ASCAC Panel Report on the Fusion Simulation Project

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Panel Chair
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Outline

- Introduction
- ASCR FSP Alignment and FSP Project
- FSP Critical Technology Challenges for ASCR
- Role of ASCR in FSP
- ASCR Challenges in FSP Execution
- Conclusions

The Charge

- Dr. Orbach's charge of October 12, 2007:
  - Consider what is being proposed for the Fusion Simulation Project (FSP)
  - Pay particular attention to the most critical challenges in applied mathematics, computer science, and computational science
  - Recommend an appropriate and mutually beneficial role for ASCR in FSP

The Panel

- F. Ronald Bailey, CSC/NASA Ames
- Don Batchelor, ORNL
- David Brown, LLNL
- Steve Jardin, Princeton Univ. Plasma Physics Lab
- Doug Kothe, ORNL
- Rusty Lusk, ANL
- Tom Manteuffel, Univ. of Colorado
- Juan Meza, LBNL
- David Schissel, General Atomics Energy Group

Panel Approach

- Reviewed FSP reports:
  - FSP Workshop Report (2007)
  - FESAC FSP Report (2007)
  - Dahlburg Report (2002)
  - Post Report (2004)
- Conducted one-day workshop (April 30, 2008)
- Held working sessions (May 1-2, 2008)
- Held several telephone conference calls

Slide 5

A1 Holly Amundson, 7/29/2008

The Fusion Simulation Project

- 15-year project at approx. $25M/yr.
- **After 5 years**: Integrated whole-device framework for the simulation of tokamak plasmas to support ITER diagnostics and design, and to review decisions.
- **After 10 years**: Simulation facility for meeting scientific and engineering objectives of ITER capable of comprehensive integrated timeline analysis for control system design.
- **After 15 years**: Validated simulation facility for DEMO reactor world-class simulation capability to maximize ITER benefit.

ASCR Alignment

- ASCR historically strong contributor to magnetically confined fusion simulation
  - PEtSc
  - SciDAC National Fusion Collaboratory
  - MFECC
- FSP well aligned with ASCR goals
  - "FSP agenda for applied math and computer science lies squarely on top of ASCR's 10-year vision.." FSP Workshop Report

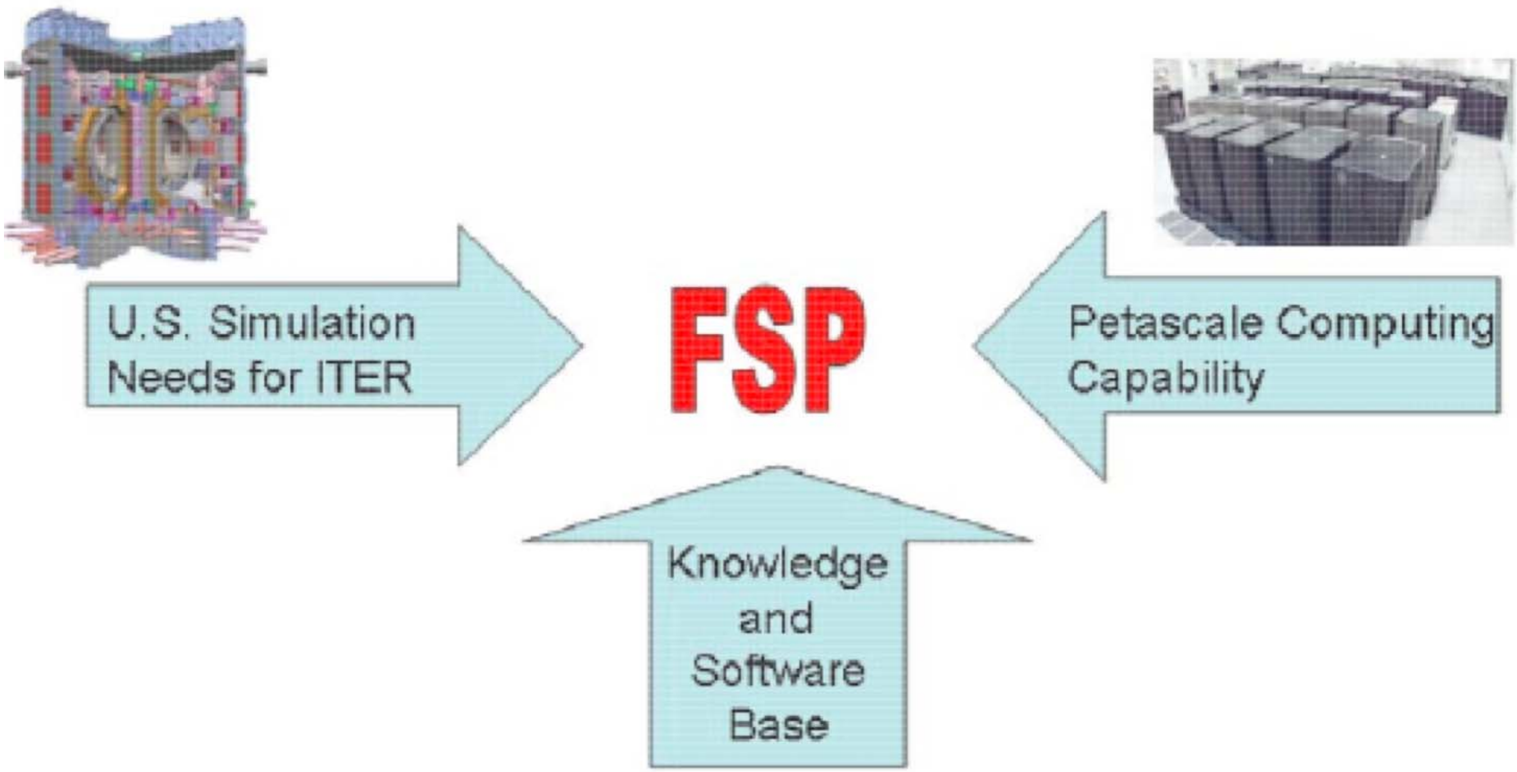
ASCR Alignment Findings

- The needs and goals of FSP for computer science and applied mathematics support are very well aligned with the capabilities and goals of the ASCR Program.

ASCR Alignment Recommendations

- The Panel strongly recommends ASCR seize the opportunity to participate in this exciting project of national importance in partnership with FES.

FSP Result of Unique Convergenece



OFES Theory Program	OFES Exp. Program	OFES SciDAC	OASCR SciDAC	OASCR Math Program	OASCR CS Program

FSP as Defined

- FSP result of over 5 years study and review given good understanding of broad scientific and technical issues

- Rather vague in many respects
  - Research program
  - Integrated computer program
  - Software framework
  - Software toolkit
  - Identification of stakeholders, customers and users

FSP Project Findings

- FSP's true scope is not yet fully defined with regards to technical products, performance, and schedule.

- Stakeholders, customers, and users are not well defined.

FSP Project Recommendations

- A documented requirements specification defining what is needed and at what level of acceptable risk, and an identification of the intended use of FSP products and their intended users is needed.

- ASCR participate with FES in the Project Definition Phase to begin producing such a document.

FSP Critical Technology Challenges for ASCR

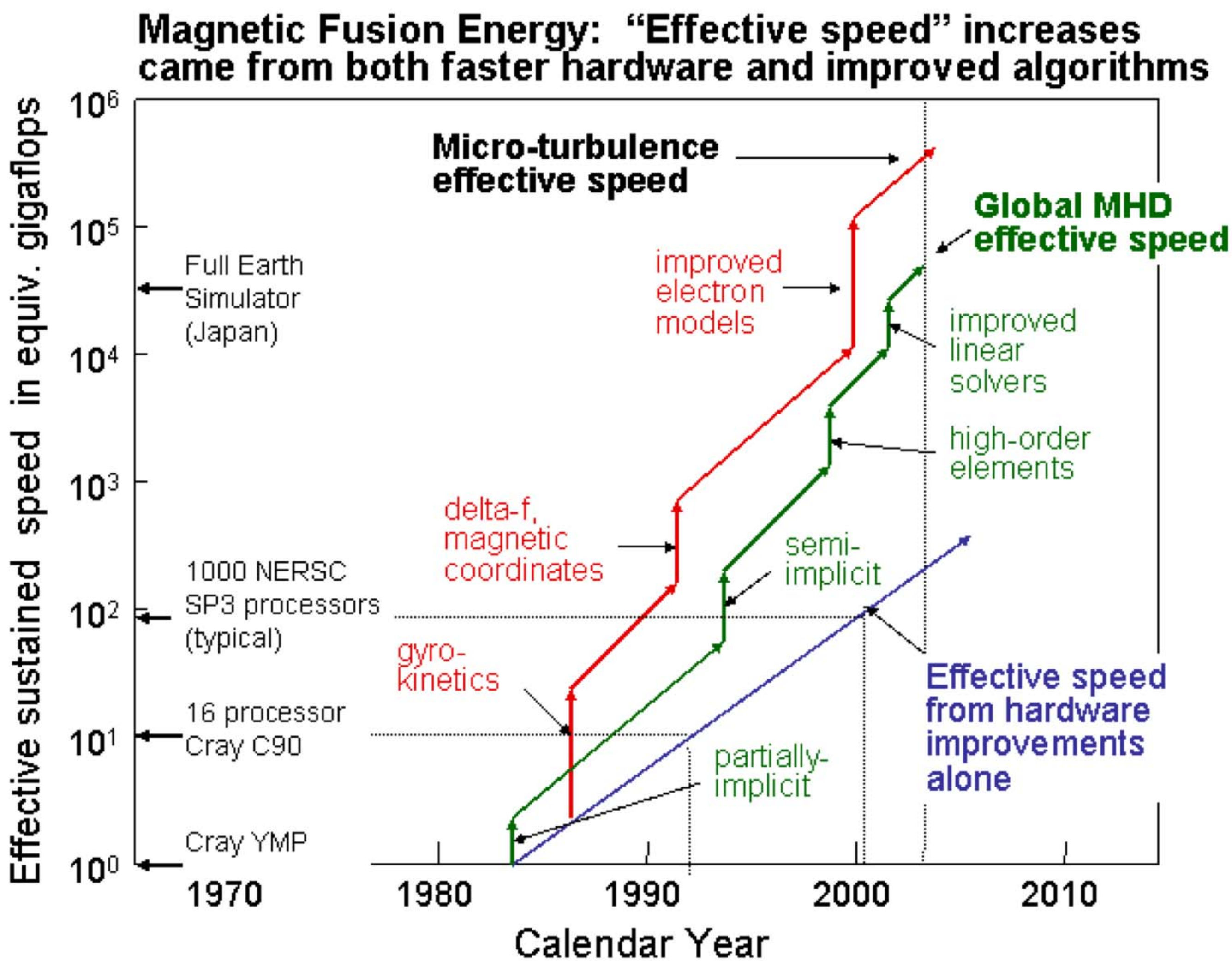
- **Areas addressed**:
  - Critical technologies previously identified
  - Applied mathematics
  - Computer science
  - Computational science

Estimate for Brute-Force Scaling Sawtooth Crash Simulations to ITER

name	symbol	units	CDX-U	DIII-D	ITER
Field	B_0	Tesla	0.22	1	5.3
Minor radius	a	meters	.22	.67	2
Temp.	T_e	keV	0.1	2.0	8.
Lundquist no.	S		1×10^4	7×10^6	5×10^8
Mode growth time	$\tau_A S^{1/2}$	s	2×10^{-4}	9×10^{-3}	7×10^{-2}
Layer thickness	$aS^{-1/2}$	m	2×10^{-3}	2×10^{-4}	8×10^{-5}
zones	$N_R\times N_\theta\times N_\phi$		3×10^6	5×10^{10}	3×10^{13}
CFL timestep	$\Delta X/V_A$ (Explicit)	s	2×10^{-9}	8×10^{-11}	7×10^{-12}
Space-time pts			6×10^{12}	1×10^{20}	6×10^{24}

Assuming explicit, uniform grid (Keyes, 2008 FSP Panel Workshop)

Faster Hardware & Improved Algorithms Lead to Faster Speed



(SCaLes Report, Vol 2, 2003)

Identification of FSP Critical Technologies Findings

- The 2007 FSP Workshop identification of critical technologies in applied mathematics, computer science, and computational science was reasonably complete.

- Experience in large-scale fusion energy simulations shows coordinating and combining research results from all such areas produces superior results.

Identification of FSP Critical Technologies Recommendation

- ASCR should coordinate its FSP research efforts in applied mathematics, computer science, and computational science to enhance focus and results for FSP.

Critical Challenges Addressed in Applied Mathematics

- Multi-physics, multi-scale
- Data-model fusion
- Uncertainty quantification
- Realistically computable models
- Data visualization and analysis

Critical Challenges in Applied Mathematics Findings

- The FSP is rich with opportunities for the development of new mathematical models, analysis techniques, and algorithms.

Critical Challenges in Applied Mathematics Recommendation

- FSP should engage the applied mathematics community in many areas including:
  - Methods for modeling multi-scale phenomena and multi-physics coupling
  - Sensitivity analysis and uncertainty quantification, data-model fusion
  - Development of computable models
  - Effective methods for the analysis of computational and experimental datasets

Critical Challenges Addressed in Computer Science

- Sustained Performance on FSP Applications
  - Heterogeneous, multi-core architectures
  - Need for programming models
  - Rapid pace of change
- Data Management, Visualization and Collaboration
  - Several orders-of-magnitude more data
  - Visual understanding
  - Distributed multi-disciplinary teams

Critical Challenges in Computer Science Finding 1

- Achieving sustained performance for FSP applications over time and across multiple platforms is made much more complex by the trend of ultra-scale computers toward many-core, heterogeneous architectures.

Critical Challenges in Computer Science Recommendation 1

- ASCR should support FSP by developing technology that ensures performance meets expectations as simulation applications move among diverse petascale to exascale platforms.

Critical Challenges in Computer Science Finding 2

- To meet its project goals, FSP requires the management of simulation-generated datasets, the visualization of these data, and the facilities and tools for collaboration by a worldwide research community.

Critical Challenges in Computer Science Recommendation 2

- FES and ASCR should dedicate resources to developing and deploying:
  - Distributed data management technologies that will provide rapid and easy access to FSP data
  - Visualization technologies that can be efficiently utilized for the anticipated large-scale data repository, as well as for the requirement of real-time graphical information sharing
  - Collaboration technologies aimed at unifying a distributed scientific team

Critical Challenges Addressed in Computational Science

- Frameworks
  - Enforces software engineering discipline
  - Reduces complexity and enhances productivity
- Workflow
  - Currently has limited use
  - Extension needed for capability-based actors and provenance
- Verification and Validation
  - Learn lessons from NNSA ASC

Critical Challenges in Computational Science Finding

- Computational frameworks, utilization of workflow tools, and systematic V&V methodology are all important for the success of FSP.

Critical Challenges in Computational Science Recommendation

- ASCR has considerable experience and expertise in each of these areas and should take the lead in recommending appropriate solutions to FSP.

The Role of ASCR in FSP

- **Two fundamental roles**:
  - Collaborator
  - Provider of basic research, technology, and facilities/infrastructure

ASCR Collaborator Role

- Envision FSP led by FES with highly collaborative support and targeted co-investment by ASCR
- SciDAC has led the way
- Integrated teams with physics-side management

ASCR Collaborator Role Finding

- The technical and project demands of FSP will call for very close teamwork between ASCR and other FSP scientists and engineers.

ASCR Collaborator Role Recommendation

- ASCR should adopt a policy of its scientists participating in integrated task teams when dictated by the needs of FSP. We envision the project management structure will remain on the physics side, with each ASCR scientist interacting closely with a number of physicists on specific subprojects in the FSP structure.

Role of Basic Research in Applied Mathematics and Computer Science Finding

- A strong element of basic research including basic research in applied mathematics and computer science will be important to the success of FSP.

Role of Basic Research in Applied Mathematics and Computer Science Recommendations

- The SciDAC model (collaboration encouraged and supported through co-funding of efforts between ASCR and science offices), may be employed in developing partnerships at the base research program level.

- In addition to promoting collaboration through an appropriate funding model, mechanisms need to be provided which encourage frequent interaction among the researchers involved.

Role of Applied Research Finding

- ASCR applied research will play a critical role in practical application of new fusion simulation-specific, as well as general knowledge in applied mathematics and computer science as a necessary step to meeting FSP goals.

Role of Applied Research Recommendation

- In addition to playing a strong collaborative role in FSP applied research, ASCR should take steps to ensure applicable results of other applied research supported by ASCR be made available and if necessary, tailored to FSP. *(see http://www.mcs.anl.gov/hs/software/ASCR_SW_Catalog.html)*

Role of Facilities

- **Areas identified**:
  - Hardware Infrastructure
  - Software Infrastructure
  - User Services
  - Network Infrastructure

Role of Facilities Finding

- The FSP will have special computational needs with regard to capability, capacity, on-demand computation, and data-storage.

Role of Facilities Recommendation

- A partnership between ASCR and FES to determine an appropriate set of hardware requirements for FSP would benefit both offices. Special solutions will need to be developed such as separate queues, dedicated systems, and special data repositories.

ASCR Challenges in FSP Execution

- FSP Sociology
  - Project pressures
  - Lack of publications
- ASCR Technology Insertion into FSP
  - Chain: basic research to applied research to engineering
- Software Engineering
- Application Development Productivity

ASCR Challenges in FSP Execution Findings

- ASCR has a predominately research culture, and participation in FSP will present significant challenges including:
  - Transitioning research results into production software
  - Attracting and retaining researchers
  - Maintaining good software engineering practices
  - Maintaining a productive development environment for high-quality software

ASCR Challenges in FSP Execution Recommendations

- ASCR should:
  - Develop and implement methods to attract, motivate, and reward researchers to participate in FSP
  - Early on, address the challenge of fostering a culture in which research creativity exists alongside project engineering discipline, one capable of transferring new applied mathematics and computer science knowledge from a research paper to FSP production code
  - Establish and enforce good software engineering standards
  - Establish a software quality activity tasked to gather and disseminate SQA best practices into FSP (especially in the areas of software verification and testing);
  - Leverage existing software development productivity tools and further efforts to improve software development environment.

Conclusions

- FSP is well-aligned to ASCR goals and recommend ASCR participate in implementing the project.
- A detailed planning effort is desperately needed
- FSP Workshop Panel did reasonable identification of critical technologies – the panel added some emphasis
- Two ASCR roles: Close collaborator with FES and provider of science, mathematics, technology, and facilities
- ASCR will need to address challenges in executing FSP including: Sociological, technology insertion, software standards, and software development productivity.