Fusion Simulation Project (FSP) Workshop Report

Presented by

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with acknowledgement to

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on behalf of the

FSP Committee, FSP Workshop Panels,

and FESAC Review Panel

ASCAC Meeting, 6 November 2007

Motivation for FSP

- **FSP poised at confluence of three developments**
  - **Inflexible schedule for burning plasma simulation capability (by ~2012)**
  - **Emergence of petascale computing capability (by 2009)**
  - **Assembly of knowledge and software under OASCR and OFES research programs, including 6+ years of rich SciDAC collaboration**

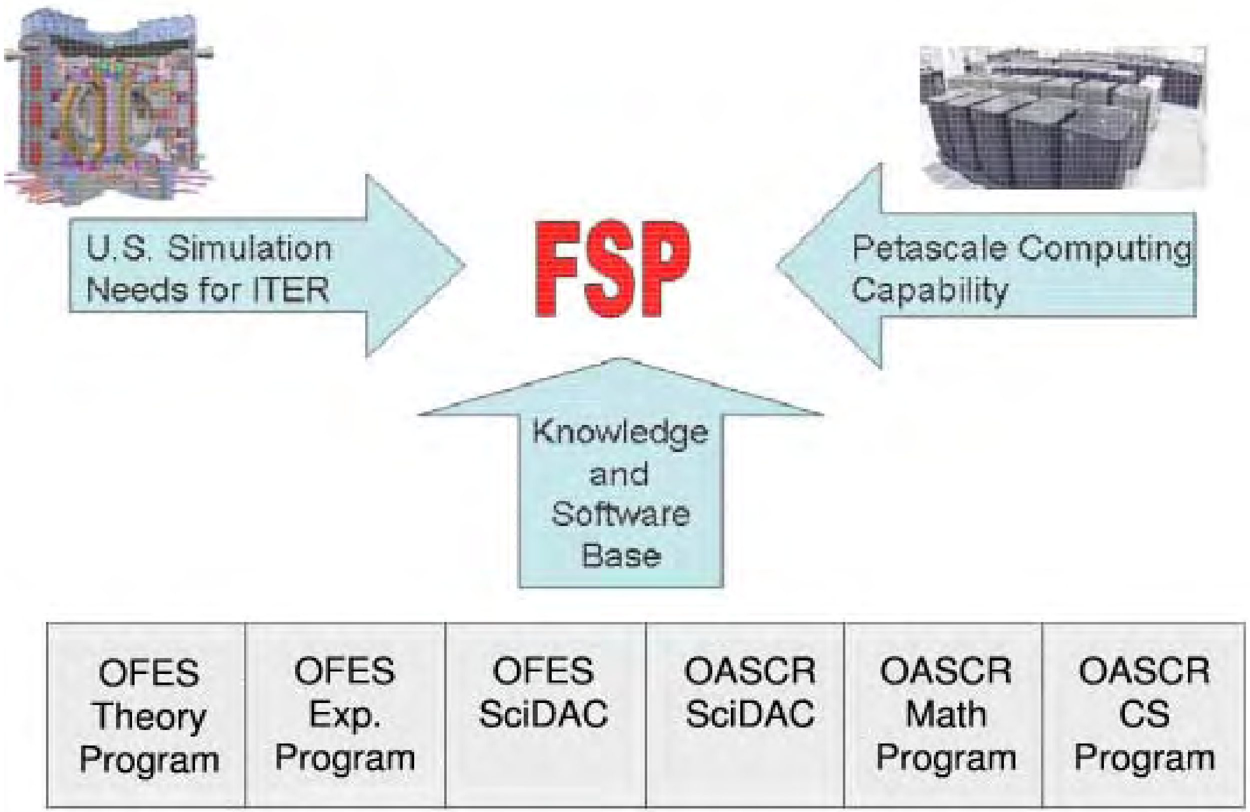
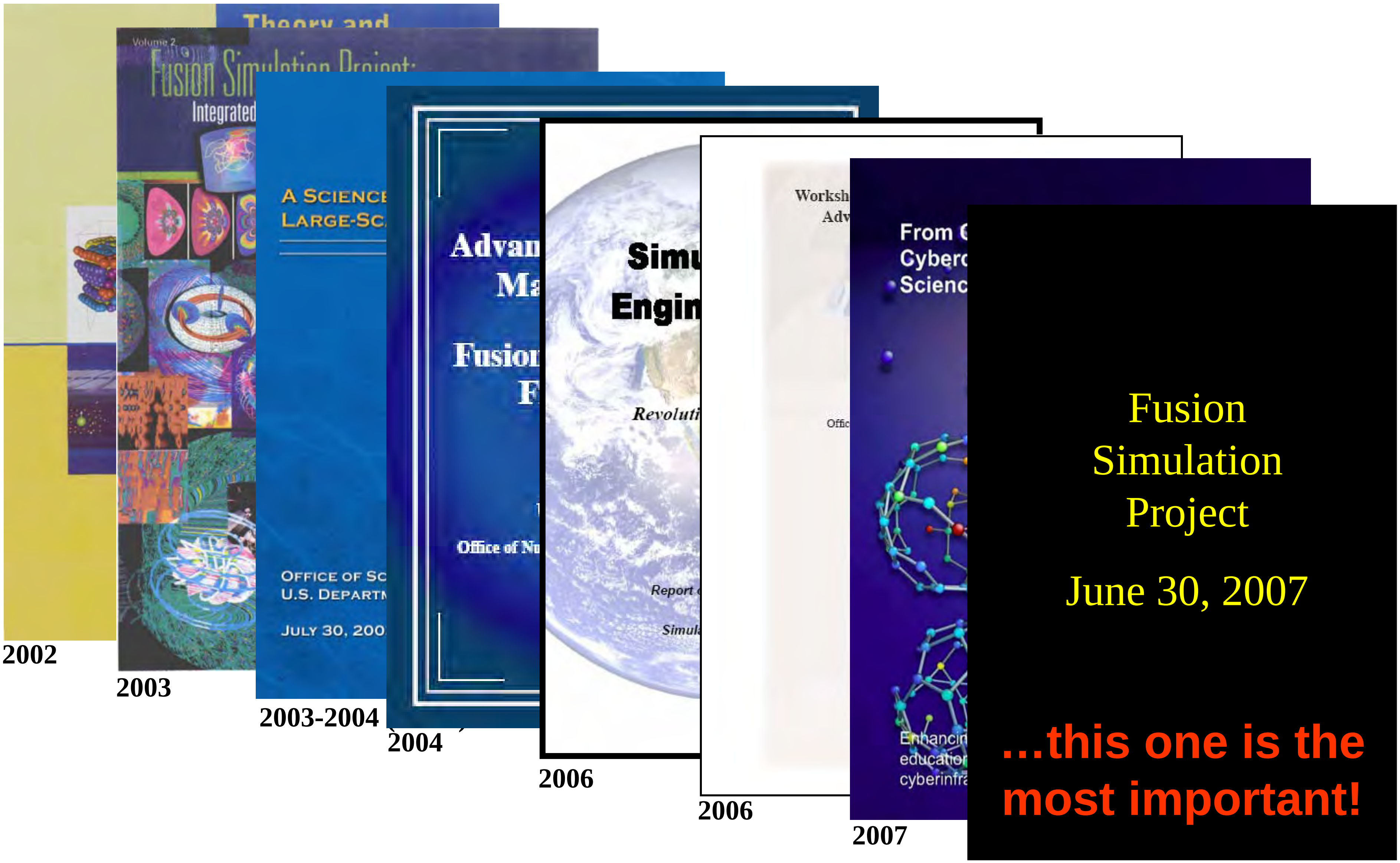


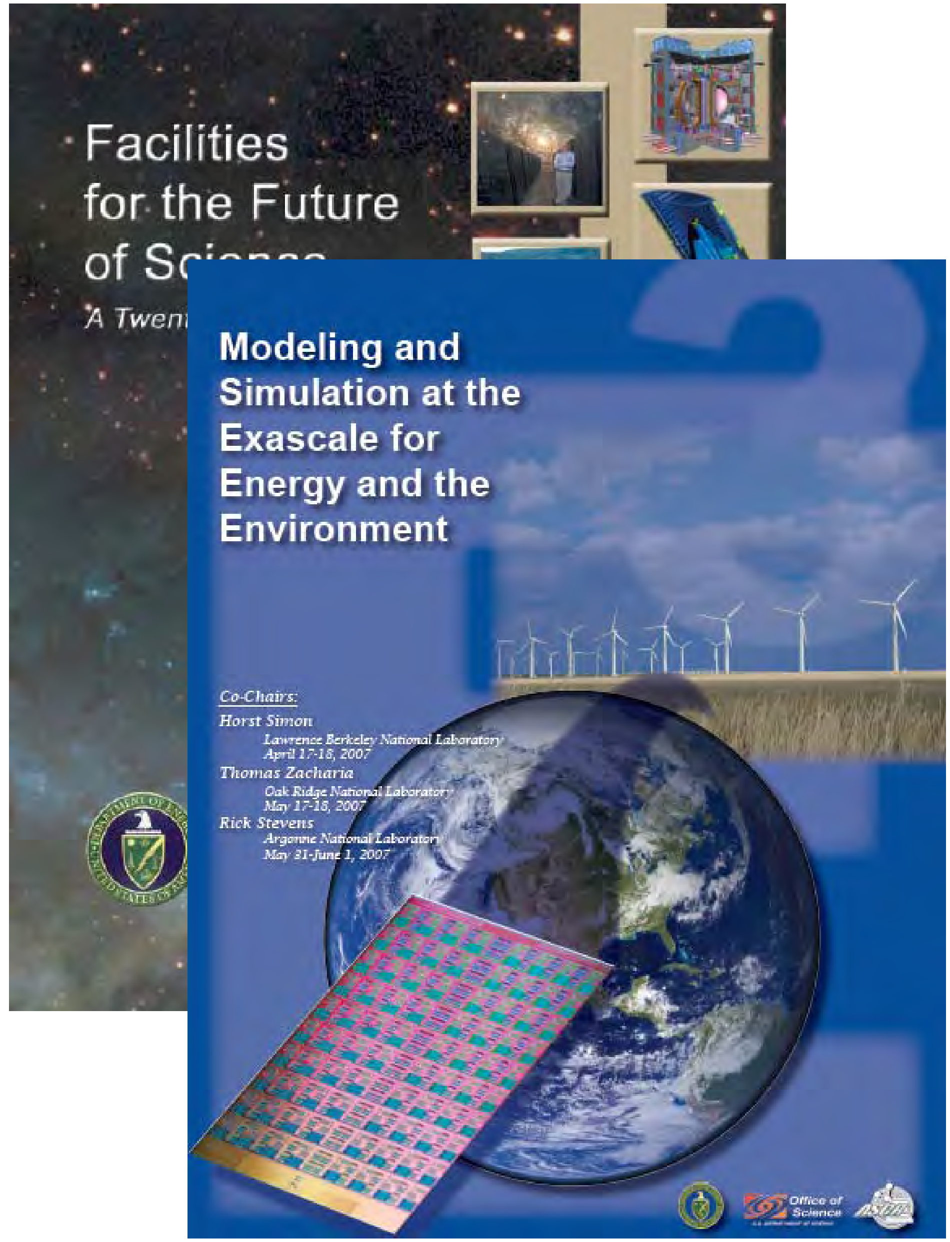
Figure 1 from the FSP Report

Of the reports to which I've recently contributed…



Why is this one the most important?

- **Historic opportunity for simulation**
- **Arrives "just in time" to help deliver civilization's arguably most important technology: essentially inexhaustible, essentially proliferation-free carbon-neutral energy – *the summum bonum***
- **FSP pushes ASCR-resident disciplines to new heights**
- **FSP demands the highest capability machines ASCR can muster**
- **OASCR and OFES are a proven team**
- **Simulation underprovisioned in ITER**
- **U.S. currently positioned to lead in large-scale integrated simulations of magnetically confined fusion plasmas**
- **FSP lies in the crosshairs of priorities #1 and #2 of *Facilities for the Future of Science* and also of the 2007 *"E3"* initiative**



20-year DOE SC facilities plan

Status of Facilities in 20-Year Outlook

By the end of FY 2007

Near-Term

Priority	Program	Facility		R&D	Conceptual Design	Engineering Design	Construction	Operation
1	FES	ITER						
2	ASCR	UltraScale Scientific Computing Capability						
Tie for 3	HEP	Joint Dark Energy Mission						
	BES	Linac Coherent Light Source						
	BER	Protein Production and Tags →	Bioenergy Research Centers*					
	NP	Rare Isotope Beam Facility (previously RIA) #						
Tie for 7	BER	Characterization and Imaging →	Bioenergy Research Centers*					
	NP	CEBAF Upgrade						
	ASCR	ESnet Upgrade						
	ASCR	NERSC Upgrade						
	BES	Transmission Electron Aberration Corrected Microscope						
12	HEP	BTeV #		Terminated				
13	HEP	International Linear Collider						

Context of this presentation

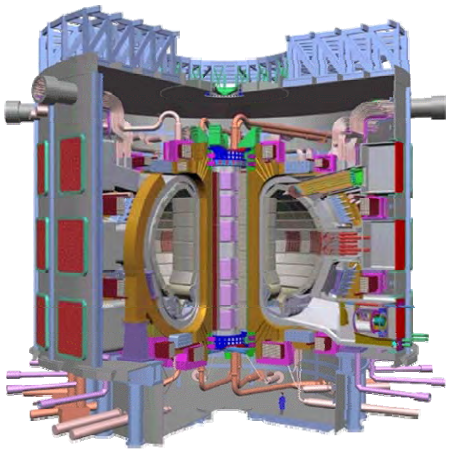
- Previous presentations of 2007 FSP workshop report emphasized OFES motivations
  - To FESAC
  - To PSACI (Plasma Sciences Advanced Computing Institute)
  - To FESAC FSP subpanel
- OFES has extensively vetted the FSP report
  - Including participation of experimental and theoretical communities
- Here, OASCR motivations emphasized
  - A few physics details retained, but see other the other reports for completeness
  - Mathematics and Computer Science agendae are mainstream and amortizable
- Both offices have strong interests in the FSP
  - To serve nation and world
  - To accelerate important research capabilities of their own
- Five years of studies should now move to a very specific project proposal stage
  - Beyond the report's intentionally inclusive (and code-name-neutral) sweep to a *particular* refereed project plan
  - In analogy to the way DOE SC procures facilities and talent for large experimental campaigns

FSP objective and motivation

- **Primary objective of the Fusion Simulation Project (FSP)**
  - **Create high-performance software to carry out comprehensive predictive integrated modeling simulations, with high physics fidelity, relevant to ITER and other toroidal fusion devices**
    - **Leadership class computers are also necessary to achieve this objective**
- **Urgent need for FSP, motivated by physics associated with ITER discharge scenario planning and control**
  - **Each discharge in ITER is expected to cost about a million dollars**
    - **Predictive whole device simulations needed to optimize discharge scenarios**
    - **Experimental teams with best scenario modeling have competitive advantage**
  - **Prior to completion of ITER construction, controls must be developed to suppress large-scale instabilities that can adversely affect confinement**
  - **Accurate predictions are needed for**
    - **Edge transport barrier that enhances the core plasma confinement**
    - **Edge instabilities that cause fluctuations in power to the divertor and first wall**
- **Fully verified and validated comprehensive integrated modeling capability is essential to support burning plasma experiments**

ITER integrated modeling needs

From May 2007 workshop presentation by W. A. Houlberg (on behalf of D. Campbell and the ITER International Organization)

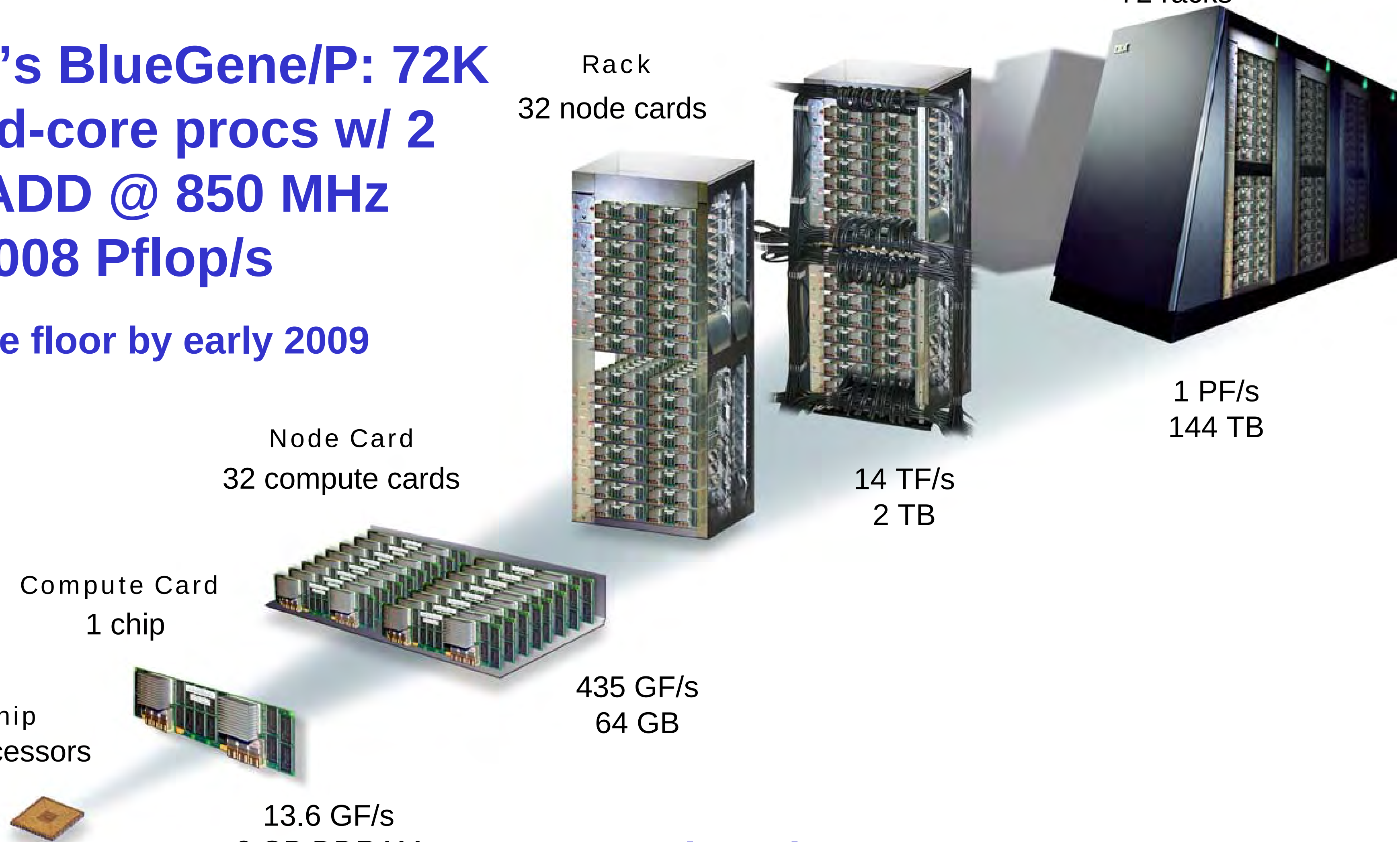


- The ultimate success of ITER will rely heavily on national programs such as FSP
  - Need to know basic interactions among the physics processes, diagnostics and auxiliary systems in order to define the details of ITER control systems
  - ITER IO will rely heavily on the resources of the domestic agencies
    - Domestically funded programs will be coordinated on an international level
- Schedule for initial modeling capabilities for ITER is aggressive
  - Currently re-analyzing the ITER design
    - Performance predictions will have to adapt to evolution in the design
  - Work on the plasma control system is underway
  - Planning for ITER operation requires intense involvement with the FSP
  - Operational program, with detailed scenario development including sequences of pulses, will need to begin around 2012
- Self-consistent modeling tools needed for scenario planning
  - Requires significant advances in modeling and computing capabilities

Emergence of petascale platforms

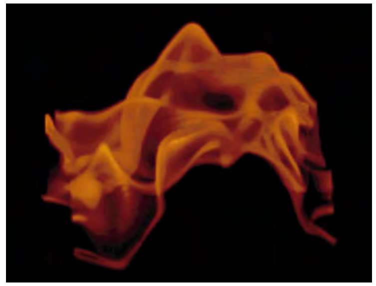
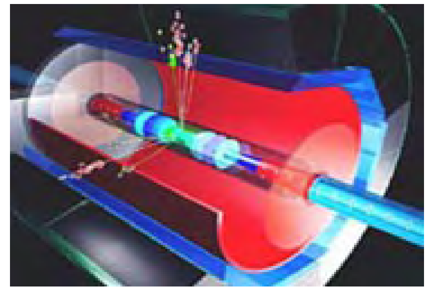
IBM's BlueGene/P: 72K quad-core procs w/ 2 FMADD @ 850 MHz = 1.008 Pflop/s

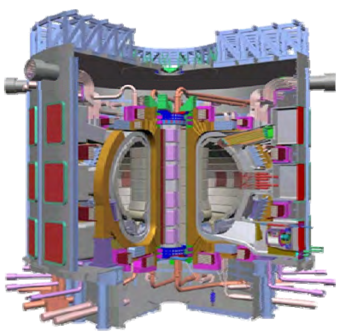
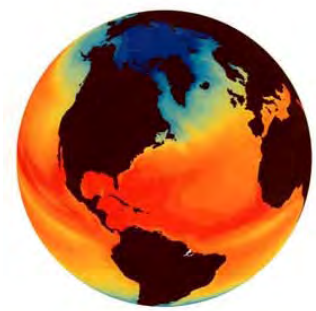
On the floor by early 2009



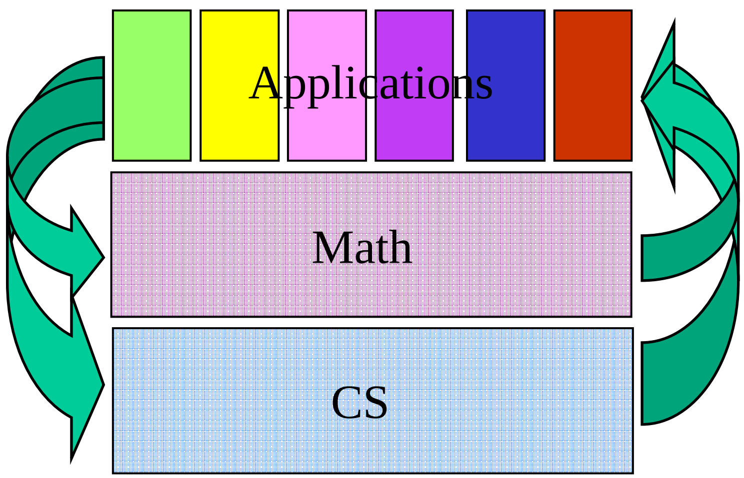
Thread concurrency: 288K (or 294,912) cores

SciDAC: amortizing general-purpose enabling technologies over many apps

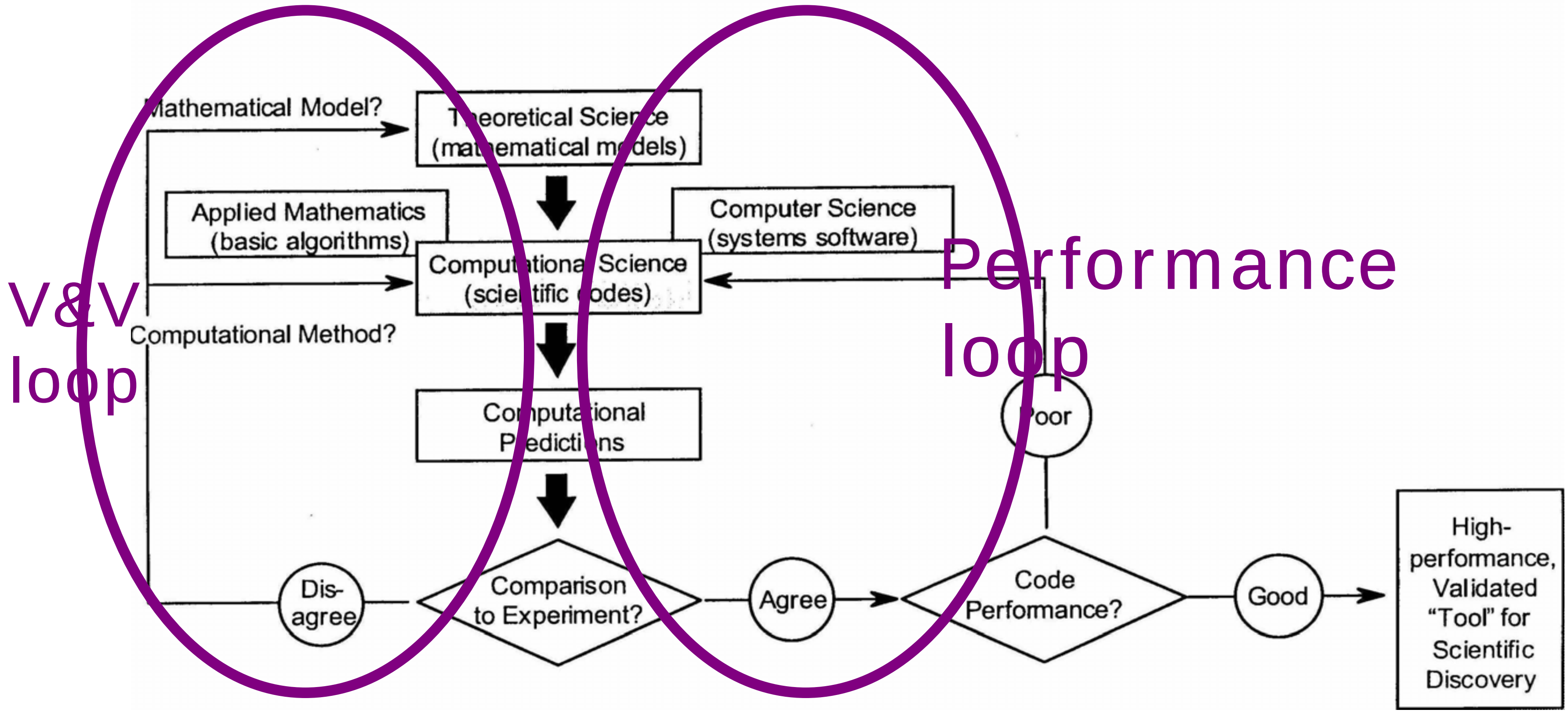



Many applications drive



Enabling technologies respond

Designing a simulation code – SciDAC-style



c/o SciDAC report, U.S. DOE, 2000

FSP background

- **Previous Fusion Simulation Project (FSP) report addressed questions outlined in charge letter of 22 February 2002**
  - **Outline 5-6 year initiative, the goal of which is develop an improved capacity for Integrated Simulation and Optimization of Fusion Systems (ISOFS)**
- **FESAC appointed committee to develop a roadmap ("Dahlburg report")**
  - **Final FESAC Report December 2002 (2 volumes)**
    - **http://www.isofs.info/ FSP_Final_Report.pdf**
    - **http://www.isofs.info/FSP_Appendix.pdf**
  - **Part I published in *Journal of Fusion Energy*, 2002**
  - **Fusion Simulation Project (FSP) envisioned as a 15-year, $25M/year multi-institutional project**
    - **Develop a comprehensive simulation capability for magnetic fusion experiments with a focus on ITER**
  - **Recommended an approach through Focused Integration Initiatives**
    - **Coupling pairs of components before moving to whole device modeling**
- **OFES formed an FSP Steering Committee in 2003 ("Post report")**
  - **Develop project vision, governance concept, and roadmap for the FSP**
  - **Recommends that the FSP consist of three elements:**
    - **Production component, a research and integration component, and a software infrastructure component**
  - **Final report in *Journal of Fusion Energy*, 2004**

Context for FSP

- Plasma physics simulations have become significantly more sophisticated in recent decades
  - The first round of SciDAC projects concentrated on first principles simulations of individual physical phenomena
    - Development of high fidelity physics models for individual physical processes needs to continue
  - The second round of SciDAC projects combines pairs of processes
  - FSP is intended, after 15 years, to combine all relevant physical phenomena in comprehensive tokamak plasma simulations
    - In the first 5 years, there will be focus on a limited number of problems for which advanced simulation capability can provide exciting scientific deliverables that substantially impact realistic predictive capabilities
- Hardware is evolving and software needs to keep up
  - Within two years, we will be in the era of petascale computing (10^{15} flop/s) with massively parallel distributed memory multicore computers
  - Each physics model challenging at this scale because of the huge number of threads required
  - Integrated modeling challenging beyond individual codes because of the diverse physics and algorithmic modules
- FSP will develop comprehensive modeling of whole tokamak plasma
  - With simultaneous interactions of multiple physical processes treated in a self-consistent manner
  - Use modules with much improved physics fidelity

Preparation for FSP workshop

- **From March 2007 establishment until May 2007 workshop, four panels had weekly teleconferences**
  - **Project Management and Structure**
  - **Status of Physics Components**
  - **Integration and Management of Code Components**
  - **Mathematical/Computational Enabling Technologies**
- **Teleconference call minutes were recorded and posted on the Fusion Simulation Project website**
  - **www.lehigh.edu/~infusion**
- **Many draft statements and paragraphs evolved during this period**
  - **Drafts evolved through e-mail and wikis**
- **Teleconferences were open to all members of all panels**
  - **Usually, panel conference calls were attended by some members of other panels for cross-fertilization of ideas**
- **Thanks largely to *Martin Greenwald, Arnold Kritz, Cynthia Phillips, Tom Rognlien*, and *Xianzhu Tang* of OFES and to *Phil Colella, Dan Meiron,* and *Pat Worley* of OASCR, the best-prepared report-writing workshop I've been involved with**

Workshop panels

Status of Physics Components

* Scott Parker U. Colorado
* Cynthia Phillips PPPL
* Xianzhu Tang LANL

Glenn Bateman Lehigh
Paul Bonoli MIT
C-S Chang NYU
Ron Cohen LLNL
Pat Diamond UCSD
Guo-Yong Fu PPPL
Chris Hegna Wisconsin
Dave Humphreys GA
George Tynan UCSD

Required Computational and Applied Mathematics Tools

* Phil Colella LBNL
* David Keyes Columbia
* Pat Worley ORNL

Jeff Candy GA
Luis Chacon LANL
George Fann ORNL
Bill Gropp ANL
Chandrika Kamath LLNL
Valerio Pascucci LLNL
Ravi Samtaney PPPL
John Shalf LBNL

Project Structure and Management

* Phil Colella LBNL
* Martin Greenwald MIT
* David Keyes Columbia
* Arnold Kritz Lehigh

Don Batchelor ORNL
Vincent Chan GA
Bruce Cohen LLNL
Steve Jardin PPPL
David Schissel GA
Dalton Schnack Wisconsin
François Waelbroeck Texas
Michael Zarnstorff PPPL

Integration and Management of Code Components

* Dan Meiron Cal Tech
* Tom Rognlien LLNL
* Andrew Siegel ANL/U. Chicago

Michael Aivazis CalTech
Rob Armstrong Sandia
David Brown LLNL
John Cary Tech-X
Lang Lao GA
Jay Larson ANL
Wei-Li Lee PPPL
Doug McCune PPPL
Ron Prater GA
Mark Shepherd RPI

* Indicates Fusion Simulation Project Committee Member

FSP workshop report (June 30, 2007)

- **The FSP workshop report:**
  - Identifies key scientific issues that can be addressed by integrated modeling that takes advantage of the physics, computer science, and applied mathematics knowledge base
  - Identifies the critical technical challenges for which predictive integrated simulation has a unique potential for providing answers in a timely fashion
    - In a way that traditional theory or experiment by themselves cannot
  - Establishes a plan to improve the fidelity of the physics modules required for predictive tokamak whole device modeling
    - Well supported theory and experimental fusion programs are essential
  - Identifies the critical areas of computational science and infrastructure in which investments would likely produce the tools required for the FSP to achieve its goals
  - Addresses issues associated with project structure and management of the proposed FSP
- **The FSP panels concluded that it is essential to produce, in a timely way, advanced whole plasma simulation capability using high-performance computers to:**
  - Provide key scientific deliverables
  - Make accurate predictions for burning plasma experiments

Fusion Simulation Project (FSP)

- **FSP mission: Develop a predictive capability for integrated modeling of magnetically confined burning plasmas**
  - **Create high-performance software to carry out comprehensive predictive integrated modeling simulations, with high physics fidelity**
    - **For ITER, future demonstration fusion reactors, and other toroidal plasma devices**
- **Petascale computers are necessary to achieve this mission – *after* algorithmic advances**
- **FSP goal: Predict reliably the behavior of plasma discharges in toroidal magnetic fusion devices on all relevant time and space scales**
  - **FSP must bring together into one framework a large number of codes and models that presently constitute separate disciplines within plasma science**
- **FSP integrated modeling capability will embody the theoretical and experimental understanding of confined thermonuclear plasmas**
  - **Theoretical models will be implemented and used in the context of self-consistent simulations that can be compared with experimental data**
  - **Experimental data will be analyzed and organized in a way that can be compared with simulation results**

FSP will benefit the U.S.

Benefits of FSP to U.S. ITER team drove the workshop

- FSP provides an opportunity for the United States to leverage its $1B+ investment in ITER
  - Access for experimental campaigns on ITER must survive highly competitive scientific review process
  - FSP predictive simulation capability will enhance credibility of proposed U.S. experimental campaigns, thereby maximizing U.S. access to ITER operation
  - Enhanced scientific understanding of data from ITER discharges will provide an opportunity for scientific discovery
- FSP will capitalize on and exemplify the benefits of DOE investments in high-performance computing both hardware and software
  - Massively parallel computers will provide platforms for the demanding calculations entailed by FSP simulations
- Integrated simulation modeling efforts in Europe and Japan are briefly described in the workshop report
  - EFDA integrated modeling effort is underway in Europe
  - TASK and TOPICS integrated modeling codes are being developed in Japan
- FSP will confer competitive advantage over other partners in design, development and operation of future DEMO-class fusion power plants

FSP vision

- The vision for FSP was well stated in the 2002 Integrated Simulation of Fusion Systems Report [http://www.isofs.info/FSP_Final_Report.pdf]:

  The ultimate goals of the Fusion Simulation Project are to predict reliably the behavior of plasma discharges in a toroidal magnetic fusion device on all relevant time and space scales. The FSP must bring together into one framework a large number of codes and models that presently constitute separate disciplines within plasma science …

- FSP panels sought to establish well defined, realizable visions for five, ten and fifteen years keyed to needs of ITER and DEMO projects:
  - **Five years:** **Assemble a new powerful integrated whole-device modeling framework that uses high-performance computing resources for the simulation of tokamak plasmas**
  - **Ten years:** **Develop a simulation facility that is required to meet the national scientific and engineering objectives for ITER throughout the remainder of its operational lifetime**
  - **Fifteen years:** **Develop a simulation facility that will be sufficiently well validated to extrapolate with confidence to a DEMO reactor based on the tokamak concept or other more advanced magnetic confinement concepts**

Driving questions for FSP

- **To motivate the FSP, it was decided at the workshop to answer these questions for each modeling capability proposed ("gaps analysis"):**
  - **What are the critical compelling scientific and technical issues that the fusion program faces *for which computation is required*?**
    - **What substantial contribution can computer simulation make that traditional theory or experiment, by themselves, cannot?**
  - **For each critical issue, *what is the current state of the art and what is missing* from the current capability?**
    - **What are the underlying models and algorithms that are used in computer simulations relating to the critical issues?**
      - **Modules that are required are often scattered among a variety of codes and are not consistent in level of sophistication**
  - **For each critical issue, *what new capabilities are needed* in order to produce simulations that will aid in addressing critical issues?**
    - **What investments in fusion science as well as computational science and infrastructure must be made to obtain solutions for the critical issue?**
- **Many critical issues require advanced simulation capability**
- **Five critical issues were selected for more detailed consideration**

Critical issues for burning plasma experiments to be addressed by FSP (slide 1 of 2)

1. Disruption effects and mitigation

- ITER can sustain only a limited number of full-current disruptions
- Important to predict the onset of a disruption and to take actions that minimize damage when a disruption occurs

2. Pedestal formation and transient heat loads on the divertor

- Pedestal height controls confinement
  - Simulation of onset and growth of pedestal needed to predict confinement
- Large ELM crashes can damage the divertor
  - Require prediction of frequency and size of ELMs as well as the effect of stabilization techniques

3. Tritium migration and impurity transport

- Since tritium can migrate through the edge plasma to locations where it is hard to remove, we must predict the transport of tritium
- Since impurities can dilute the deuterium-tritium fuel and degrade fusion power production, we must predict impurity influx and transport

Critical issues for burning plasma experiments to be addressed by FSP (slide 2 of 2)

4. Performance optimization and scenario modeling

- **Performance includes sustaining maximum fusion power production**
  - Since each ITER discharge will cost about $1M, it is important to plan each discharge and to evaluate the results of each discharge carefully
- **Scenario modeling is used to plan new experiments**
  - Since multiple experimental teams will be competing for ITER running time, teams with best scenario modeling capability may obtain more running time
- **Scenario modeling is used in data analysis**
  - Validated simulations provide a way to embody our knowledge of fusion plasmas

5. Plasma feedback control

- **Burning plasma regime is fundamentally new, with stronger self-coupling and weaker external control than ever before**
  - Burning plasma experiments are designed to operate near parameter limits but must avoid damaging disruptions
- **Real-time feedback control essential to avoid disruptions and to optimize the performance of burning plasma experiments**
  - Instability control includes the use of modulated heating and current drive, as well as the application of non-axisymmetric fields

Physics “components” essential for integrated burning plasma simulations

- Many physics “components” are important in addressing critical issues in the integrated modeling of burning plasma experiments
- In order to optimize burning plasma performance, many of these components require substantial physics and computational advances
- To illustrate the advances required, four components required in an integrated simulation of a burning plasma were identified :
  - Core and edge turbulence and transport
  - Large-scale instabilities
  - Sources and sinks of heat, momentum, current and particles
  - Energetic particle effects
- These are on-going research areas in plasma fusion, to be harvested continually for the FSP
- It is recognized that other components might have been chosen to illustrate the advances required
  - For example, edge physics, equilibrium, wall material physics, atomic physics …

Physics components are interactive

- Many physical processes in tokamaks interact strongly as illustrated in Table 2.1 in the report
  - Whole device integrated modeling codes are needed to simulate strongly interacting physical processes observed in experiments
- Examples of interacting processes:
  - Large scale instabilities can strongly modify plasma profiles which, in turn, can affect the driving mechanisms producing instabilities
    - Sawtooth oscillations (internal kink/tearing modes) redistribute current density, thermal particles and fast particle species and seed neoclassical tearing modes
    - Neoclassical tearing modes (NTMs) are very sensitive to current and pressure profiles and produce flat spots in those profiles
    - Energetic alpha particles (fusion products) can excite global instabilities that can redistribute or remove these particles before they deposit their energy
  - Boundary conditions strongly affect core plasma profiles
    - H-mode pedestal height, normally limited by ELM crashes, controls core temperature profiles since anomalous transport is “stiff”
    - Wall conditioning has a strong effect on discharge performance
  - Distortion of velocity distribution due to slowing down of fast ions from NBI, RF and fusion reactions need to be included in gyrokinetic turbulence codes
    - Fast ions are redistributed by large scale instabilities and slowing down time is affected by plasma profile changes caused by sawtooth crashes

Integration and management of code components

- FSP represents a new level of the integration of leading edge simulation components
  - Very large project, which requires geographically distributed collaboration because expertise is currently distributed
  - Legacy and recently written codes will play a role in early stages of FSP
    - FSP should make use of the expertise embodied in existing codes
    - FSP must satisfy the large user base of currently used codes
- Required advances in component architecture are critical
  - To facilitate large number of people working simultaneously on a large code
  - FSP will require a variety of levels of integration across time scales, spatial regions, different physical phenomena
- Investments are needed for software design, repository management, release management, regression suites and documentation
  - There is trade-off between rapid development and code stability
  - Software tools will help manage code development and maintenance
- Software tools are also needed to enhance connection between simulations and experiments

FSP and OASCR vision

- FSP agenda for applied mathematics and computer science is at the top of the OASCR ten-year vision statement “Modeling and Simulation at the Exascale for Energy and the Environment”
  - Integration focusing on whole-system behavior, going beyond traditional reductionism focused on detailed understanding of components
  - Interdisciplinary simulations incorporating all relevant expertise
  - Validated simulations capitalizing on the ability to manage, visualize, and analyze ultra-large datasets
- FSP programmatic themes support the OASCR vision
  - Engagement of top scientists and engineers to develop the science of complex systems and drive computer architectures and algorithms
  - Investment in pioneering science to contribute to advancing energy, ecology, and global security
  - Development of scalable algorithms, visualization, and analysis systems to integrate ultra-scale data with ultra-scale simulation
  - Build-out the required computing facilities and an integrated network computing environment
- The readiness of the OFES customer is exemplary

Mathematical and computational enabling technologies

- Research topics and techniques, important to the success of FSP are identified in the areas of
  - Applied mathematics, data management, analysis, visualization, and performance engineering
- Investment in these critical areas is required for FSP to achieve its goals
- Efficient implementation of mathematical and computational methods on petascale and exascale resources requires applied mathematics progress on
  - Spatial and temporal discretizations of higher accuracy
  - Scalable solver methods for efficient utilization of computing resources
  - Inverse problem capabilities
  - Mathematical optimization and control techniques
- FSP will produce massive amounts of data that must be managed, mined, visualized and will benefit from advances in
  - Efficient storage techniques
  - Scientific data mining
  - Advanced visualization techniques
  - Scientific workflow technology

Applied Mathematics research areas in FSP

The list below is not an exhaustive list but rather a list of more likely research topics in applied mathematics within the scope of the FSP

- **Application of fully implicit Newton-Krylov methods**
  - **For research codes (*e.g.* extended MHD)**
  - **For coupled systems ("implicit" coupling)**
  - **Physics-based preconditioners**
- **Adaptive Mesh Refinement methods**
  - **Higher order spatial and temporal**
  - **Time implicit AMR methods**
- **Scalable solvers**
  - **Iterative**
  - **Sparse but special structures (block-dense)**
- **Adaptive fast-transform and pseudo-spectral methods**
- **Applied math issues in multi-physics coupling**
  - **General applied math issues concerning consistency of coupled formulation, convergence, accuracy**
  - **Methods such as projective integration may be useful for linking disparate time scales**

Computer Science research areas in FSP

- Scientific data management and mining
  - Transparent sharing of simulation and experimental data
  - Utilize modern database-like file storage approaches
  - Exploit scientific data mining for predictive simulations and to interpret experiments
- Scientific data analysis and visualization
  - Develop reliable quantitative scientific insight from raw data
- Software engineering
  - Trusted, maintainable, extensible, flexible, predictive integrated simulation
  - Automatic input checking for consistency and accuracy
- Performance engineering
  - Performance portability, performance instrumentation, frequent performance assessment and regression studies, performance characterization
- Successful exploitation of high performance computing resources
  - Identify achievable performance and suitability for massively parallel computing, for code, for algorithm, and for problem instance
- User interface to make complex FSP code usable

Verification and Validation (V&V)

- Verification and validation are essential for the role envisioned for FSP
- Verification assesses the degree to which a code correctly implements the chosen physical models
  - Sources of error include algorithms, spatial or temporal gridding, lack of convergence, coding errors, or compiler bugs
  - Verification activities include:
    - Software quality assurance, which is particularly difficult on massively parallel computers
    - Removing deficiencies in numerical algorithms, which involves comparing computational solutions with benchmark solutions, analytical solutions, manufactured solutions, and heroically resolved numerical solutions
- Validation assesses the degree to which a code describes the real world
  - Model validation emphasizes the quantitative comparison with dedicated high-quality validation experiments
  - Predictive estimation is characterization of errors from all steps in sequence of modeling process
    - Leads to probabilistic description of possible future outcomes based on all recognized errors and uncertainties
    - Research challenges: development of new sampling methods; uncertainty propagation for systems of systems; and extrapolation to higher levels in the validation hierarchy

Verification and Validation (V&V)

- Current approaches to V&V in simulations of magnetically confined fusion plasmas are often informal and *ad hoc*
  - Advent of FSP will provide an opportunity to introduce more uniform and rigorous verification and validation practices
    - This will aid in establishing the fidelity of the advanced physics modules
- A formal approach to model validation requires forging a strong collaboration with experimental facilities
  - To develop data sets that challenge the computational models
- Code developers and device operators must be assured that FSP codes are sufficiently accurate in their predictions
  - Particularly important if predictions are to be useful for modeling prospective scenarios or avoiding deleterious regimes in ITER
- Several FSP panels contributed to V&V considerations
- Verification and Validation are important confidence building exercises
  - Must be based on well established scientific approaches that allow *a priori* or *posteriori* estimates of calculational uncertainties
  - Serious approach to V&V requires that tests, once performed, are well documented

Five-year Deliverables

- New powerful integrated whole device modeling framework that uses high-performance computing resources to include the most up-to-date:
  - Global nonlinear extended MHD simulations of large scale instabilities, including effects of energetic particle modes
  - Turbulence and transport modeling (core and edge)
  - Radio frequency, neutral beam, and fusion product sources of heating, current, momentum and particles
  - Edge physics, including H-mode pedestal, edge localized modes, atomic physics, and plasma-wall interactions
  - Range of models that include fundamental computations
- Stringent verification methods and validation capabilities
  - Synthetic diagnostics and experimental data reconstruction to facilitate comparison with experiment
- State-of-the-art data archiving and data mining capabilities
- Production system to provide wide accessibility to a large user base
  - Verification and Validation achieved through widespread use of code
  - State-of-the-art visualization capabilities
- Provide capability to address critical burning plasma issues using high fidelity physics models and a flexible framework on petaflop computers

Ten and Fifteen-year Deliverables

10-year goal: Develop advanced and thoroughly tested simulation facility for initial years of ITER operation

- **Use high-performance computations to couple turbulence, transport, large scale instabilities, radio frequency, and energetic particles for core, edge and wall domains across different time and spatial scales**
  - **Pair-wise coupling will evolve to comprehensive integrated modeling**
- **Ability to simulate active control of fusion heated discharges using heating, fueling, current drive, and 3-D magnetic field systems**

15-year goal: Unique world-class simulation capability that bridges the gap between first principles computations on microsecond time scales and whole device modeling on the time scales of hundreds of seconds

- **Provide integrated high fidelity physics simulations of burning plasma devices that include interactions of large scale instabilities, turbulence, transport, energetic particles, neutral beam and radio frequency heating and current drive, edge physics and plasma-wall interactions**

FSP project management

- **FSP is a scientific development and focused research effort of unprecedented size and scope in U.S. fusion theory and supporting computational science and applied mathematics research programs**
  - **A strong and well-coordinated management structure is required**
    - **OFES and OASCR will specify the requirements in the request for proposals**
    - **Submitted proposals will provide detail on how the project will be structured and managed to achieve its goals**
  - **Effective management is required to ensure that deliverables and goals are achieved**
  - **Though unprecedented in size and scope for OFES and OASCR theory and simulation communities, experience from experimentalists in OFES informed the report**
- **Thirteen issues that management will have to address are identified**
  - **Management tasks associated with each of these issues are described**
  - **Management approach for these issues will be specified in the proposals that are submitted**

Management issues

- **Accountability**
  - Make clear who is ultimately responsible for project deliverables as a whole as well as for the individual parts of the project
- **Utility**
  - Mechanisms to evaluate the usefulness of the project, in whole and in parts
- **Delivery**
  - Ensure that release schedules and required capability are achieved
- **Expertise, advice, and evaluation**
  - Identify mechanisms, such as advisory committees and/or panels, by which required expertise is brought into the project
- **Communication**
  - Disseminate project requirements, schedules, progress and issues to the multi-institutional, geographically distributed workforce
- **Best practices and interdisciplinary integration**
  - Project structure should ensure that tasks are executed by teams that have embraced the expertise needed from all appropriate fields
- **Motivation and evaluation**
  - Establish mechanisms to ensure accomplishments are appropriately rewarded

Management issues

- Technical decision making
  - Project structure should allow for technical decisions to be made in a manner in which all participants are confident that they are heard
- Conflict resolution
  - Management structure must be able to identify the person and/or mechanism by which conflicts will be resolved
- Delivery and quality
  - Identify the mechanisms to insure deliverables are provided on time and that all quality standards are enforced
- Staffing and resource management
  - Dynamically assign resources and staff and establish a mechanism for reassignment of tasks, in partnership with the Department of Energy
- Risk assessment and mitigation
  - Quantify risk for each part of the software project and have appropriate backup solutions and/or have recovery methods in place
- Mentoring and education
  - Ensure that mechanisms exist for bringing into the project scientifically capable personal and establish liaisons with educational institutions

Fusion Simulation Project structure

Sample FSP Structure

- Lead institution for FSP that is chosen by an open, competitive process
  - Responsible to DOE for meeting the project goals and milestones
- High-level Program Advisory Committee (PAC)
  - Report to the top management of the lead institution
  - Composed of scientists external to the project
- Management Advisory Committee
  - Project Director and additional members chosen from institutions participating in the project
  - Represent the broad community and institutional interests
- FSP Project director (at lead institution)
  - Assemble management team that will coordinate and insure the success of the elements of the project
- Scientific Steering Committee
  - Addresses all activities of the project including research, production computing, and software design
- Software Standards Committee,
- Verification and Validation Committee,
- User Advisory Committee

Relation to the OFES base program

- **FSP requires well supported theory and experimental fusion programs**
- **Base theory program, in particular, is needed to provide improvements to the physics models, the algorithms and the computer science that are at the foundation of FSP components**
  - **Improved models are essential for physics fidelity of FSP simulations**
- **Improved diagnostics in experimental program are needed to provide accurate experimental data for validation of FSP simulation results**
- **It is expected that FSP personnel will work closely with plasma physics theoreticians and experimentalists at each stage in the development of the project**
- **New contributions and scientific discovery can result from significant advances in physics models, algorithms, software, computer hardware**
- **A dramatic increase in funding is required for FSP to reach its goals while maintaining a strong base research program**

Possible FSP budget scenario

OFES and OASCR Fusion SciDAC Funding (Million FY2008 $)				
	Core SciDAC Funding	FSP Funding		
Fiscal Year	SciDAC R&D (OFES)	Proto-FSP / FSP (OFES)	Proto-FSP / FSP (OASCR)	Total SciDAC Funding
2007	3.5	3/0	3/0	9.5
2008	4.0	3/0	3/0	10
2009	4.0	TBD	TBD	~12
2010	4.0	TBD	TBD	~16
2011	4.0	TBD	TBD	~22
2012	4.0	TBD	TBD	~25
2013	4.0	TBD	TBD	~28
2014	4.0	TBD	TBD	~28
2015	4.0	TBD	TBD	~28
2016	4.0	TBD	TBD	~28
2017	4.0	TBD	TBD	~28
2018	4.0	TBD	TBD	~28

FESAC recently concluded a review of the FSP report: charge questions*

1. **Has the report identified key scientific issues and grand challenges that can be addressed by this approach to linking the scientific knowledge base for fusion energy?**

2. **Have all the critical technical challenges been identified for which predictive integrated simulation modeling has a unique potential for providing answers in a timely fashion, in a way that traditional theory or experiment by themselves cannot?**

3. **Is there a clear plan to establish the fidelity of the advanced physics modules, including a sound plan for validation and verification?**

4. **Does the FSP Workshop clearly identify the critical areas of computational science and infrastructure in which investments would likely produce the tools required for the FSP to achieve its goals?**

5. **Have the issues associated with project structure and management of the proposed FSP been properly addressed?**

***Endorsed by FESAC yesterday; Stewart Prager, FESAC Chair, is transmitting the report to Undersecretary Orbach**

FESAC FSP Subcommittee

* **William Tang (PPPL and Princeton U.) Chair**: Chief Scientist, Princeton Plasma Physics Laboratory (PPPL) and Associate Director for Princeton Institute for Computational Science and Engineering at Princeton University

* **Riccardo Betti (U. Rochester)**: Professor of Mechanical Engineering & Physics at U. Rochester; *Member of FESAC*

* **Jeffrey Brooks (ANL)**: Senior Computational Nuclear Engineer at ANL

* **Vincent Chan (GA)**: Director of Theory and Computational Science at General Atomics; *Member of FESAC*

* **Thom Dunning (U. Illinois)**: Distinguished Professor of Computational Chemistry & Director of NSF's NCSA (National Center for Supercomputing Applications); *First Director of DOE's SciDAC Program*

FESAC FSP Subcommittee

* **Charles Greenfield (GA)**: Deputy Director of Experimental Science Division at General Atomics; *Deputy Director of the national Burning Plasma Organization (BPO)*

* **Brian Gross (GFDL)**: Deputy Director and Head of Computing at the Geophysical Fluid Dynamics Laboratory -- NOAA's National Laboratory for Climate Modelling

* **Michael Norman (UCSD)**: Professor of Physics and Center for Astrophysics & Space Sciences

* **Miklos Porkolab (MIT)**: Professor of Physics and Director of Plasma Science & Fusion Center (PSFC) at MIT

* **Rick Stevens (U. Chicago & Argonne National Lab)**: Professor of Computer Science at U. Chicago and Associate Director for Computational and Life Sciences at Argonne National Laboratory; *member of ASCAC*

Charge Question 1: Has the report identified key scientific issues and grand challenges that can be addressed by this approach to linking the scientific knowledge base for fusion energy?

Response: **Conditional "YES"**

- **The five critical science issues identified as most urgent for burning plasmas/ITER are *important and compelling***

--- similar list from independent assessment by European community (Reference -- *A. Becoulet, et al. IAEA '06, Paper TH/P2-22*)
--- each is a computational "grand challenge" in own right requiring integrated simulation capability

- **Fig. 2.2 (of Workshop Rpt.) captures *scientific complexity* of interacting physical processes within a tokamak discharge with *---- each topic in its own right requiring improved detailed physics understanding***

- **Table 2.1 (of Workshop Rpt.) illustrates how properties of tokamak plasmas depends on large variety of processes where "nearly everything depends on everything else" *---- makes case that an integrated approach is needed from a scientific perspective***

Charge Question 2: Have all the critical technical challenges been identified for which predictive integrated simulation modeling has a unique potential for providing answers in a timely fashion, in a way that traditional theory or experiment by themselves cannot?

Response: Conditional "YES"

- **The critical technical challenges identified are appropriate, and, as in the earlier reports from Dahlburg and Post, *<u>at least first major phase of FSP should be on a subset of these issues</u>* to ensure useful deliverables in a timely way**

- **<u>Expectations of FSP</u> productivity should be *<u>realistic and commensurate with actual funding support</u>***
  - **--- $3M in SciDAC FES for individual physics components, followed by $6M (3 yrs. later) for SciDAC "proto-FSP" integration projects (in "binary" sense)**

- **<u>Uniqueness aspect</u>:** ***Simulation bridges gap between experiment and traditional theory via state-of-art advances in Applied Math, Computer Science, and HPC together with V&V for improved predictive capability***
  - **--- Experiment encompasses all realistic physics but limited in *scalability of predictions* by natural bounds of hardware**
  - **--- Traditional Theory makes approximations to 1st-Principles equations to produce analytic and simplified numerical predictive solutions in *special limits of validity***

Charge Question 3: Is there a clear plan to establish the fidelity of the advanced physics modules, including a sound plan for validation and verification?

Response: **Conditional "YES" -- FSP Workshop Report clearly recognizes major importance of establishing the physics fidelity of advanced physics modules & associated essential role of Verification & Validation (V&V)**

- **While present vision for FSP provides reasonable framework and mechanism to move in right direction, it *needs a clear plan for V & V that benefits from/relies upon base programs for theory and experimental research***

- **Verification** ***assesses degree to which a code correctly implements the chosen physical model***
--- FESAC FSP Panel believes that this is more than "essentially a mathematical problem" --- Special emphasis should be placed on code verification via cross-code benchmarking and comparisons with theoretical predictions

- **Validation** ***assesses degree to which a code describes the real world --- Report in need of more specificity; i.e., example "action items"***

Charge Question 4: Does the FSP Workshop clearly identify the critical areas of computational science and infrastructure in which investments would likely produce the tools required for the FSP to achieve its goals?

Response: **Conditional "YES" -- FSP Workshop Report describes well the CS methodologies needed to produce needed tools including enabling mathematical techniques and infrastructure**

- **Chapters 3-6 of Report provide strong testimonial to *excellent working relationship between prominent researchers supported by OASCR and OFES***

- **More *specificity desirable on identifying most important software deliverables* and how they would be applied to FSP codes**
  --- specificity regarding code names & algorithms relevant to FSP more evident in earlier Dahlburg Report
  --- vision needed for how formidable *macro/micro-physics coupling* challenge will be addressed even if provided "infinitely powerful" compute power in future
  --- vision for *systems architecture & operational infrastructure* needed to address future "deadline-driven" data assimilation methods (for interpretation of shot-data for time-urgent experimental planning)

- **Dealing with programming strategies for the *multi-core architectures* expected to dominate future leadership class systems pose a huge challenge for FSP**

Charge Question 5: Have the issues associated with project structure and management of the proposed FSP been properly addressed?

Response: Conditional "YES" -- While the FSP Workshop Report does properly identify and address the issues associated with project structure and management, *prioritization with respect to the most critically important ones is needed*

- **FSP needs to be able to quantify *Risk Assessment/Mitigation***
  -- needed for project of this magnitude (comparable to experiments) together with backup solutions/recovery methods identified

- **FSP should have a detailed *Work Breakdown Structure (WBS)* in line with best practices guidelines (Example from Combustion Systems Simulation)**
  -- needed for technical decisions for *integrated product in which scientific basis for some components still evolving*

- **FSP as a large, multi-institutional, geographically-distributed project, demands *crisp communications* on requirements, schedules, progress, & timely issues**

- **FSP's project management & structure need to ensure high motivation & reward system for participants *within project and also within home institution***

Conclusions of FSP Review

• FSP Workshop Report represents impressive collaborative effort from a large segment of OFES and OASCR communities to help formulate an exciting project to produce realistic simulations of fusion systems with unprecedented physics fidelity

• Integrated modeling capability from FSP should be *embodiment of the state of theoretical & experimental understanding of confined thermonuclear plasmas*

-- provide reliable predictive capability with V & V to accelerate progress on answering outstanding scientific questions in field

• A successful FSP will better enable study of burning plasmas, aid the US role in operation of ITER, and help position the US for DEMO

--- powerful (peta- to exascale) platforms of future likely needed for effectively participating in ITER and for designing DEMO

• While the *Workshop Report is convincing on need for and benefits of FSP*, the associated *plan demands more specificity in a number of ways*
Nevertheless, it contains sufficient information for making the case that the *FSP can succeed in answering questions in a timely way that experiment and traditional theory by themselves cannot*.

Recommendations of FSP Review

• In order to be successful, the FSP should not be "everything to everyone." It must be *focused and project-driven with well-identified deliverables* that the stakeholders fully support.

• The FESAC FSP Subcommittee agrees with the five critical scientific issues identified in the Workshop Report as important areas of focus appropriate for the FSP. However, an integration effort encompassing all five of these challenging issues from the beginning looks to be too large a step. To be practically achievable, the *FSP should begin with more modest integration efforts that exhibit a compelling level of verification and validation*. This recommendation is in line with a similar position taken in the original FSP Report from Dahlburg, et al.

• The FSP should be a <u>repository of the latest physics as it evolves</u>. In this sense it cannot be a "stand-alone" project. It must be properly coordinated with theory, experiment and fundamental simulation. More specifically, a proper implementation of the *FSP will demand an effective plan for developing "advanced scientific modules" via utilization of results from the OFES base theory program, the SciDAC FES program, new insights from joint experiment-theory-modelling efforts, and the expertise residing in OASCR's computer science and applied math programs*.

Recommendations, cont.

• The FSP cannot succeed without a *viable validation and verification effort*, and this will imply expanding the diagnostic effort and linking it better to the FSP, for example through an *increased synthetic diagnostic development effort*. This will require special personnel with an appreciation of both diagnostic methods and code expertise.

• The management of the FSP should be organized with clear accountability and oversight and work out a *clear and compelling work-breakdown-structure (WBS).* It should also seek advice and guidance from a broad community of stakeholders, experimentalists, analytic theorists, fusion engineering scientists, applied mathematicians and computer scientists.

• The FSP should establish and maintain strong *connections with relevant international projects* and also draw on the large experience base from existing *scientific software development projects from other fields, such as ASCI*.

• The DOE should properly launch a true FSP only if a *sufficient critical funding level can be realistically met and sustained*.

Recommendations of FSP Review

Observation from FESAC FSP Subcommittee:

The effective "enfranchising" of the fusion community -- especially the experimentalists and technologists as well as analytic theorists -- into the Fusion Simulation Project (FSP) will require that this program produces first-rate scientific capabilities that help advance the research of a large user base of scientists working in these areas, particularly as their work relates to ITER and burning plasmas.

Finally, with regard to Dr. Orbach's request in the letter of charge to "recommend a course of action," the FESAC FSP Subcommittee would respond as follows:

Since the FSP Workshop Report has affirmed, strengthened, and generally updated the case made by the earlier reports from J. Dahlburg, et al. (2002) and D. Post, et al. (2004), we recommend that the FSP move forward to a Project Definition phase of development, keeping in mind the specific suggestions made in this FESAC FSP Subcommittee Report that are connected to the five questions posed in the letter of charge.

FSP and SciDAC: a personal view

From *SIAM News*, Volume 39, Number 7, September 2006

Taking on the ITER Challenge, Scientists Look to Innovative Algorithms, Petascale Computers

By Michelle Sipics

The promise of fusion as a clean, self-sustaining and essentially limitless energy source has become a mantra for the age, held out by many scientists as a possible solution to the world's energy crisis and a way to reduce the amounts of greenhouse gases released into the atmosphere by more conventional sources of energy. If self-sustaining fusion reactions can be realized and maintained long enough to produce electricity, the technology could potentially revolutionize energy generation and use.

ITER, initially short for International Thermonuclear Experimental Reactor, is now the official, non-acronymic name (meaning "the way" in Latin) of what is undoubtedly the largest undertaking of its kind. Started as a collaboration between four major parties in 1985, ITER has evolved into a seven-party project that finally found a physical home last year, when it was announced that the ITER fusion reactor would be built in Cadarache, in southern France. (The participants are the European Union, Russia, Japan, China, India, South Korea, and the United States.) In May, the seven initialed an agreement documenting the negotiated terms for the construction, operation, and decommissioning of the ITER tokamak, signifying another milestone for both the project itself and its eventual goal of using fusion to facilitate large-scale energy generation for the world.

Problems remain, however—notably the years, and perhaps decades, of progress needed to attain such a goal. In fact, even *simulating* the proposed ITER tokamak is currently out of reach. But according to David Keyes, a computational mathematician at Columbia University and acting director of the Institute for Scientific Computing Research (ISCR) at Lawrence Livermore National Laboratory, the ability to perform such simulations may be drawing closer.

Hardware 3, Software 9

"Fusion scientists have been making useful characterizations about plasma fusion devices, physics, operating regimes and the like for over 50 years," Keyes says. "However, to simulate the dynamics of ITER for a typical experimental 'shot' over scales of interest with today's most commonly used algorithmic technologies would require approximately 10^{24} floating-point operations." That sounds bleak, given the 280.6 Tflop/s (10^{12} flops/s) benchmark performance of the IBM BlueGene/L at Lawrence Livermore National Laboratory—as of June the fastest supercomputer in the world. But Keyes is optimistic: "We expect that with proper algorithmic ingenuity, we can reduce this to 10^{15} flops."

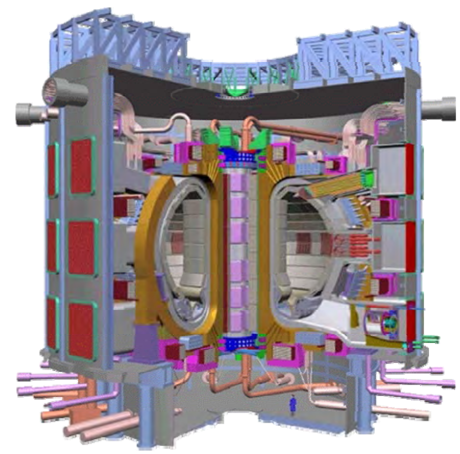
Optimizing the algorithms used, in other words, could lower the computing power required for some ITER simulations by an astounding nine orders of magnitude. Even more exciting, those newly feasible simulations would be at the petascale—ready to run on the petaflop/s supercomputers widely expected within a few years.

The ingenuity envisioned by Keyes even has a roadmap. Together with Stephen Jardin of the Princeton Plasma Physics Laboratory, Keyes developed a breakdown that explains where as many as 12 orders of magnitude of speedup will come from over the next decade: 1.5 from increased parallelism, 1.5 from greater processor speed and efficiency, four from adaptive gridding, one from higher-order elements, one from field-line following coordinates, and three from implicit algorithms.

Scaling fusion simulations up 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}

10^{12} needed (explicit uniform baseline)



International
Thermonuclear
Experimental
Reactor

in Cadaraches, France, operational by 2017

FSP ASCAC *6 November 2007*

Where to find 12 orders in 10 years?

Hardware: 3

- 1.5 orders: increased processor speed and efficiency
- 1.5 orders: in… ased … curren…

Software: 9

- 1 order: highe… eti… ns
  - Same … r elements
- 1 order: … g
  - Less … es
- 4 orde…
  - Zones r… d resolution requir… evere
- 3 orders: imp…
  - Mode growth time 9 … ders l… er th… Alfven-limited CFL

Algorithmic improvements bring yottascale (10^{24}) calculation down to petascale (10^{15})!

Comments on ITER simulation roadmap

- Increased processor speed
  - 10 years is 6.5 Moore doubling times
- Increased concurrency
  - BG/L is already 2^{17} procs, MHD now routinely at ca. 2^{12}
- Higher-order discretizations
  - low-order preconditioning of high-order discretizations
- Flux-surface following gridding
  - in SciDAC, this is ITAPS; evolve mesh to approximately follow flux surfaces
- Adaptive gridding
  - in SciDAC, this is APDEC; Cartesian AMR
- Implicit solvers
  - in SciDAC, this is TOPS; Newton-Krylov w/multigrid preconditioning

Concluding thoughts

- **The national fusion simulation effort needs a strong computational base, *fully worthy of the state of the discipline***
  - ***"Scientific codes embody the current state of understanding of natural and engineered systems" – Thom Dunning, Jr., SciDAC Report, 2000***
  - **Especially so, as the U.S. no longer enjoys experimental dominance and has no immediate plans to regain it (instead, to share it widely as a partner)**
  - **U.S. lead in simulation can easily be lost; our international partners are on the move in simulation**
  - **OASCR's OFES partners have ambitious simulation plans and need OASCR's help**
- **FSP is not just for leadership in plasma fusion science in the ITER campaign; it is foundational for subsequent commercial demonstration in DEMO**
  - **The U.S. should not be dependent on overseas capabilities for the latter**
- **FSP will provide a showcase application for current OASCR investments in petascale hardware**
- **FSP provides an ideal environment for displaying the fruits of decades of OASCR investments in people and scientific software**

Additional slides

FSP workshop agenda

Workshop was held at the Atrium Court Hotel, Rockville, MD on May 16-18, 2007

	Wednesday, 5/16/2007
	Plenary Session
8:30	**David Keyes / Arnold Kritz** Welcome and Organizational Announcements and Introduction
8:35	**Michael Strayer**, Associate Director for ASCR Introductory Remarks – *Fusion Simulations at Extreme Scale*
8:55	**Steve Eckstrand**, OFES Introductory Remarks—*Initiating the Fusion Simulation Project*
9:15	**Wayne Houlberg**, ORNL *ITER Integrated Modeling Needs*
9:50	Questions and discussion regarding ITER requirements
10:00	Coffee Break
10:15	**Marty Marinak,** LLNL *Role of Simulation in the ICF program*
10:50	Discussion on what can be learned from simulation experience in the ICF program
11:00	**Don Batchelor** Report on behalf of the Project Management & Structure (M&S) panel – Project scope, structure, and management
11:30	Feedback to M&S panel from all panel members and observers
12:00	**Working Lunch**; M&S Panel discusses feedback; other panels discuss and finalize their presentation

	Plenary Session Continues
1:00	**Xianzhu Tang** Report on behalf of the Status of Physics Components and Scientific Issues for Burning Plasmas panel
1:20	Discussion of Physics Components and Scientific Issues panel presentation
1:40	**Dan Meiron** Report on behalf of the Integration and Management of Code Components panel
2:10	Discussion of Integration and Management of Code Components panel presentation
2:30	**Patrick Worley** Report on behalf of Mathematical and Computational Enabling Technologies panel
2:50	Discussion of Computer Science / Applied Math panel presentation
3:20	Brief Comments by Workshop Observers
3:30	Break
	Breakout Sessions
3:50	Panel breakout sessions to evolve panel reports
5:30	Dinner (Panel Chairs meet to discuss evening work)
8:00	Panel breakout sessions to evolve panel reports

FSP workshop agenda – cont.

	Thursday, 5/17/2007
	Breakout Sessions
8:30	Panel breakout sessions to evolve panel reports
	Plenary Session
12:00	Brief presentations, during lunch, describing objectives and status of existing SciDAC-2 focused initiatives **John Cary** – FACETS **CS Chang** – CPES **Don Batchelor** – SWIMM
1:00	**Steve Jardin** Summary of FSP Management and Structure report. Feedback by members of other panels and by observers
1:30	**Cynthia Phillips** Summary of FSP Physics Components and Scientific Issues report. Feedback by members of panels and by observers
2:00	**Dan Meiron** Summary of FSP Integration and Managements of Code components report. Feedback by members of panels and by observers
2:30	**Patrick Worley** Summary of FSP Mathematical and Computational Enabling Technologies report. Feedback by members of panels and by observers
3:00	Break
	Plenary Session Continues
3:15	**Ray Fonck**, Associate Director for OFES Comments on the fusion simulation project, the workshop, and the planned report
3:30	**Walt Polansky,** Acting Director OASCR Computational Science Research and Partnerships Comments on the fusion simulation project, the workshop, and the planned report
	Breakout Sessions
3:45	Each panel resumes working on the FSP workshop report taking into account comments made in the plenary session
	Friday, 5/18/2007
9:00	FSP Committee, scribes, and DOE Office of Science organizers meet to assemble the first draft of the workshop report **Adjourn @ 2pm**

Approximately 75 attendees at workshop

Complete minutes of plenary sessions, including comments, questions and responses are available as a result of effort contributed by Antoinette (Tina) Macaluso of SAIC

1. Disruption effects and mitigation

- Disruptions are initiated by large-scale instabilities
  - Conditions for disruptive instabilities determined by evolution of plasma profiles, which are a consequence of sources and sinks and transport
- Disruption simulation capability is scattered across many codes that are not seamlessly integrated together into a coherent framework
  - Complete nonlinear evolution disruptions extremely difficult to compute
- For comprehensive analysis of disruption onset and effects, as well as accurate prediction and design of mitigation approaches, required new and integrated physics elements include:
  - Plasma-wall interaction, impurity transport, atomic radiation physics
  - Equilibrium and kinetic profile evolution
  - Nonlinear evolution of large scale instabilities
  - Runaway electron production
  - Effects of axisymmetric control actuators such as poloidal field coils
  - Effects of non-axisymmetric control actuators such as resonant magnetic field perturbation coils

2. Pedestal formation and transient divertor heat loads

- First-principles gyrokinetic simulations of the pedestal and scrape-off-layer are being developed by:
  - Center for Plasma Edge Simulation and the Edge Simulation Laboratory
- Gyrokinetic codes used to simulate pedestal formation and growth
  - Spatially axisymmetric gyrokinetic codes simulate neoclassical effects
  - Full 5-D turbulence simulation codes are nearing completion
    - Need to develop fully electromagnetic edge gyrokinetic simulations
- Two-fluid codes have been applied to modeling of the pedestal on transport and turbulence timescales
- Monte Carlo and fluid formulations used to model neutral transport
- Linear and nonlinear extended MHD codes used to model ELM triggering and ELM crash evolution
  - Kinetic effects on ELMs may well play a significant role
- Require multi-scale integration between plasma phenomena operating on turbulence, neoclassical, large-scale MHD, various atomic physics, and transport timescales, as well as coupling to core plasma

3a. Tritium migration

- Modeling of deuterium and tritium recycling involves wall material simulations, presently performed by simple 1D diffusion codes
  - Present experimental results indicate D/T penetrates much deeper into the material than simple models indicate
  - Impact of energy pulses from ELMs is believed important
- Plasma tritium transport modeled by 3D Monte Carlo ion/neutral codes
  - Rates for the large number of molecular and surface processes often have a large number of adjustable coefficients to fit complex experimental results
    - Adjusted to values substantially larger than expected from simple theory
- Time-dependent diffusion simulations of tritium retention within first few microns of wall materials must be coupled to edge transport codes
  - Multi-species, 2D, two-velocity kinetic ion transport codes need to evaluate collisional, neoclassical impurity transport in edge region, coupled to core
- Inter-atomic potentials need to be developed for ITER mixed materials
  - For use in 3D molecular dynamics simulations of sputtering
- Molecular dynamics results need to be supplemented by 2D kinetic Monte Carlo simulations of slower wall surface chemistry processes that also generate hydrocarbons

3b. Impurity production and transport

- **Impurities produced by plasma-wall interactions and fusion products**
  - **Physical and chemical sputtering and evaporative release contribute**
    - **Impurity influx complicated by the presence of various wall materials, such as beryllium, carbon, tungsten, in different locations of the wall**
    - **Further complicated by impact of heat fluctuations during ELM cycles**
  - **Sufficiently high impurity influx can rapidly degrade fusion performance**
- **Chemical sputtering is not well understood, particularly for carbon wall**
  - **Empirically parameterized models, which utilize experimental data on material composition, surface conditions, wall temperature, incident plasma flux, and sometimes long-time exposure history**
  - **Extensions of the molecular dynamic sputtering database, mixed material simulation, and kinetic Monte Carlo simulations are needed**
- **Impurity transport simulations in scrape-off-layer need improvements:**
  - **Need to include 3D turbulence impact on multi-species impurities and coupling to kinetic transport**
  - **Gyrokinetic simulations of core, pedestal and scrape-off-layer are needed to predict impurity concentration and resulting effects on fusion performance**

4. Performance optimization and scenario modeling

- **Full-featured integrated modeling codes such as TRANSP or ONETWO are large codes that were started 30 years ago**
  - **They consist of a patchwork of contributions from a large number of people who were often working on isolated tasks under time pressure**
  - **The required models are often scattered among a variety of codes and are not consistent in their level of sophistication**
  - **Most of the codes are not modular, they do not use modern software engineering methods, and the programming practices do not always conform to accepted standards for reliability, efficiency, and documentation**
  - **As a result, these codes are difficult to learn, to run correctly, and to maintain**
- **A new comprehensive whole device integrated modeling code framework is needed for scenario modeling**
  - **In addition to a comprehensive collection of physics modules, the framework should include synthetic diagnostics and the tools needed to make quantitative comparisons between simulation results and experimental data**
  - **Tight coupling is needed for strongly interacting physical processes**
  - **Integrated framework should have options for first-principles computations**
  - **Simulations can make a substantial contribution in a way that traditional theory and experiment, by themselves, cannot**

5. Plasma feedback control

- ITER will be the most control-demanding tokamak ever built, at time of its commissioning, as first burning plasma experiment
  - Feedback control used to avoid disruptions and optimize performance
  - The need to certify high confidence control performance will place extreme demands on the physics simulation community
    - Will require an unprecedented amount of integration between frontier physics understanding and mission-critical control solutions
- Currently, 1-1/2D simulation codes include feedback actuator modules
  - Connection between these simulations and real-time control platforms has been demonstrate and used routinely on some devices
  - However, currently, there is minimal integration with other physical effects
  - Varying levels of accuracy, completeness, and validation, which are often insufficient for ITER requirements
- Needed for ITER Control Data Access and Communications system:
  - Control design models derivable from more detailed physics models
  - Full or partial shot integrated control scenario simulation capability
  - Modular infrastructure for flexibly using these products

1. Core and edge turbulence and transport

- Current research issues for core and edge gyrokinetic codes:
  - Electron thermal transport (resolving electron and ion dynamics together)
  - Effects of zonal flows and magnetic shear
  - Electromagnetic (finite beta) effects
- There is a debate in the field concerning the relative advantages of particle-in-cell vs. continuum approaches to gyrokinetic simulations
  - Special gyrokinetic codes have been developed for the edge, with its steep gradients, geometrical complexity, impurity and neutral-particle dynamics
- FSP needs to bridge gap between turbulence and transport time scales
  - One approach is to develop comprehensive reduced transport models from advanced gyrokinetic simulation results
    - Time-slice gyrokinetic simulations can recalibrate reduced models as needed
  - It is particularly challenging to simulate transport barriers
- Gyrokinetic codes must be developed to investigate turbulence in:
  - 3D plasma equilibria, such as regions with helical magnetic islands
  - Open flux surface regions in the scrape-off-layer at the edge of the plasma
- Core and edge turbulence simulations must be coupled

2. Large-scale instabilities

- **Includes neoclassical tearing modes, edge localized modes, sawtooth oscillations, resistive wall modes, and Alfven eigenmodes**
- **Nearly all of the forefront research in macroscopic instability modeling involves nonlinear mode evolution using extended MHD models**
  - **Extended MHD includes physics relevant to long mean free path plasmas, effects of energetic particles, two-fluid effects, and magnetic reconnection**
- **Modules are needed for computing mode stabilization such as**
  - **Localized current drive used for stabilization of neoclassical tearing modes**
  - **Rotation used to stabilize resistive wall modes**
- **Extended MHD models need rigorous closure on higher order moments for long mean free path fusion plasmas**
  - **Framework needed that yields concurrent solutions for**
    - **Fluid-moment-based extended MHD equations**
    - **Drift kinetic equation for long mean free path moment closure, and**
    - **Gyro-kinetic equation for effect of micro-turbulence on instabilities**
- **Improved numerical algorithms needed, particularly scalable solvers for implicit time advancement of strongly hyperbolic partial differential equations such as the extended MHD**
  - **Aggressive grid adaptation scheme needed that concentrates grid resolution near the location of the dynamically moving narrow layers**

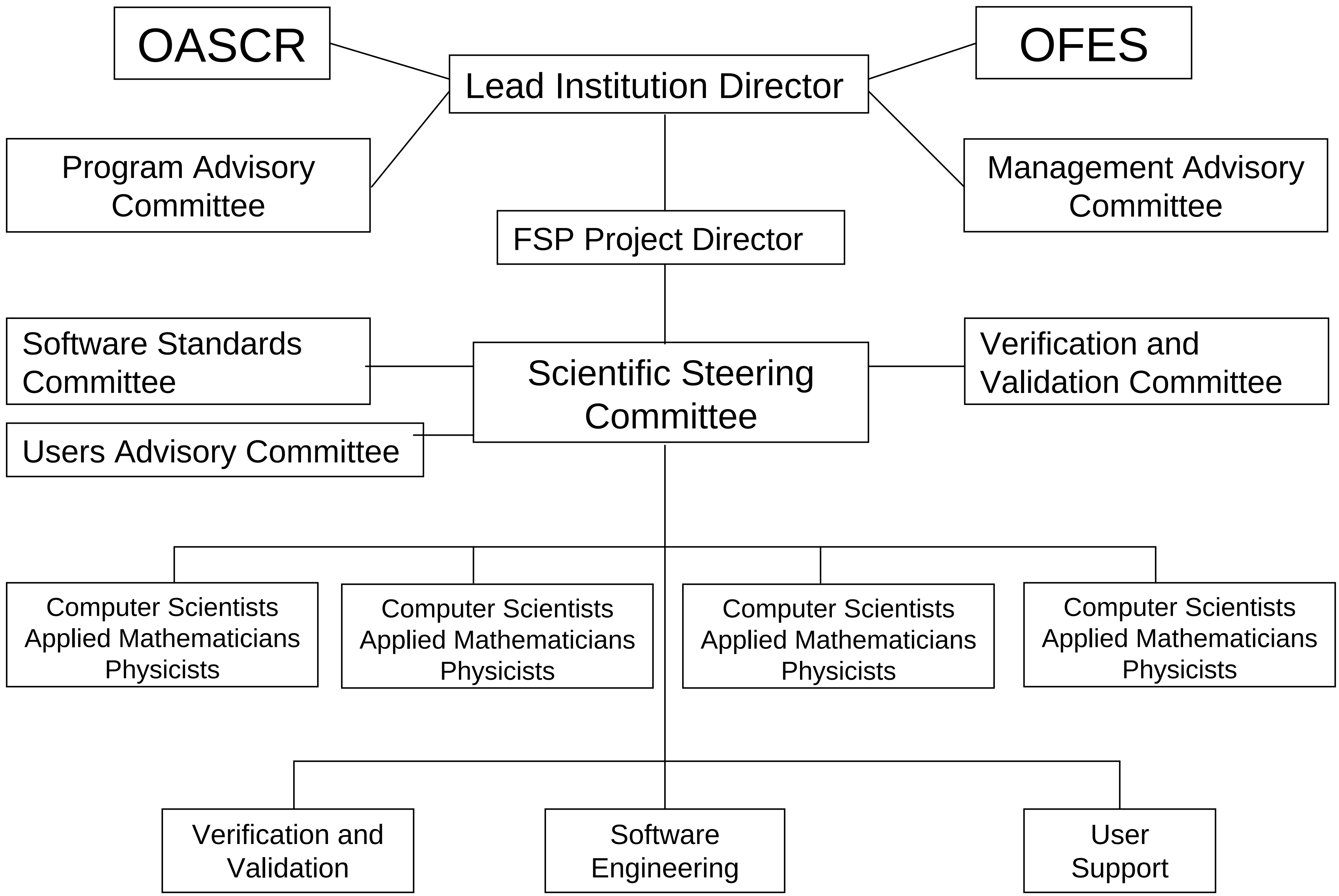
3. Sources and sinks of heat, momentum, current, and particles

- Includes radio frequency, neutral beam, fusion reactions, edge neutrals
- RF codes include:
  - Sheath physics near antennas
  - Full-wave electromagnetic field solvers
  - Bounce averaged Fokker-Planck codes for slowing down of fast particles
- Monte Carlo technique is most widely used to model slowing down of energetic particles from neutral beam injection and fusion reactions
  - Includes effects of large scale instabilities, magnetic ripple, banana orbits and finite gyro radius, charge exchange losses and the recapture of fast ions
- Improvements needed for RF codes:
  - Improved simulations need terascale and petascale computing platforms
  - Nonlinear formation of near and far-field RF sheaths implementing metal wall boundary conditions for the sheaths in ICRF full-wave solvers
  - Self-consistent coupling of Monte Carlo orbit codes to ICRF full-wave solvers
  - Inclusion of magnetic islands, scrape-off-layer, and more complete collision operator for slower ions needed in Monte Carlo codes

4. Energetic particle effects

- Expected to significantly affect behavior of burning plasmas
  - Can drive instabilities, which can eject energetic particles
  - Possibility of driving plasma rotation in ITER is an open issue
  - Energetic particle-driven Alfven instabilities can induce zonal flow which may suppress core plasma turbulence
  - Fusion alpha particles can stabilize the internal kink mode leading to monster sawteeth and can also stabilize resistive wall modes
- Codes currently simulate one cycle of growth, saturation, and decay of energetic particle-driven Alfven modes for moderate mode numbers
  - Codes are limited in physics and numerical efficiency for self-consistent high-resolution simulations of high-*n* modes in burning plasmas.
- Self-consistent nonlinear simulations of energetic particle-driven modes are needed on transport timescales
  - Need to investigate fast ion transport, driven by interactions of the energetic particles with Alfven instabilities with high mode number
  - Factor of ten higher resolution (in each dimension) and a factor of ten longer physical time period needed for alpha particle-driven Alfven instabilities

Sample FSP management structure



Schematic: Model FSP Organization Chart