Scientific and Computational Challenges of the Fusion Simulation Program (FSP)

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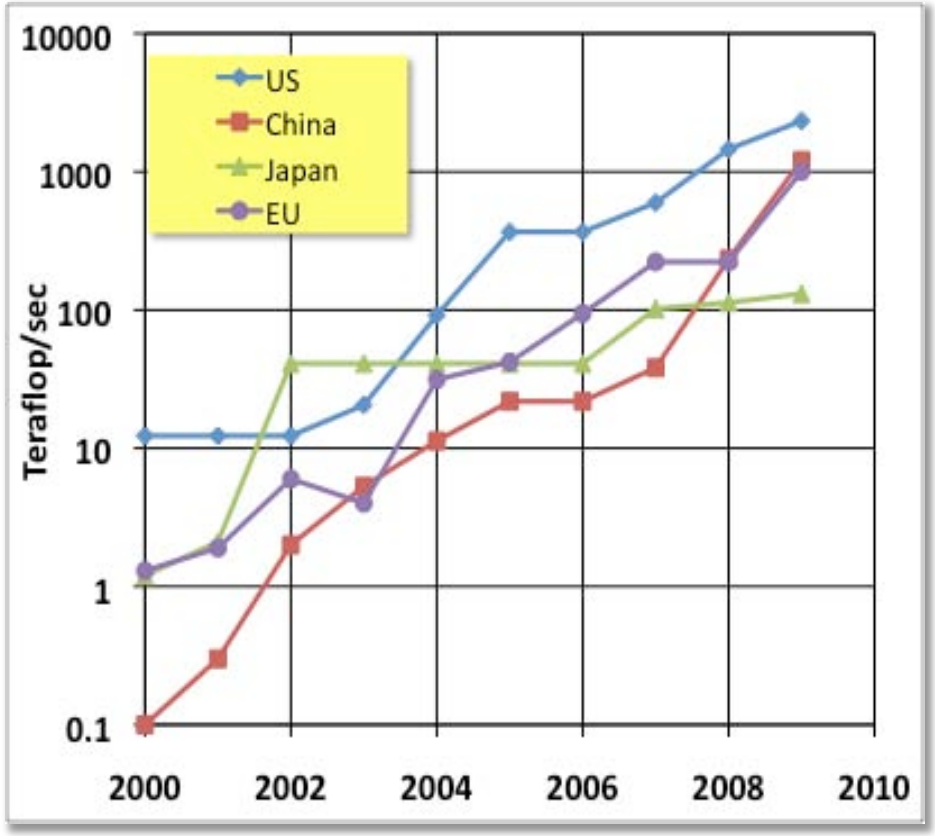
Computational Science, Exascale Computing & Leadership in Science & Technology (*S. Koonin, US Energy Undersecretary*)

- **Scientific & technological challenges:**
  - *New fuels and reactors (fission & fusion)*
  - *Stewardship without nuclear tests*
  - *Carbon sequestration alternatives*
  - *Regional climate impacts*
- **Broader application of exascale computing can significantly accelerate progress in both applied and fundamental science**
  - *Renewable energy and energy storage*
  - *Prediction and control of materials in extreme environments*
  - *Understanding dark energy and dark matter*
  - *Clean and efficient combustion in advanced engines*



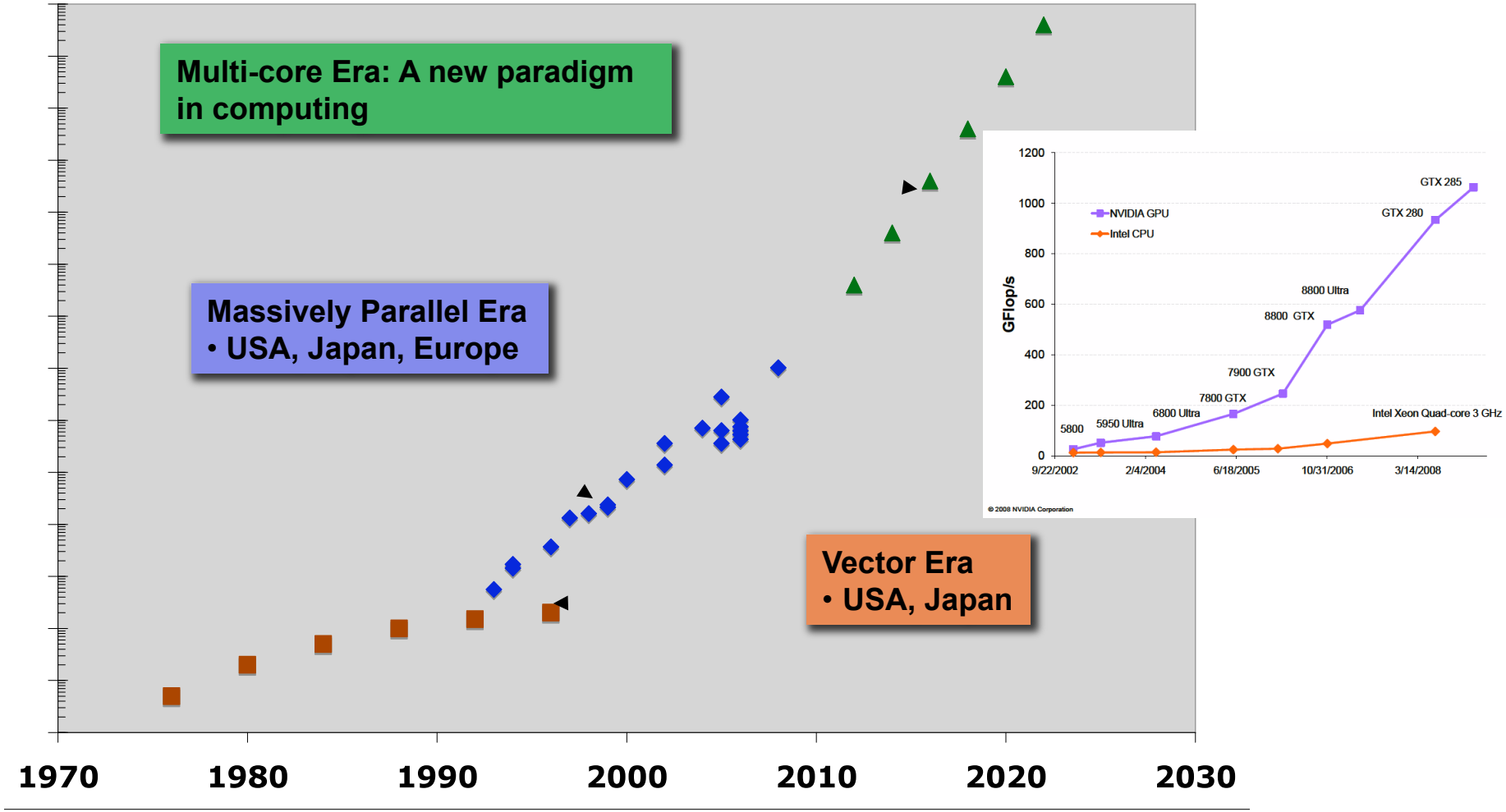
International Competition in HPC

Chart shows most capable system for each year in TOP500

Teraflop = 10^{12} floating point operations per second

Pre-eminence in 21st Century science & technology requires leadership in computational science and high performance computing => "exascale" (10^6 Teraflops) applications

- **Domain Applications *(e.g., FES)* Should be Prepared to Exploit *Local Concurrency* to Take Advantage of Future Supercomputing Systems *(e.g., CPU-GPU hybrid such as Tienhe-1A)***



Advanced Computing can Transform Many Domain Applications Areas (including FES)

- ***Practical Considerations:*** **[achieving "buy-in" from general scientific community]**
  - **Need to distinguish between *"voracious"* (*more of same - just bigger & faster*) vs. *"transformational"* (*achievement of major new levels of scientific understanding*)**
  - **Need to improve *significantly* on *experimental validation* together with *verification & uncertainty quantification* to enhance realistic predictive capability**

- ***Associated Extreme Scale Computing Challenges:***
- ***Hardware complexity*: Heterogenous multicore *(e.g., cpu+gpu -- LANL, ORNL, …)*, power management, memory, communications, storage, …**
- ***Software challenges*: Operating systems, I/O and file systems, and coding/algorithmic needs in the face of *increased computer architecture complexity* … *"parallelism doubles every two years" (as a new form of Moore's Law)***

  (MPI + threads; CUDA; rewriting code focused on data movement over arithmetic; …..)

  ***People:** *Major challenge to attract, train, & assimilate the next generation of simulation/modeling-oriented CS, Applied Math and applications-oriented computational scientists and engineers.*

Advanced Scientific Codes --- *"a measure of the state of understanding of natural and engineered systems"* (T. Dunning, 1st SciDAC Director)

Problem with Computational Method?

Problem with Mathematical Model?

Theory
(Mathematical Model)

Applied Mathematics
(Basic Algorithms)

Computational Physics
(Scientific Codes)

Computer Science
(System Software)

"Performance" Loop

Computational Predictions

"V&V" Loop

Inadequate

No

Agree* w/ Experiments?

Yes

Speed/Efficiency?

Use the New Tool for Scientific Discovery

Adequate

(Repeat cycle as new phenomena encountered)

*Comparisons: *empirical trends; sensitivity studies; detailed structure (spectra, correlation functions, …)*

Verification, Validation, & Uncertainty Quantification Challenges

- **Establishing the physics fidelity of modern plasma science simulation tools demands proper Verification & Validation (V&V) and Uncertainty Quantification (UQ) -- *Reliable codes demand solid theoretical foundations and careful experimental validation***

  • **Verification assesses degree to which a code (*both in the advanced direct numerical simulation (DNS) and reduced models categories*) correctly implements the chosen physical model**
  --- more than "essentially a mathematical problem"
  e.g., accuracy of numerical approximations, mesh/space and temporal discretization, statistical sampling errors, etc.
  --- also requires*:* (1) comparisons with theoretical predictions; and (2) cross-code benchmarking (codes based on different mathematical formulations/algorithms but targeting the same generic physics)

  • **Validation assesses degree to which a code (within its domain of applicability) "describes the real world"**
  --- also requires: (1) deployment of modern diagnostics; and (2) application of "synthetic diagnostics" in advanced simulations

  • **Uncertainty Quantification is the quantitative characterization & reduction of uncertainty in applications related to variability of input data/model parameters & uncertainties due to unknown processes or mechanisms (e.g., sensitivity analysis)**

ITER Goal: *Demonstration of the Scientific and Technological Feasibility of Fusion Power*

- ITER *is a dramatic next-step for Magnetic Fusion Energy (MFE)*:

  -- Today: 10 MW(th) for 1 second with gain ~1
  -- ITER: 500 MW(th) for >400 seconds with gain >10

- Many of the technologies used in ITER will be the same as those required in a power plant *but additional R&D will be needed*

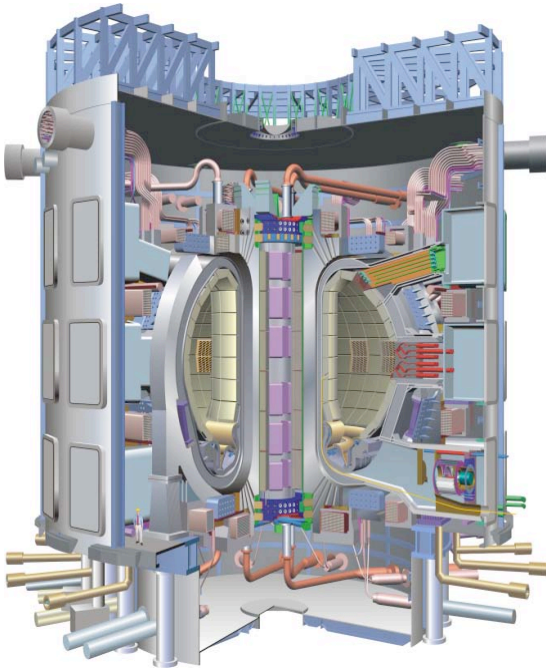
  -- "DEMO": 2500 MW(th) continuous with gain >25, in a device of similar size and field as ITER

  * Higher power density
  * Efficient continuous operation

- Strong R&D programs are required to support ITER and leverage its results.

  -- Experiments, theory, computation, and technology that support, supplement and benefit from ITER

ITER



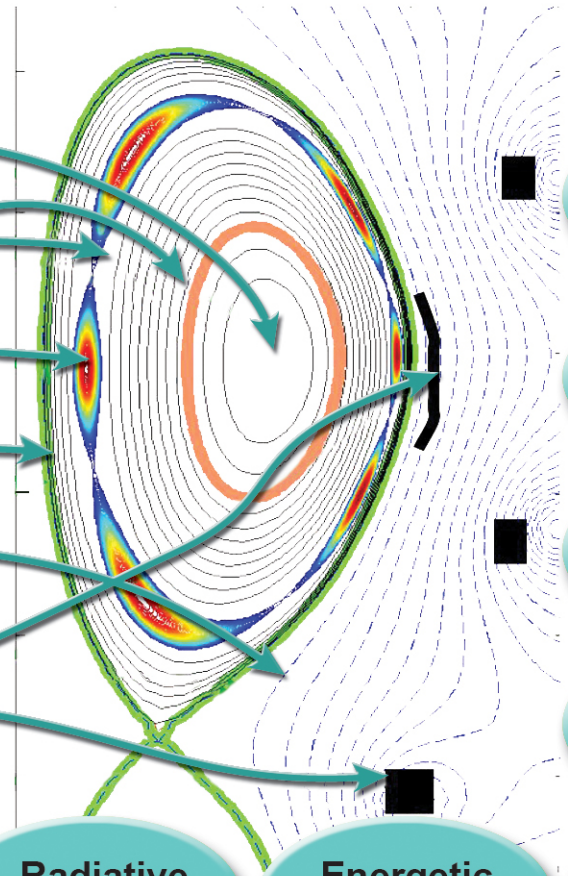
FSP -- A Strategic *Opportunity* to Accelerate Scientific Progress in FES

- Need for reliable predictive simulation capability for *BP/ITER (especially in the US)*
- Powerful ("Leadership Class") Computational Facilities moving rapidly toward petascale & beyond
- Interdisciplinary *collaborative experience*, knowledge, & software assembled over the course of nearly a decade under SciDAC plus OFES and OASCR base research programs in the US

OFES Theory Program	OFES Experimental Program	OFES SciDAC	OASCR SciDAC	OASCR Math Program	OASCR CS Program

Elements of an MFE Integrated Model

- Sawtooth Region (q < 1)
- Core confinement Region
- Magnetic Islands
- Edge Pedestal Region
- Scrape-off Layer
- Vacuum/Wall/ Conducctors/Antenna



Core & Edge Transport

Plasma Turbulence

Large Scale Instabilities

MHD Equilibrium

Plasma-Wall Interactions

Atomic Physics

Radiative Transport

Energetic Particles

Heating & Current Drive

MFE Science Drivers

- ***Disruptions*: Large-scale macroscopic events leading to rapid termination of plasma discharges**

Goal: Avoid or mitigate because ITER can sustain only a limited number of full-current disruptions with ***severe heat loads, JxB forces, run-away electron generation***

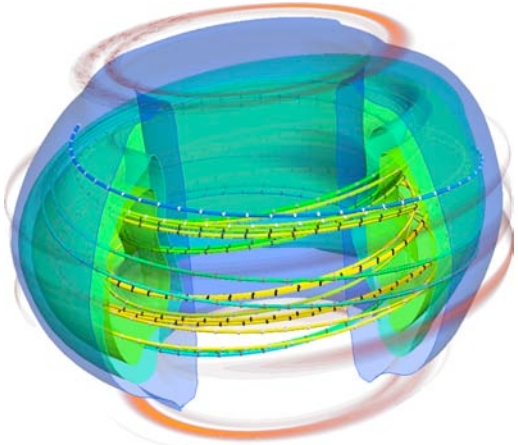
- ***Pedestals*: Steep spatial gradients whose formation leads to transient heat loads in plasma periphery (divertor region)**

Goal: Predict (i) onset & growth because pedestal height observed to control confinement; (ii) frequency and size of edge localized mode (ELM) crashes to ***mitigate erosion of divertor and plasma-facing components***

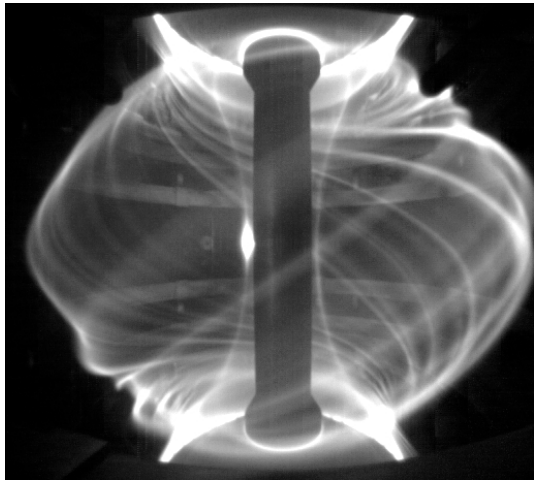
- ***Core Profiles*: Plasma profiles in core confinement region of MFE plasmas.**

Goal*: (i) determine operational limits (e.g., sustainable plasma pressure) and ***optimize plasma performance*** (e.g., fusion yield); and (ii) provide confidence in extrapolating core confinement predictions to future devices

****Requires prediction of temperature, density, current, and rotation profiles in plasma core, including the internal transport barrier region***



Plasma Disruptions in DIII-D



ELMs in MAST

MFE Science Drivers

- ***Wave-Particle Interactions*:** **Dynamics between energetic particles and EM waves impacting efficiency of auxiliary heating and the fast-particle confinement of fusion products & supra-thermal particles from RF and energetic beam heating**

Goal: ensure steady-state (long-pulse) performance in burning plasmas such as ITER

-- ***Burning plasma regime is fundamentally new with stronger self-coupling and weaker external control***

- ***Plasma Boundary*:** **Region at plasma periphery where complex plasma-materials interactions occur**

Goal: effective modelling of heat loads impacting: (i) divertor design and operational strategies; (ii) erosion of divertor and plasma facing components; and (iii) ***tritium retention and removal***

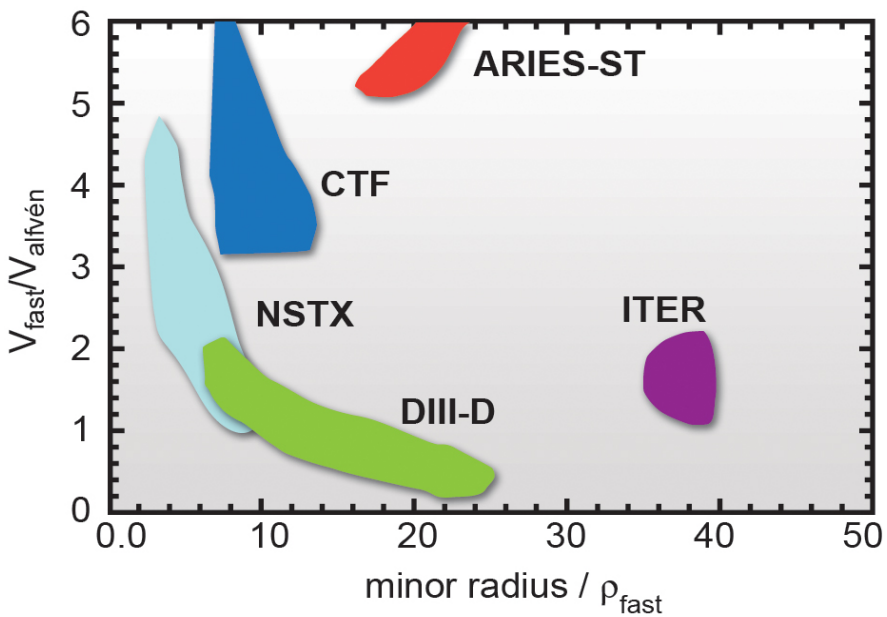
- ***Whole Device Model*:** **Experimentally-validated integrated predictive code to simulate entire MFE system, including dynamics of other 5 Science Drivers**

Goal: provide reliable ***scenario modelling*** for existing and planned (ITER) experimental systems & enable effective design of future devices (DEMO)

Plasma Boundary Layer
Plasma-wall interactions

Magnetically Confined Burning Plasmas:
Unique opportunities for scientific discoveries

- BP/ITER physics elements raise mission-critical questions
  - Unprecedented size
  - Self-heating
  - Large energetic particle population
  - Multiple instabilities with unknown consequences for fast ion confinement



Predicting fast ion confinement: Critical for sustaining a burning plasma

- What is nonlinear interaction between energetic particles and "sea of Alfvén modes?"
- How is transport affected by presence of multiple instabilities?
- How can predictive numerical tools be properly validated?
- What scale of computational resources will be needed to answer BP/ITER mission-relevant questions?

Recent "Leadership Computing Facility" (LCF) - enabled simulations provide new insights into nature of plasma turbulence

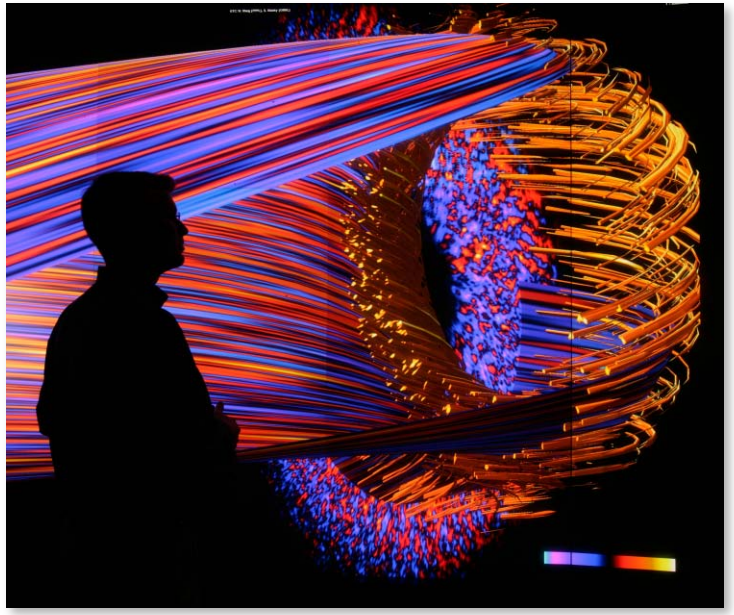
Teraflops-to- petaflops computing power have accelerated progress in understanding heat losses caused by plasma turbulence

Multi-scale simulations accounting for fully global 3D geometric complexity of problem (*spanning micro and meso scales*) have been carried out on DOE-SC LCF's

Excellent Scalability of Global PIC Codes *enabled by strong ASCR-FES collaborations* in SciDAC

Exascale-level production runs are needed to enable running codes with even higher physics fidelity and more comprehensive & realistic integrated dynamics

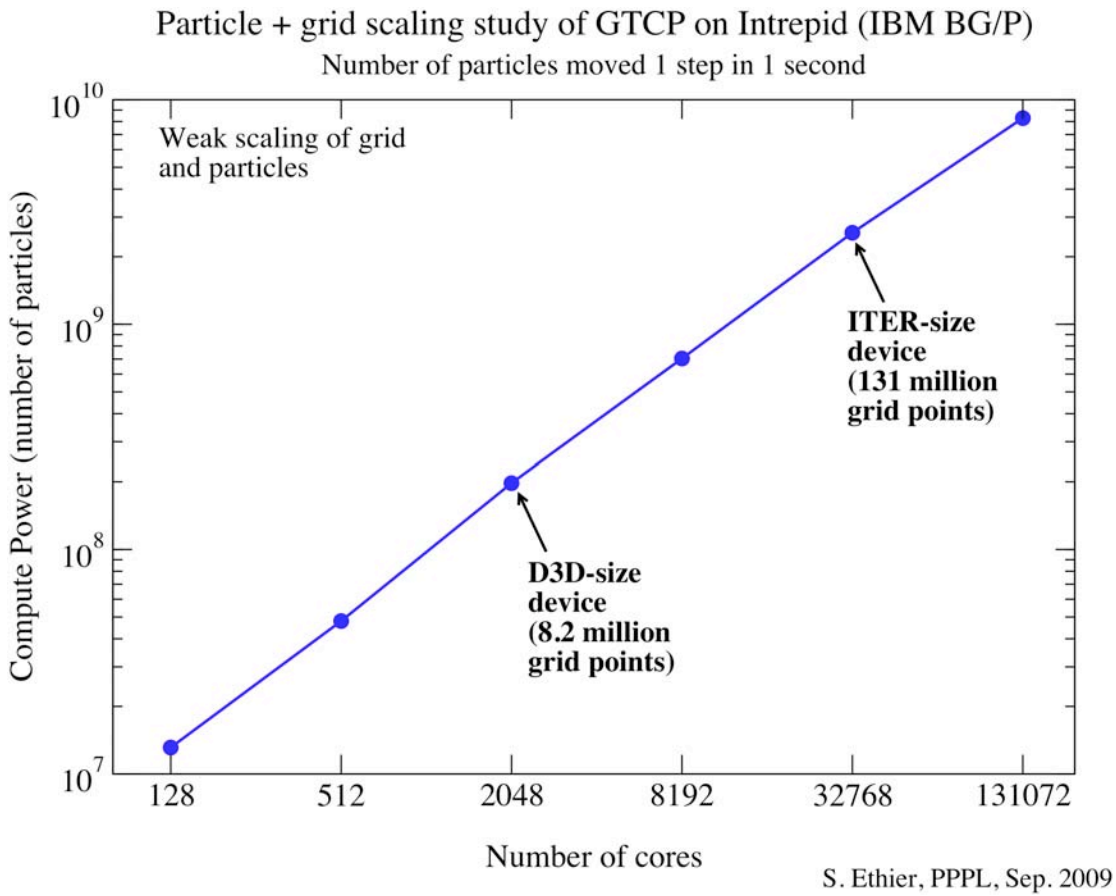
e.g. -- *Current petascale-level production runs on ORNL's Jaguar LCF require 24M CPU hours (100,000 cores × 240 hours)*



Mission Importance:

Fusion reactor size and cost are determined by balance between loss processes and self-heating rates

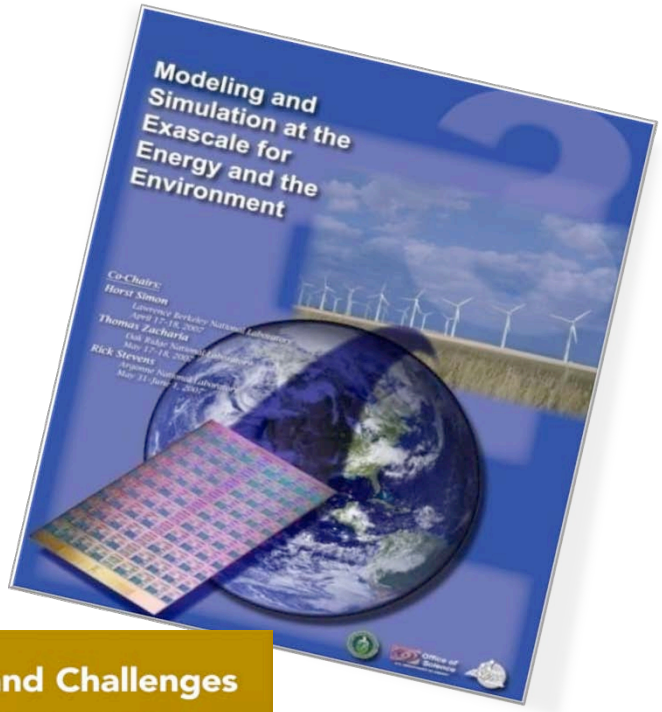
Scaling GTC-P on IBM BG-P at ALCF



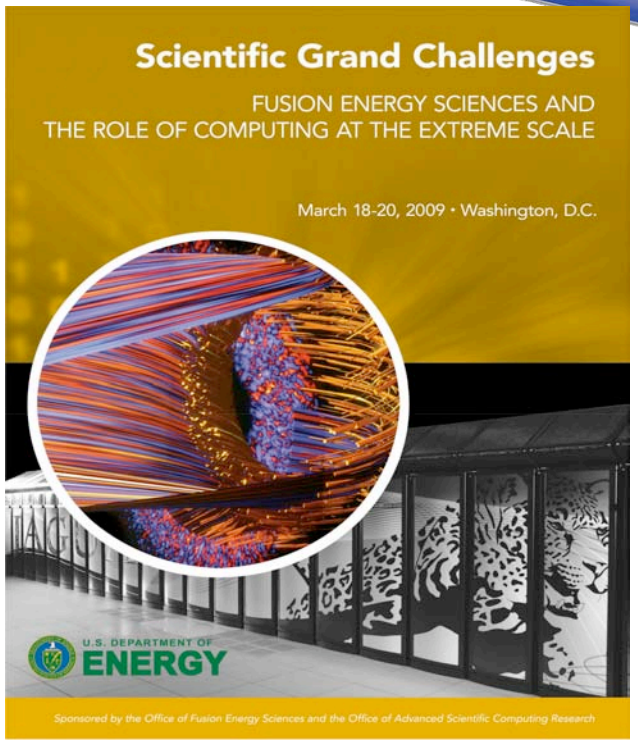
Excellent scalability demonstrated – promising basis for performance on new (multi-petaflop) IBM BG-Q

Moving to the "Exascale"
(10^{18} floating point operations per second)

- US DoE held a series of major workshops in 2009-2010 to assess the ***opportunities and challenges of exascale computing for the advancement of science, technology, and associated missions***



- ASCR strategy involves working with:
  - -- domain applications areas such as FES to scale/adapt applications to new leadership computer systems
  - -- LCF's at ORNL & ANL that provide series of increasingly powerful computer systems



HPC Challenges in Moving toward Exascale

Locality: *Need to improve data locality (e.g., by sorting particles according to their positions on grid)*

-- due to physical limitations, ***moving data between, and even within, modern microchips is more time-consuming than performing computations!***

-- scientific codes often use data structures that are easy to implement quickly but limit flexibility and scalability in the long run

Latency: *Need to explore* ***highly multi-threaded algorithms*** *to address memory latency*

Flops vs. Memory: *Need to utilize Flops (cheap) to better utilize Memory (limited & expensive to access)*

Emerging Architectures: *Need to deploy innovative algorithms within modern science codes on* ***low memory per node architectures*** – ***(e.g, Tienhe-1A and Fujitsu-K)***

-- multi-threading within nodes, maximizing locality while minimizing communications

-- large future simulations *(e.g., PIC ➔ need to likely work with >10 billion grid points and over 100 trillion particles!!)*

FSP Activities Status *(National Planning Team from 6 national labs, 9 universities, & 2 companies)*

• Science Plans for the 6 FSP Science Drivers developed with ~70 leading scientists from FES & ASCR community -- ***Oct, 2010***

-- *prioritization with awareness of customer needs via connections to exp. facilities (national & international), ITER, BPO, ITPA,…);*

➔choice of *consolidated* Integrated Science Applications (ISA's)

(i) Whole Device Modeling + Disruption Avoidance:
=> ***Discharge optimization and prediction, especially the avoidance of disruptions***

(ii) Edge Physics: Boundary + Pedestal:
=> ***Heat and particle loads with associated impact on Plasma-Material Interactions (PMI) and including the nature and impact of Edge Localized Modes (ELM's)***

• Report from 2nd FSP Planning Workshop with over 80 participants @ GA, Feb. 8-11 posted on FSP web-site - http://www.pppl.gov/fsp/ (*Report, March, 2011*)

• **"FSP PAUSE"**: (E. Synakowski at FESAC, March 6, 2011): *"budget pressures, esp. with ITER growth, may make it difficult to execute the FSP at the funding levels previously envisioned.*

➔ *This is the optimal time to pause and take advantage of completion of the planning prior to execution of the FSP itself*

➔ *FSP Plan to DoE-SC: 1st complete draft - July 31, 2011; final due – Sept. 31, 2011)*

- **U. S. Energy Undersecretary** *Steven Koonin:*

3 November 2009 – American Physical Society Meeting, Atlanta,Georgia

"Validated predictive simulation capability is key to advancing fusion science towards energy … the Fusion Simulation Program is a start along this path."

- **U.S. Energy Secretary** *Steven Chu:*

27 September 2010 – "All Hands Meeting" at PPPL, Princeton, NJ

"The world's energy challenge requires a strong continued commitment to plasma and fusion science."

"Progress in fusion has to be grounded in validated predictive understanding: the DoE is clearly interested in your planning and progress for a strong Fusion Simulation Program (FSP)."

➔ **U. S. Energy Undersecretary** *Steven Koonin:*

18 March 2011 *-- House Sub-Committee on Energy & Water Testimony, DC*

"With respect to US investment in ITER … need to make sure our program is best positioned to take advantage of that … so we'll put a lot of money into diagnostics, simulation, and the human capability … Executing simulation is in part about the hardware but it's also about the software and the expertise to meld experiments and observations together with the codes .. and there the U.S. is second to none."

Future Challenges and Opportunities

(1) *Energy Goal* in FES application domain is to increase availability of clean abundant energy by first moving to a *burning plasma experiment* -- the multi-billion dollar *ITER* facility located in France & involving the collaboration of 7 governments representing over half of world's population

-- ITER targets 500 MW for 400 seconds with gain > 10 to demonstrate *technical feasibility of fusion energy* & *DEMO* (*demonstration power plant*) will target 2500 MW with gain of 25

(2) *HPC Goal* is to harness increasing HPC power ("Moore's law) to ensure timely progress on the scientific grand challenges in FES as described in DoE-SC report (2010) on *"Scientific Grand Challenges: Fusion Energy Sciences and Computing at the Extreme Scale."*

(3) *Interdisciplinary Computational Sciences Goal* is to leverage advances/"lessons learned" from successful U.S. DoE national cross-disciplinary programs such as SciDAC .

Mission of FSP (Fusion Simulation Program):

Accelerate progress in delivering reliable integrated predictive capabilities -- benefiting significantly from access to HPC resources – from petascale to exascale & beyond -- together with a vigorous verification, validation, & uncertainty quantification program