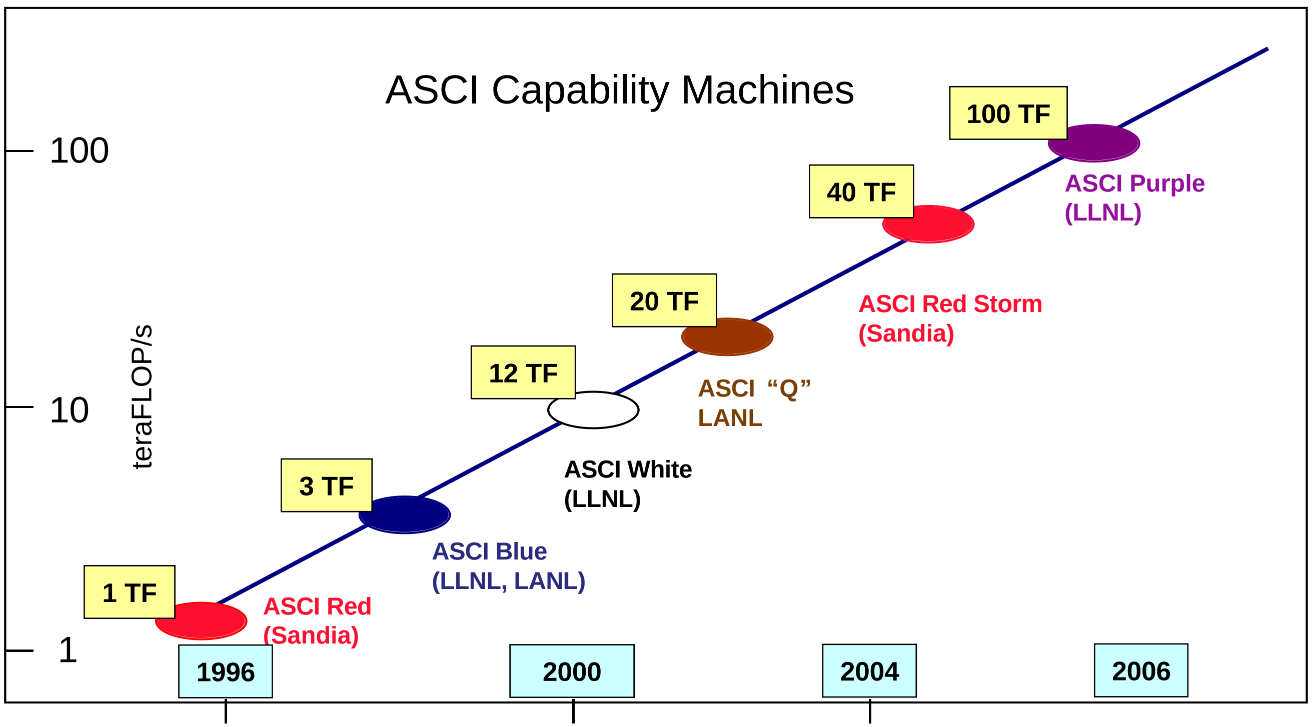
Document the requirements to move beyond a 100 TF ASC computing platform to a petaflop platform

- **Task of tri-lab team was to produce a report by December 31, 2004**
- **The focus of the milestone is on *capability* (not *capacity*)**
  - **Without sufficient capacity, capability will be sacrificed**
  - ***Capability***
    - **Maximum processing power possible that can be applied to a single job**
  - ***Capacity***
    - **The total processing power available from all machines capable of operating ASC codes**
- **We assumed the stockpile mission would not change drastically**

> ***"Within 10 years… 1 Petaflop will be needed to execute the most demanding jobs."***
>
> **– *Requirements for ASCI*, JASON, 2003**

Initial ASCI plans called for 100 Tflop "entry-level" platform

- Errors associated with numerical approximations mask physics issues when not converged
- With 100 TF, we can have adequate resolution to begin to study these physics issues without them being masked by numerical errors



Maintaining a robust, reliable, safe, and secure stockpile requires an operational 1-2 petaflop platform by 2010

Certifying a changing stockpile

- **Assuring robust, reliable performance without nuclear testing**
  - Requires high fidelity and increased “science”
  - A responsive infrastructure requires flexibility in weapons configurations/manufacturing

Responding to a changed world

- **Increased security threats place new demands on use control, security, safety, and survivability**
  - Enhanced surety through microsystems
  - Analysis of the facilities vulnerability
  - Sandia Pulse Reactor (SPR) replacement

Enabling and exploiting breakthroughs

- **Computing can enable breakthroughs in NNSA experimental facilities**
  - Z, NIF

NNSA’s leadership in the pursuit of 1 PF will ensure that SSP needs are met

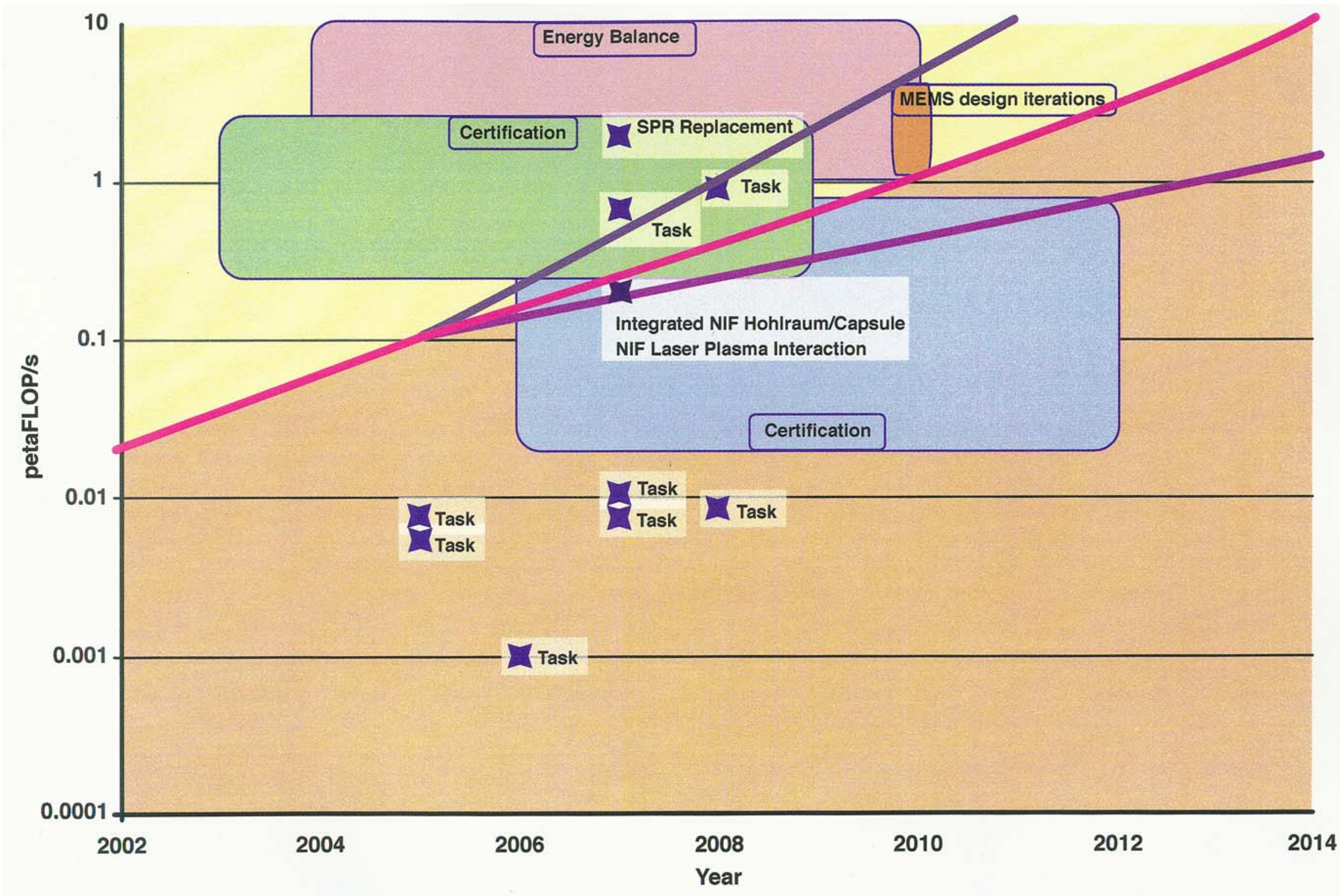
- The ASC investment strategy in platform development has enabled the spectacular advance in mission-driven simulations
- ASC’s leadership is based on sustained procurements and aggressive goals
- There is a risk of the industry developing platforms that will not meet our needs if ASC is not fully involved
  - Will they achieve 1 PF when NNSA needs it?
  - Will the architecture be amenable to SSP applications?

NNSA leadership needed to ensure that 1 PF is an effective 1 PF

Petaflop computing will have a comprehensive impact on stockpile stewardship

	Application	*Desired run time (days)*	*required*
Certifying a changing stockpile	Nuclear weapon physics simulation (3D)	14	0.214
	1-ns shocked high explosives chemical dynamics	30	1
	Nuclear weapon physics simulation (3D)	14	1.24
	Nuclear weapon physics simulation (3D)	14	1.47
	Nuclear weapon physics simulation (3D)	14	2.3
	DNS simulation of near-asymptotic regime of turbulence	30	3
	Model NGT design	7	3.7
	Nuclear weapon physics simulation (3D)	48	10.2
	LES simulation of far asymptotic regime of turbulence	365	10.7
	Classical MD simulation of Pu process	30	20
Responding to a changed world	MEMs design	1	1
	Replacing SPR	14	2.7
	Facility vulnerability and mitigation analysis	7	3.1
Enabling and exploiting breakthroughs	NIF laser-plasma interaction	30	0.360
	Integrated NIF hohlraum/capsule	1	0.750
	Breakeven Z target design (3D, 300 wire resolution)	7	1.3

Urgent stockpile and science deliverables drive the need for capability computing



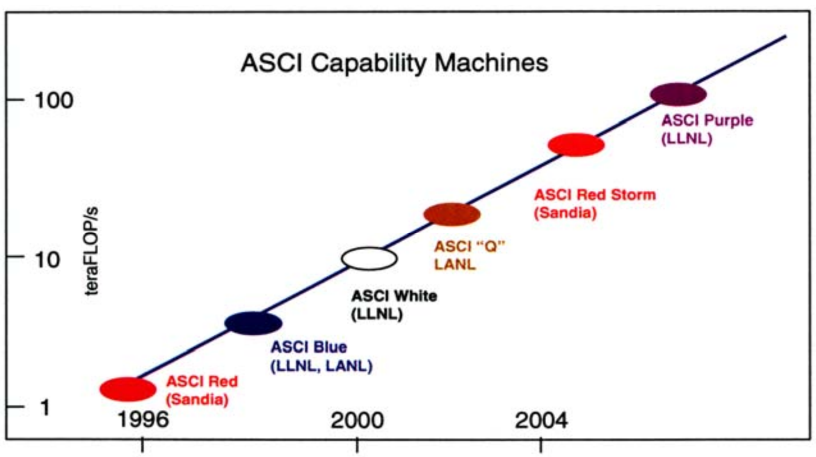
The ASCI Initiative has evolved into the ASC Program

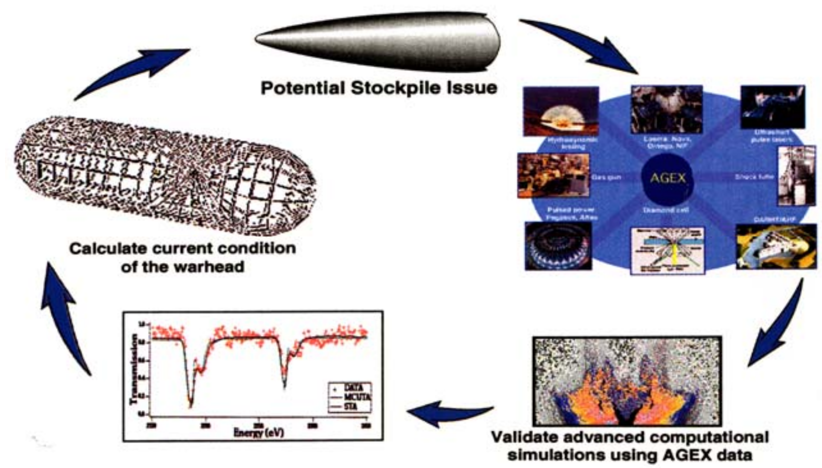
Goals for ~1996-2004
Accelerated Strategic Computing Initiative

- **Focus was on creating a new capability and demonstrating:**
  - **3D full-system simulation**
  - **Functional, scalable capability platforms**
  - **Uncertainties were substantial**

Goals for Future
Advanced Simulation and Computing

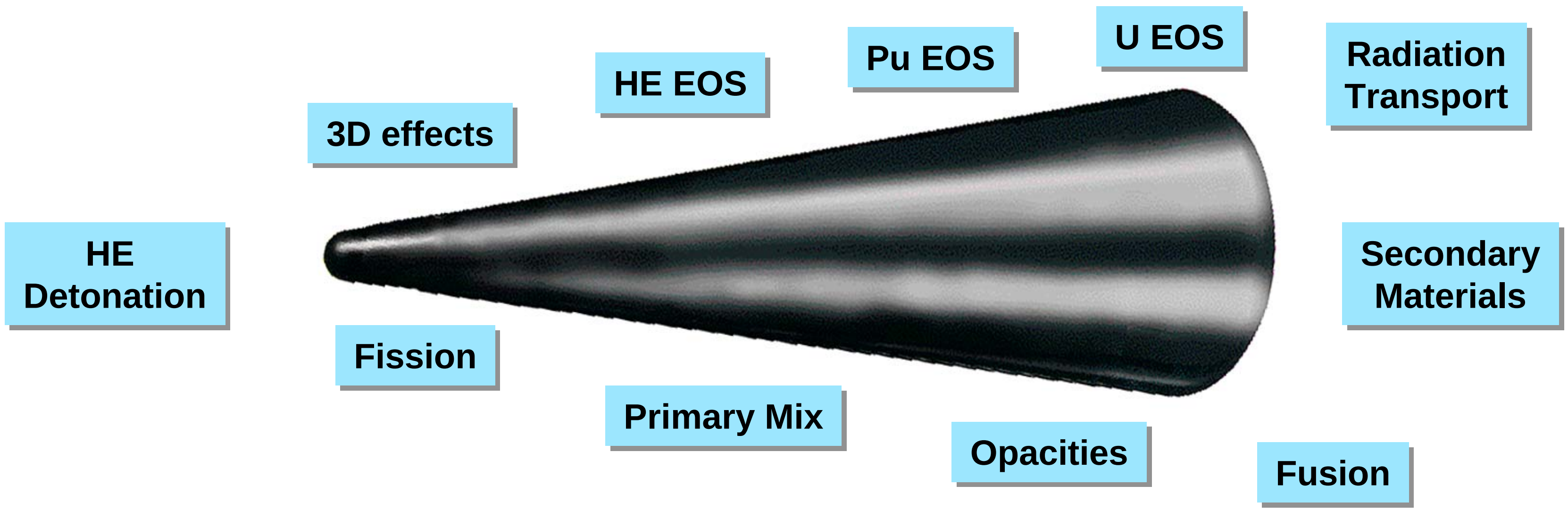
- **Focus today is on employing capabilities as an integral part of the program**
  - **Because of aging, codes must predict operation with increased confidence**
  - **Drives capability, capacity, and scientific computing**
  - **New 10-year ASC Strategy is aimed at increased predictive capability**





The Stockpile Stewardship challenge:
Maintain confidence in an aging stockpile as changes occur

Weapons simulation development effort is focused on known obstacles to predictive simulation



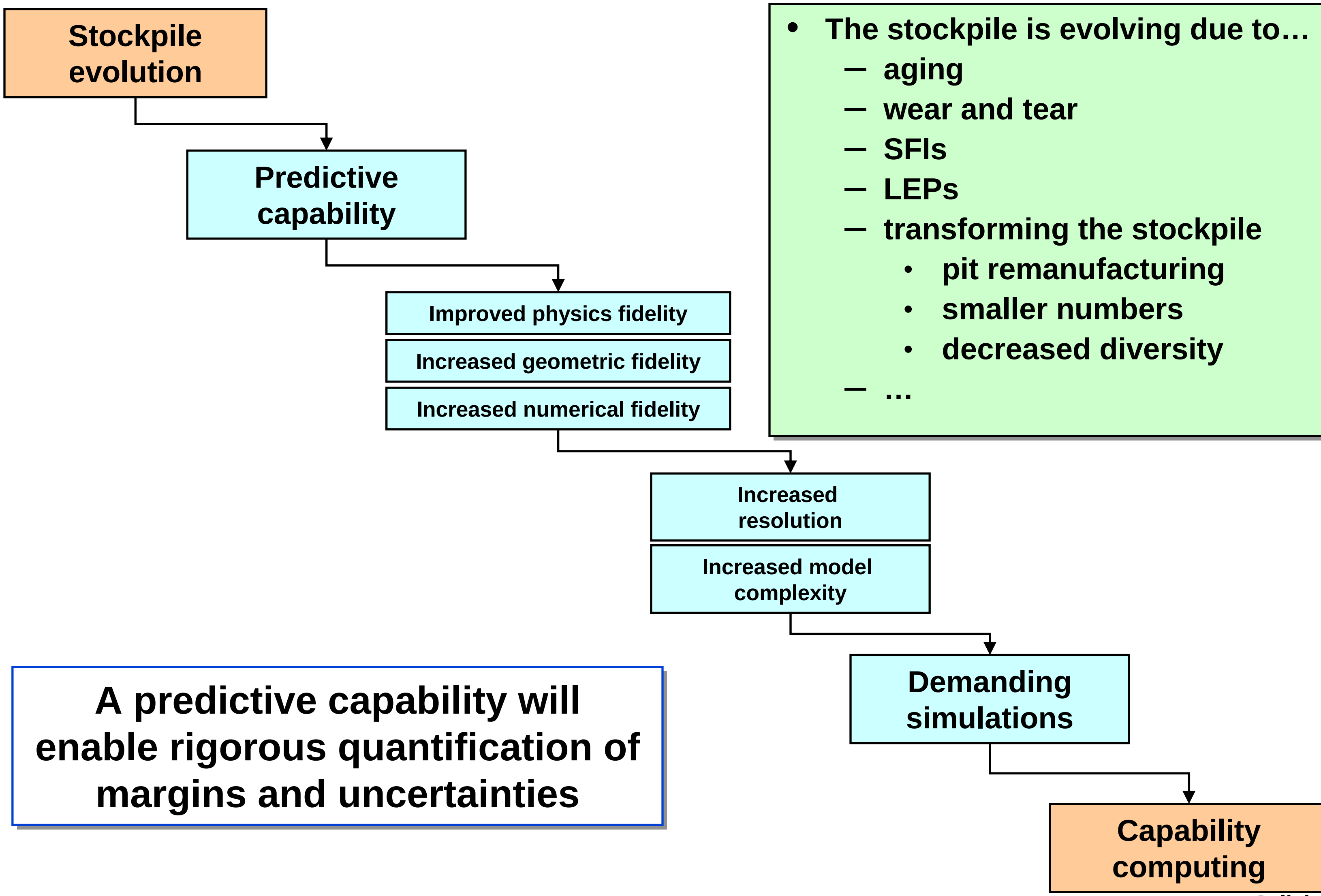
- We must eliminate/reduce known errors due to
  - Use of 1D or 2D approximations for 3D objects
  - Insufficient spatial resolution
  - Physical or numerical approximations
  - Inferior physical databases

Two types of simulations are necessary: *science* simulations and *design* simulations

- ***Design*** **simulation**
  - **Directly model the behavior of weapons systems and components**
- ***Science*** **simulation**
  - **Model the basic behavior of material at conditions present in nuclear device but not achievable in the laboratory**

Both science and design drive the need for computation capability

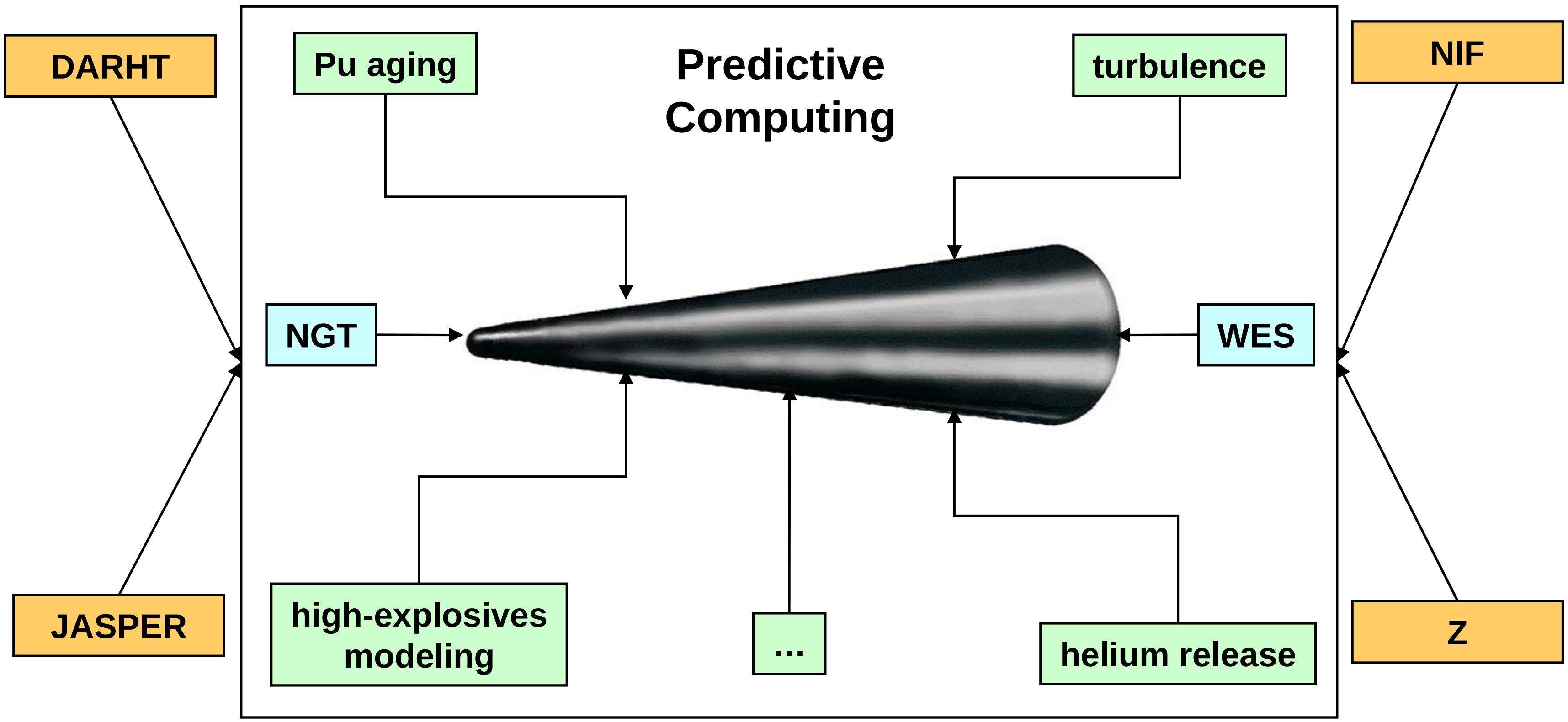
Stockpile evolution drives the need for capability computing beyond 100 TF



- The stockpile is evolving due to…
  - aging
  - wear and tear
  - SFIs
  - LEPs
  - transforming the stockpile
    - pit remanufacturing
    - smaller numbers
    - decreased diversity
  - …

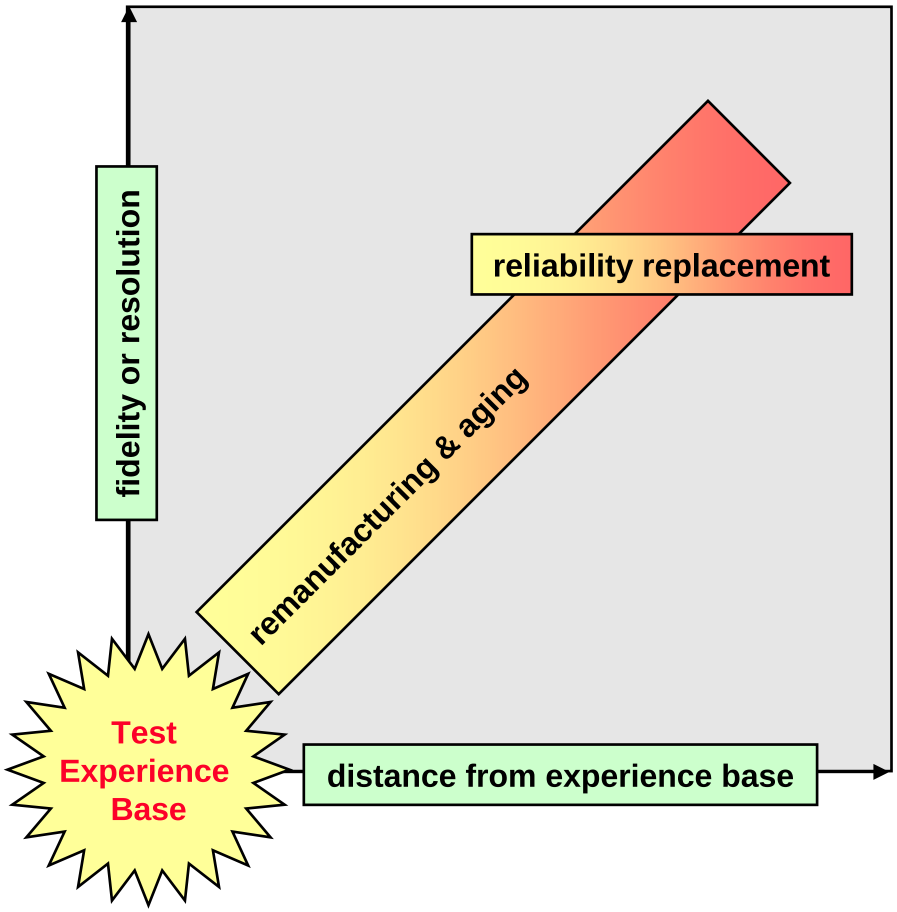
A predictive capability will enable rigorous quantification of margins and uncertainties

Predictive capability is composed of many complex interacting components



Each simulation component (*design* and *science*) has fidelity requirements

Petaflop computing enables transformation to an achievable and affordable enterprise



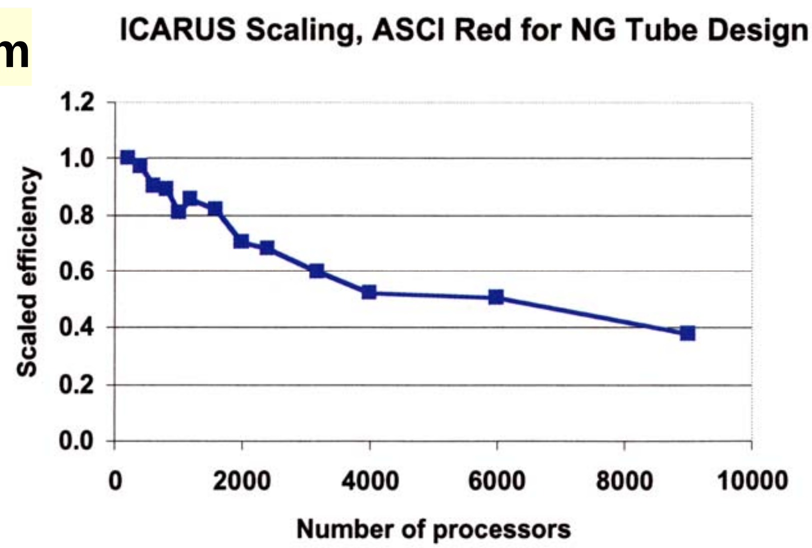
- Characteristics of the transformed enterprise:
  - Enhances surety and limits vulnerability
  - Simplifies manufacturing
  - Is safe, affordable and responsive
  - Does not require nuclear testing

Future *design* simulations require increased capability

- Simulations need improved resolution
  - More zones
- Simulations need "better physics"
  - Sub-grid models to capture improved *science*
    - Also necessitates increased resolution

Virtual design of neutron generator tubes requires a predictive computing capability

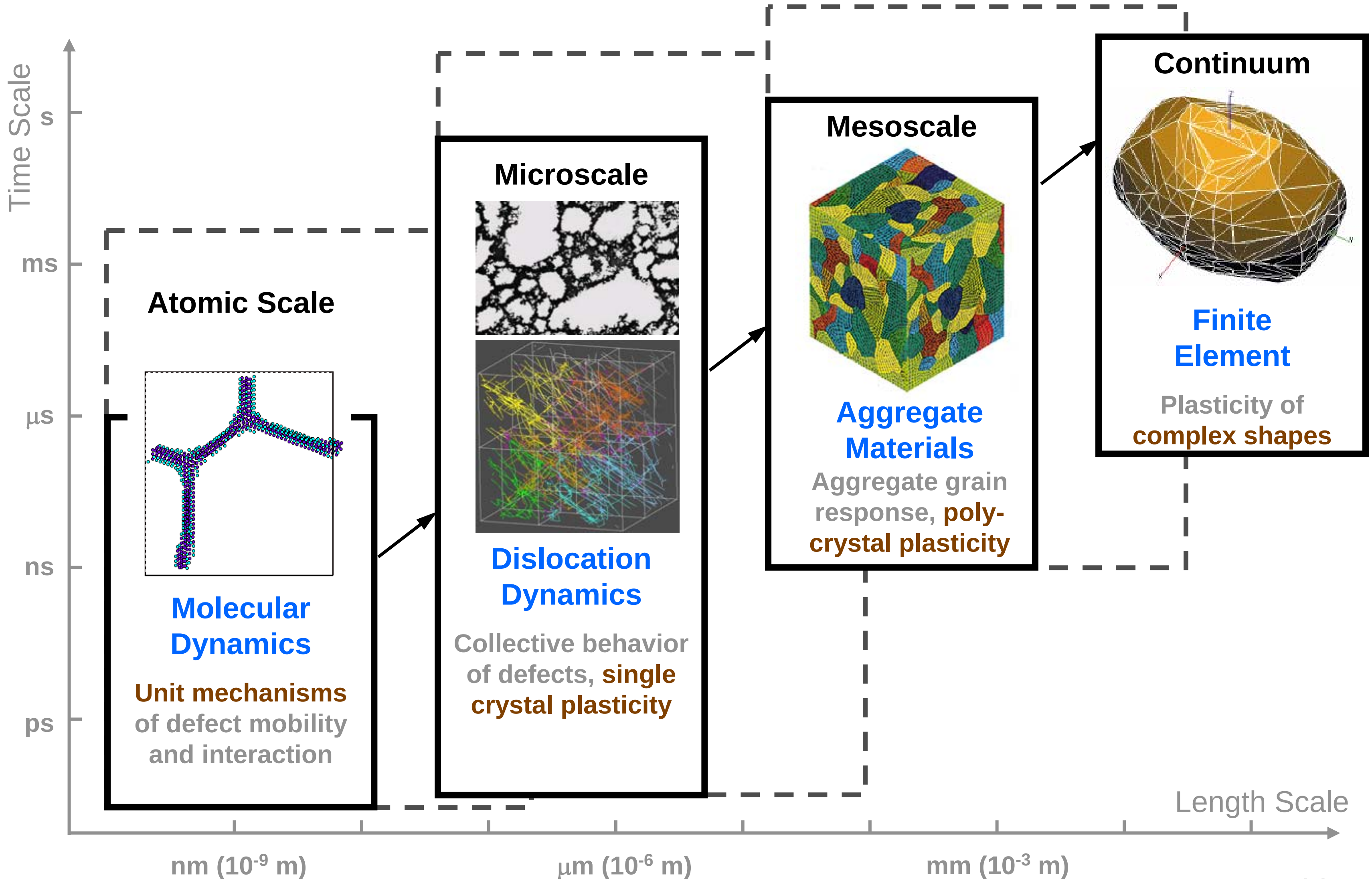
- Virtual design requires
  - Boltzmann solution over 3D geometry
  - Improved materials properties
  - Better surface chemistry
  - High voltage breakdown physics
  - Simulation of processing parameters
- Estimated capability for virtual design
  - 19 days/run on 1 PF scalable platform
  - 10 to 100 runs per design evaluation



To adequately capture physics fidelity, demanding *science* simulations are needed

- Turbulence
  - Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES) feed sub-grid models in *design* simulation
- Effect of aging on plutonium
  - Large molecular dynamic simulations
  - Quantum Monte Carlo
  - Path-integral Monte Carlo
- Helium release from metal parts in weapons components
  - Large molecular dynamic simulations of bubble growth
- High-explosives modeling
  - Molecular-scale and grain-scale simulations feed sub-grid models in *design* simulation

Multi-scale modeling allows sophisticated models to be built in a "boot-strap" approach



Predictive capability required for understanding helium release in metals

- Molecular-dynamics simulations needed to reveal mechanism of helium aggregation and migration
  - Identify lattice defects that promote He retention
  - Identify processing steps controlling lattice characteristics
- Petascale computing needed to simulation surface effects, grain size, etc., at the size and time scale of the physical mechanisms

	Current capability	*Required capability*
Atoms in simulation	345 x 10^3	10^{10}
Sustained flops	10^{15}	3 x 10^{20}
Computing platform	4 TF	1 PF
Run time (days)	28	3.5

Each materials issue needs 10s of runs; run time of 2-4 days required

High-explosive modeling is crucial to predicting nuclear weapon performance

- **Path to predicting HE performance**
  - **First-principles and semi-empirical molecular dynamics**
    - **Dynamics of chemistry of shocked HE**
    - **Rate constants and species concentrations**
  - **Grain-scale micro-structure simulations**
    - **10-1000 zones per individual grain**
    - **Detailed simulation of single zone in *design* calculation**
  - **Sub-grid models in *design* simulation demands finer resolution, smaller time-steps, and increased memory**

	Molecular-Scale		*Grain-Scale*	
	Current capability	*Required capability*	*Current capability*	*Required capability*
	200 atoms; 50 ps	1000 atoms; 1 ns	10^7 zones	10^9 zones
Platform	11 TF	1 PF	13 TF	300 TF
Run-time (days)	365	30	21	21

Accurate properties of plutonium, both new and aged, are needed to predict weapon performance

		Requirement (PF-days)		Requirement for 30-day run-time (PF)	
Material Process	*Methodology*	*Minimum capability*	*Required capability*	*Minimum capability*	*Required capability*
Process 1	QMD	1.5	3	0.05	0.1
Process 2	QMD, CMD	60	90	2	3
Process 3	CMD, DD, DD-FE	60	210	2	7
Process 4	CMD	600	600	20	20
Process 5	CMD, AS	450	450	15	15

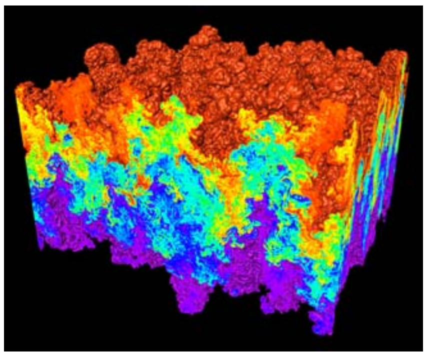
Requirements are shown here for a single point in phase space

QMD	Quantum Molecular Dynamics
CMD	Classical Molecular Dynamics
DD	Dislocation Dynamics
DD-FE	DD-Finite Element Hybrid
AS	Adaptive Sampling CMD-FE

Turbulence must be investigated through multi-scale "bootstrap" technique

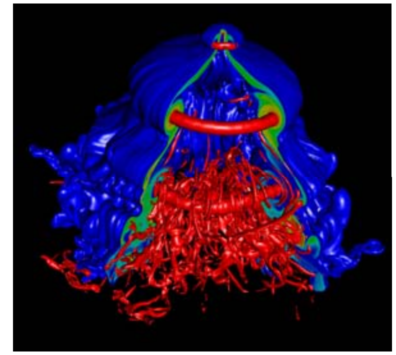
Direct Numerical Simulation (DNS)

sub-grid model



Large Eddy Simulation (LES)

sub-grid model

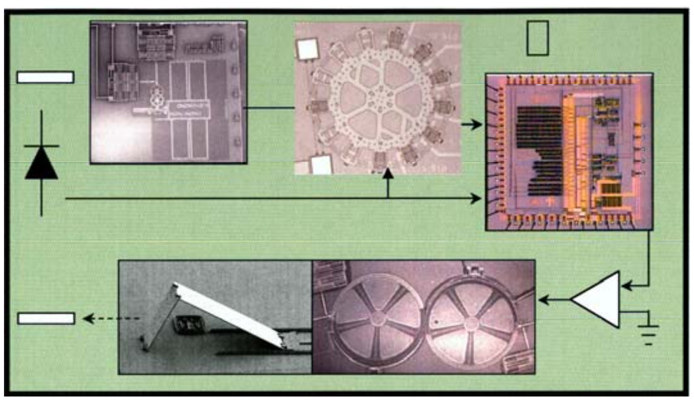


Design Simulation

		Computational Requirements		*Capability required for 30-day turn-around*	
Phase	*Reynolds Number*	*DNS*	*LES*	*DNS*	*LES*
Mixing transition	40,000	6 PF-days	0.25 PF-days	200 TF	8.33 TF
Near asymptotic regime (acceptable)	100,000	90.2 PF-days	3.9 PF-days	3 PF	130 TF
Near asymptotic regime (desirable)	200,000	721 PF-days	31 PF-days	-	1 PF

Increased threats have placed new demands on surety, safety, and survivability

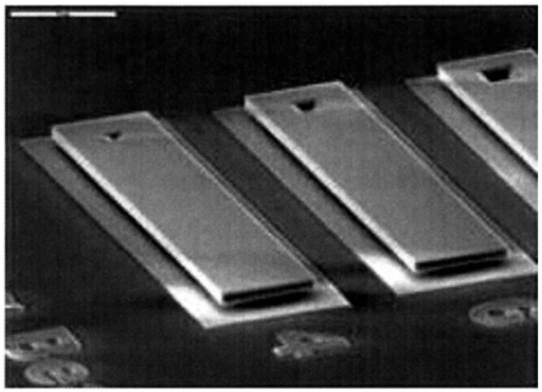
- Adapting to a world changed by terrorism
  - Enhanced surety through advanced microsystems (e.g., MEMS/nano devices)
  - Assuring facilities/weapon survivability and functionality after attack, and limiting collateral damage
  - Replacing high risk/cost facilities (e.g. SPR)



Trajectory safety subsystem on a chip

9/11 impact at the Pentagon

MEMS gas dynamics design requires petascale computing

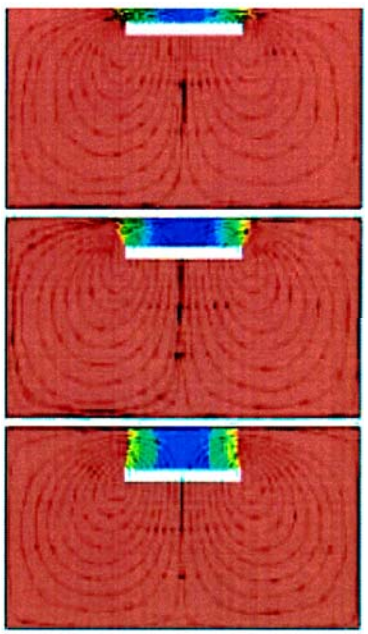


"Diving boards for bacteria"

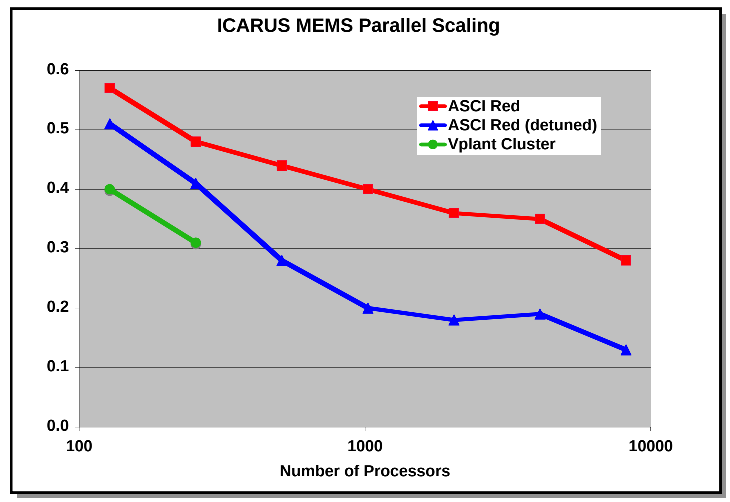
- Polycrystalline silicon
- Length: 100 microns
- Width: 20 microns
- Thickness: 2 microns
- Gap: 2-6 microns
- Frequency: 10-100 kHz

Critical challenges

- Non-continuum mechanics
- Boltzmann equation needed
- Transients relevant
- Margins important
- Need to understand space
- Full testing impractical



Characteristic	*Current capability*	*Required capability*
Geometry	2D	3D
Boundary treatment	Static	Moving
Gas flow	Steady-state	Transient
Oscillation	Sample	Full
Platform	1 TF	1 PF
Run-time (days)	3	1



1 PF needed for 1-day turnaround

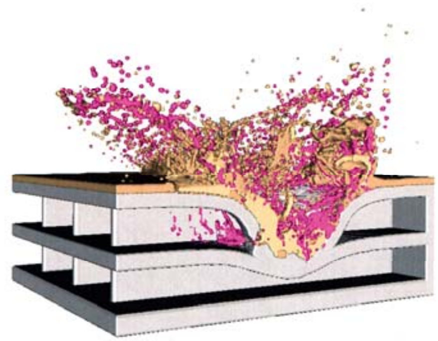
Unique aspects at MEMS scales require petascale computing

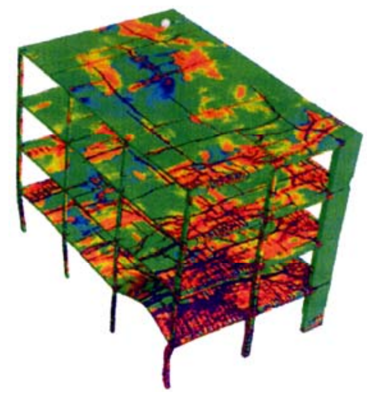
- **Material properties are not extensive**
  - differ in normal and transverse directions, and layer by layer
- **Transport properties are geometry dependent**
- **Must model at the grain level**
- **Thermal conductivity simulation, for example, requires**
  - simulation of photon scattering off boundaries
  - large spatial domain due to high-sound speed
- **Computational capability will limit both the design sophistication and the deployment rate of microsystems**

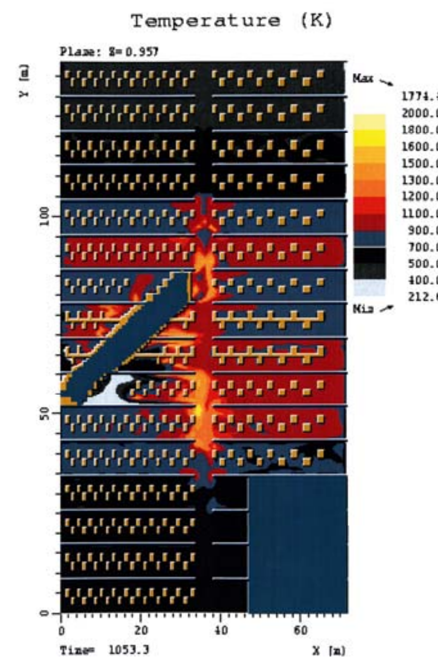
Plane atoms	*Normal atoms*	*Ops/ time-step*	*Time-steps*	*Operations*	*Platform*	*Run-time (hours)*
30 x 30	10^3	4.5×10^9	10^5	4.5×10^{14}	100 TF	13
100 x 100	10^5	5.0×10^9	10^6	5.0×10^{18}	1 PF	14

Each design cycle requires 25-75 simulations

Petascale computing will be required to perform mitigation studies on critical US facilities





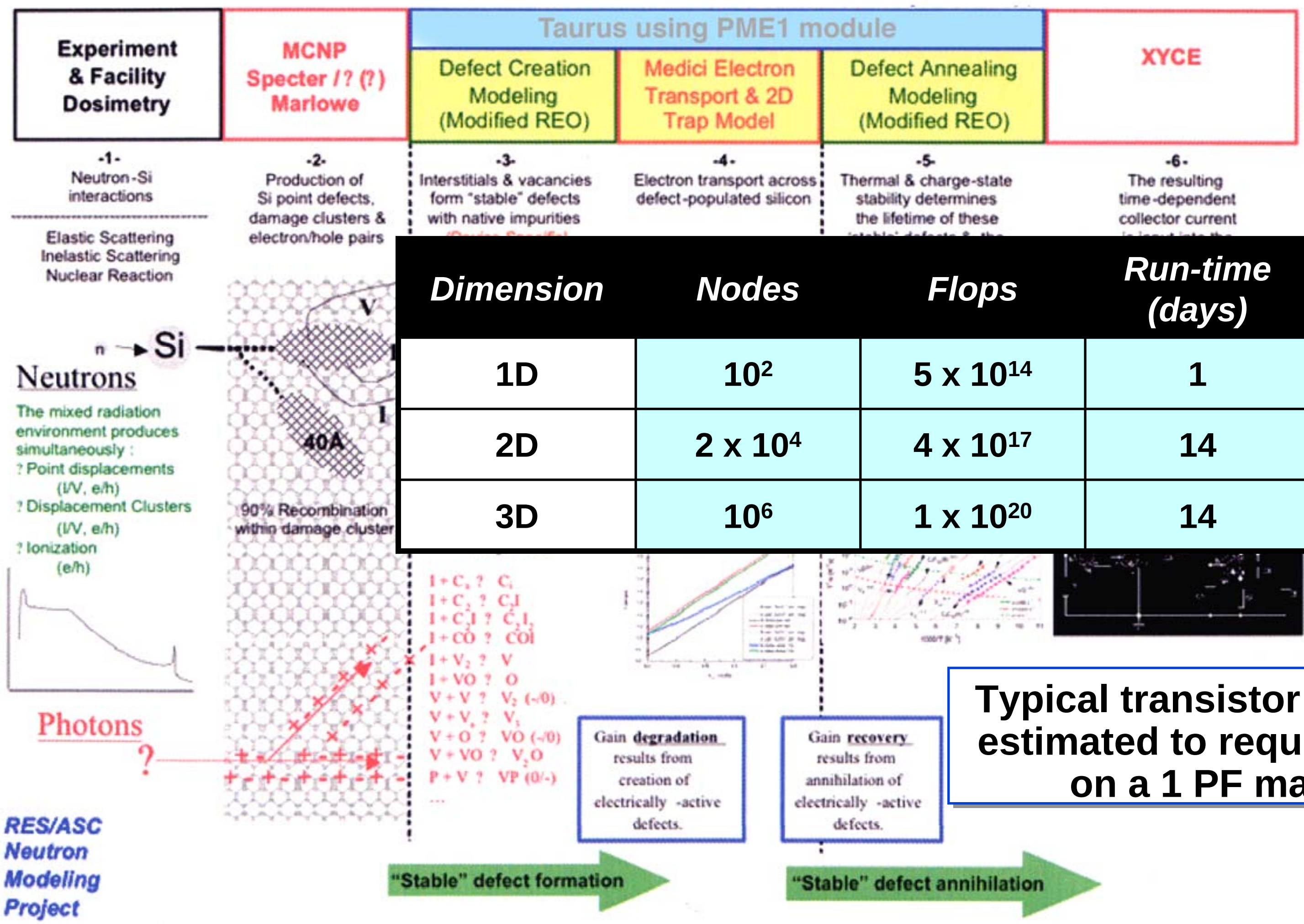


Fidelity	*Structural Dynamics*	*Fuel Dispersal*	*Fire/Thermal Response*	*Structural Collapse*
Cells	**10^9**	**10^9**	**10^8**	**10^9**
Variables	**5**	**10**	**40**	**3**
Time Steps	**10^{-6}**	**10^{-3}**	**10^{-2}**	**10^{-1}**
Run-time @ 1 PF, 10% eff.	**30 days**	**5 days**	**30 days**	**3 days**

Estimates for a non-coupled simulation of a 10,000 m^3 facility

Need 20-50 simulations per facility

Replacing SPR functionality will require petascale computation



Dimension	*Nodes*	*Flops*	*Run-time (days)*	*Platform*
1D	10^2	5×10^{14}	1	0.2 TF
2D	2×10^4	4×10^{17}	14	10 TF
3D	10^6	1×10^{20}	14	2.7 PF

Typical transistor simulation estimated to require 38 days on a 1 PF machine

Z simulations require petascale platforms to model 3D implosions complicated by MHD effects

- Geometry
  - Micron-size wires
  - Centimeter-size hohlraums
- Materials
  - Opacity
  - Conductivity
  - Equation of State
  - Reaction Rates
- Physics
  - Radiation
  - Magnetics
  - Hydrodynamics
  - Thermal Conduction
  - Ion/Electron Temperature
  - Alpha particle transport
  - Fusion burn

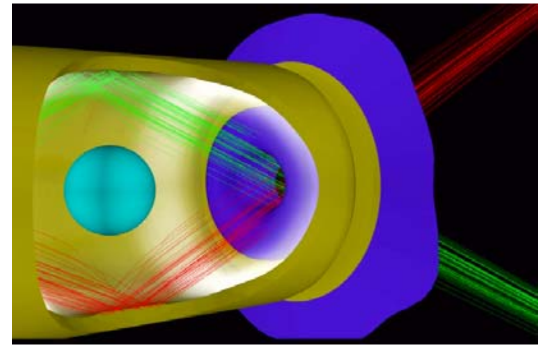
	Current capability	*Required capability*
Wires	30	300
Elements	36 M	360 M
Iterations	1	4000
Symmetry	Eighth	Half
Computing platform	1.25 TF	1.3 PF
Run time (days)	.25	7

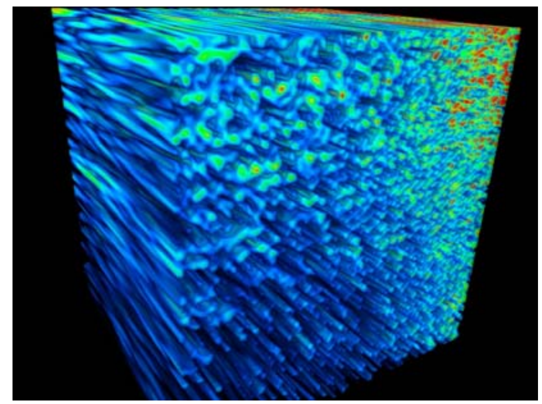
- Campaigns supported by HEDP
  - Dynamic materials
  - Secondary Certification
  - Nuclear survivability
  - Ignition & High Yield

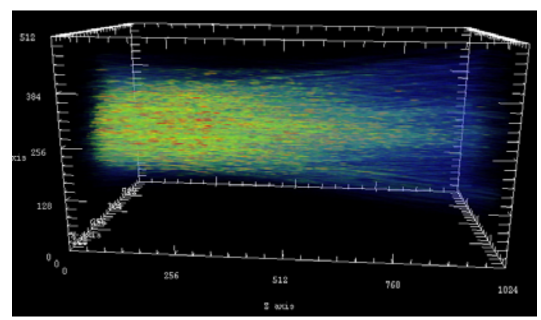
A 300-wire design calculation will require 7 days/run on a 1.3 PF platform, with 10s of runs needed per design iteration

NIF simulations require shorter turn-around times that weapons design

- Unlike predictive and postdictive weapons simulations, NIF performance simulations will be conducted in the midst of experimental campaigns
  - 1-2 day turn-around required
- Two types of capability simulations needed
  - Integrated hohlraum/capsule performance
    - resolve surface roughness effects (l=100 modes)
    - verify adequacy of routine separate hohlraum, capsule simulations
    - resolution requires full 500 TF system in FY07
  - Laser-plasma interaction
    - tune NIF beams' characteristics to
      - increase efficiency
      - reduce demands on laser (reduce likelihood of damage)
    - by FY07 need 360 TF system to achieve 30 day turn-around







Summary

- **The initial ASCI entry-level goal of 100 TF was sized to allow sufficient resolution to reduce numerical errors to permit study of physics issues**
- **NNSA needs an operational 1-2 petaflop platform by 2010 to achieve the high-resolution, high-fidelity simulations required of a predictive capability necessitated by …**
  - **the aging and changing stockpile**
  - **the need for increased safety and surety driven by the terrorist threat of the post-9/11 world**
  - **the opportunity to enable breakthroughs at NNSA experimental facilities**
- **NNSA must lead the pursuit of petaflop computing to ensure that SSP needs are met**

Petaflop capability is needed in the 2010 timeframe to fully meet stewardship obligations

Backup slides begin here…

The predictive capability requirement is set by QMU (Quantifying Margins and Uncertainties)

- **For stockpile systems with established small margins (M), uncertainty (U) must be sufficiently small to ensure acceptable M/U**
  - **the requirement of small U drives greater predictive capability**
    - **increase resolution**
    - **quantify impact of poorly understood phenomena**

Different systems require varying levels of predictive capability