Fusion Simulation Project:
Integrated Simulation & Optimization of Magnetic Fusion Systems

First report of the FESAC ISOFS Subcommittee
12 July 2002

ISOFS (Integrated Simulation & Optimization of Fusion Systems)
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Executive Summary

Fusion is a potentially inexhaustible energy source whose development entails understanding complex plasmas under extreme conditions. The development of a science-based predictive capability for high temperature, fusion-relevant plasmas is a challenge central to fusion energy science. The combination of extreme separation of time and spatial scales, extreme anisotropy, the macroscopic effects of microscopic physics, the importance of geometric detail, and the requirement of causality (inability to parallelize over time) makes this problem among the most challenging in computational physics. The exponential growth of computational capability, coupled with the high cost of operating large-scale experimental facilities, makes the development of a fusion simulation initiative a timely and cost-effective opportunity.

Numerical modeling has played a vital role in magnetic fusion for over four decades, with increases in the breadth and scope of feasible simulation enabled by improvements in hardware, software and algorithms. Currently, sophisticated computational models are under development for many individual features of magnetically confined plasmas. However, full predictive understanding of fusion plasmas also requires cross-coupling of a wide variety of physical processes. While integrated models using simplified descriptions of a number of physical processes exist and have been widely used in the program, the capabilities needed for full predictive simulation and optimization of a burning plasma require major qualitative improvements in physics models, algorithms, computational platforms, and the ability to integrate codes from a large number of research teams working on different elements of the problem. Such a capability was cited in the year 2000 FESAC IPPA integrated planning document as a ten-year goal. Worldwide progress in laboratory experiments provides the basis for a recent FESAC recommendation to proceed with a burning plasma experiment (see FESAC Review of Burning Plasma Physics Report, September, 2001). An integrated simulation capability would dramatically enhance the utilization of such a facility and the optimization of toroidal fusion plasmas in general. This undertaking represents a significant opportunity for the DOE Office of Science to create a capability that will advance the understanding of fusion plasmas to a level unparalleled worldwide.

The ISOFS subcommittee recommends that a major initiative be undertaken, referred to here as the *Fusion Simulation Project (FSP)*. The purpose of the initiative is to make a significant advance within five years toward the ultimate objective of fusion simulation – to predict accurately the behavior of plasma discharges in a toroidal magnetic fusion device on all relevant diverse time and space scales. This is in essence the capability for carrying out "virtual experiments" of a burning magnetically confined plasma, implying predictive capability over many energy-confinement times, faithful representations of the salient physics processes of the plasma, and inclusion of the interactions with the external world (sources, control systems and bounding surfaces).

Two fundamental issues are common to many fusion physics integration areas: coupling of phenomena at disparate space and time scales, and coupling models of different dimensionality. To solve these generic problems and achieve the integration we are seeking, strong collaboration and advances in physics, applied mathematics, and computer science will be required. This disciplinary integration will be an essential element of the program.

To succeed, a central feature of this initiative must also be an intensive and continual close coupling between the calculations and experiments. The phenomena in magnetic fusion devices, the equations describing them, and the interactions among the various critical phenomena are sufficiently complex that developing the most effective approximations and establishing when the models have the desired accuracy can only be accomplished by continual iteration and testing of the models against experimental data.

We envision that there will be three major categories of activity within the Fusion Simulation Project: 1) research to advance fundamental capabilities in fusion science, applied mathematics and computer science that address specific program critical needs; 2) development of applications modules, the core building blocks of an integrated modeling capability, in extended MHD, turbulence and transport, the plasma edge, and external sources, including development of the required computational science framework as well as the visualization and interpretation tools; and 3) project integration, which includes development necessary to create a comprehensive simulation including the interconnection and interoperation of multiple applications modules, oversight of software standards and release policies, collaborative tools, program governance, and accountability. It will likely be necessary to support more than one approach to various research areas in all three categories listed above.

Provided below is an overview of the Fusion Simulation Project.

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I. Background

On 22 February 2002, Dr. James Decker [then Director (acting), Department of Energy (DOE) Office of Science] issued a charge to the federal panel that provides advice to the DOE Office of Fusion Energy Sciences (OFES), the FESAC (Fusion Energy Sciences Advisory Committee). This charge, the letter of which is reproduced in the appendix of this report, requested advice on the development of a capacity for integrated simulation and optimization of fusion systems (ISOFS). The charge letter, further, indicated that the capacity should be developed by researchers from the DOE OFES in collaborative partnership with researchers from the DOE OASCR (Office of Advanced Scientific Computing Research).

Here we address the first two requests in the charge letter: to overview the current status of simulation of toroidal confinement fusion systems, and to describe a vision for a computational capacity for the full-integrated simulation of toroidal magnetically-confined fusion systems. Subsequently, and by 1 December 2002, a comprehensive plan for an ISOFS capability will be developed. This plan will include a detailed discussion of the role of applied mathematics and computer science in the initiative as well as the computational infrastructure needs of the initiative. Thus, the later report will address the remaining elements of the charge letter.

In order to address the ISOFS charge, the FESAC formed a subpanel, the FESAC ISOFS Subcommittee. Members of this Subcommittee are listed on the first page of this report. During the period 22 February to the present, the Subcommittee has taken as input for its deliberations both written and verbal contributions from members of the fusion and applied mathematics communities, and, further, convened in a workshop environment on 23-24 May 2002, to discuss the ISOFS charge. This document, which represents the results of the Subcommittee activity to date, is the first report of the FESAC ISOFS Subcommittee. The Subcommittee notes that substantial community input for the final report will be solicited at a major ISOFS workshop that is currently being planned for 17-18 September 2002; details about this upcoming meeting and extended Subcommittee activities may be found at the website: http://www.isofs.info .

II. Overview and Recommendations

Numerical modeling has played a vital role in magnetic fusion for over four decades with increases in the breadth and scope of feasible simulation enabled by improvements in hardware, software and algorithms. Recent developments in computers, computer science, and theory have created an opportunity to achieve dramatic advances from an intensive effort to harness these emerging capabilities. These advances can bring simulation to a level of sophistication enabling it to be an equal partner with basic theory and experiments in advancing the field.

The ability to understand and predict the dynamics of high temperature fusion-relevant plasmas is a formidable physics challenge that is central to the goals of the Fusion Energy Sciences program. It is widely recognized that the complexity of the dynamics of these systems is such that the development of computational models to understand their behavior is critical. Numerical modeling in magnetic fusion research, as exemplified by the fusion SciDAC projects, are providing important physics understanding and routinely stretch the limits of available supercomputers. However, crosscutting issues crucial to the further development of these models require a qualitative change in the approach to these problems. In particular, we find two fundamental issues that commonly appear in the integration of different fusion physics areas: the coupling of phenomena at disparate time scales and the necessity of coupling models of different dimensionality.

Further, research on fusion plasmas has often been compartmentalized into specific topical areas with little cross-talk between these topics – e.g., magnetohydrodynamics (MHD) and turbulent-transport. Since the dynamics of a high temperature plasma does not respect those categorizations, the inability to bridge the gap between the various models inhibits the ability to achieve the needed depth of understanding of key phenomena. Indeed, these are key issues for any challenging simulation effort such as climate modeling, inertial confinement fusion or astrophysics. To solve these generic problems and achieve the integration we are seeking, strong collaboration and advances in fusion physics models, applied mathematics, as well as computer science will be required.

A properly designed computational initiative that advances both the understanding of the key scientific processes which control plasma behavior, and the development of innovative techniques for cross linking these processes, would fundamentally advance the ability to predict the behavior of and therefore optimize fusion plasma systems. Such an initiative would:

- allow us to bring together the multiple disciplines necessary to take advantage of modern computing and advances in fusion theory;
- go beyond what is scientifically achievable by the disciplines in isolation; and,
- enable the full integration of theory, experiment, and simulation.

In view of the importance of establishing the feasibility of the potentially inexhaustible energy source, fusion energy – coupled with the complexity and variety of magnetic fusion physics, the exponential growth of computational power, the dramatic improvement in high-temperature plasma diagnostics, and the high cost of operating experimental facilities over the wide ranges of relevant scenarios – the development of a fusion simulation initiative represents a timely and cost-effective opportunity.

The ISOFS subcommittee recommends that a major initiative be undertaken, here referred to as the Fusion Simulation Project (FSP), of creating a comprehensive set of theoretical fusion models, an architecture for bringing together the disparate physics models, combined with the algorithms and computational infrastructure that enable the models to work together.

The purpose is to make a significant advance toward the ultimate objective of fusion simulation – to predict in detail the behavior of any discharge in a toroidal magnetic fusion device on all important time and space scales. This is in essence the capability for carrying out "virtual experiments" of a burning magnetically confined plasma, implying predictive capability over many energy-confinement times, faithful representations of the salient physical processes of the plasma, and the interaction with the external world (sources, control systems and bounding surfaces). The initiative should be structured to add capability incrementally and should adopt near and intermediate term objectives of: supporting basic theoretical research; supporting the understanding, interpretation, and planning of ongoing fusion experiments; exploration of new confinement concepts to improve the prospects for economical fusion power; and predicting the performance of future fusion devices.

The FSP should be comprised of three interacting levels of activities:

- Fundamentals: improvements in physics understanding in individual areas, including all relevant physical processes, validation by comparison with experiment and analytic models, development of advanced numerical approaches, and needed computer science advances;

- Applications modules: "stand-alone" integrated suites of codes, perhaps from multiple developers, that address fundamental problem areas such as MHD, turbulent transport, and external sources. Each applications module must be developed to high software engineering standards and be formulated in such a way so as to be compatible with other modules and seamlessly join to assemble the comprehensive simulation capability; and

- Integration: development necessary to create a comprehensive simulation capacity, i.e. development of flexible physics and computational frameworks which at all stages of the FSP provide all functions necessary to create a comprehensive simulation, including the inter-operation of applications modules, oversight of software standards and release policies, collaborative tools and the like. We envision a vigorous program of comparison and iteration with experiments at this level, as well as at the other levels.

The initiative should be carried out at a scale such that within five years certain goals can be achieved:

1) Robust computational modules are developed in each of the fundamental science areas representing the state-of-the-art in physics content, numerical methods, and computational science methods enabling efficient incorporation into the integration framework.

2) Approaches are developed for the fundamental problems of disparate time or space scales, and coupling of models of processes having different dimensionalities.

3) An initial inter-operable code capability that allows for three-dimensional geometry is available for widespread testing as a research tool.

4) The effectiveness of the integration approach is demonstrated by application to interpreting experimental data, and testing the validity of various physics models.

To bring these disparate components together will require the dedicated talents of many accomplished physicists, applied mathematicians and computer scientists. There is no doubt that the sociology of the FSP will be a challenge. On the one hand, a strong fusion physics effort is required, involving a number of institutions and the relevant theory, simulation, and experimental communities. On the other hand, setting priorities and a considerable degree of central direction will be essential. Even more challenging will be effective integration of first-rate computer scientists and applied mathematicians as equal partners with fusion physicists in this venture. The issue of project governance includes the establishment of an effective cooperative arrangement between and within OFES and OSCAR and clear delineations of working relationships with other initiatives and activities such as the DOE Office of Science SciDAC, OFES fusion experiments, and OSCAR computing resources. Success will require planning, leadership, and likely new management approaches.

This initiative rests entirely on a progressing science base. Therefore it is paramount that FSP funding be new to the program rather than redirected from present, critical areas. Also, it must be at a level adequate to accomplish the FSP goals. To estimate funding, we use the successful DOE Accelerated Strategic Computing Initiative (ASCI) Level 1 University Centers Program as an example, and recognize that a critical mass, as realized in that $25M/year program, must be applied to the elements of the applied and integration activities of FSP. This leads to the estimate that a total of $20M in new FSP funding will be required in the first year of the project, with an increment projected for the second year, followed by a leveling-off of funding in subsequent years of the activity. Through the course of the project, funding should be approximately equally allocated between OFES and OASCR research elements.

III. Fusion Simulation Project Elements

Bringing the power of advanced computing to the comprehensive simulation of fusion devices will entail three major categories of Fusion Simulation Project (FSP) activity: fundamental needs; applications modules; and project integration. Work within the category of fundamental needs addresses specific project critical needs. In some cases this work will include the solution of basic research problems in the areas of plasma science, applied mathematics and computer science. It will likely be necessary to support more than one approach to the same problem at this level of activity. Applications modules are the core building blocks of the initiative. These are integrated suites of codes or tools for the simulation of categories of phenomena as well as collaborative tools or algorithmic suites, as required. The project integration activity includes all functions necessary to create a comprehensive simulation including the inter-operation of applications modules, oversight of software standards and release policies, collaborative tools, program governance and accountability.

A. Fundamentals

In the past fifteen years, enormous progress has been made in the fusion program in experimental discoveries, theoretical insight, and computation. Internal transport barriers and other advanced regimes in tokamaks have been found and qualitatively explained in terms of the interaction of plasma flow shear and turbulence. Large-scale plasma turbulence simulations now promise to provide a complete quantitative description of these processes. A new understanding of tokamak disruptions has emerged. New stable MHD configurations for alternative concepts, such as stellarators, reversed-field pinches and other devices are being designed by means of advanced computational tools. Through MHD studies in the plasma edge, the limiting plasma pressure, density, and current are being better explained. The scrape-off layer outside the magnetic separatrix is being well modeled in the collisional regime by fluid codes, together with calculations of neutral-particle recycling. Instabilities driven by injected radio waves, particle beams, and, by extension, alpha particles, are being diagnosed and interpreted by theory and simulation. In addition to the above, there are many other examples.

Nevertheless, a number of major unsolved problems remain, which must be investigated and resolved in the course of this simulation initiative, including, for example, inclusion of kinetic effects in MHD fluid-like models, electron kinetics and the exploration of the electron gyroradius regime, particle and momentum transport, and the physics underlying transient and nonlocal effects. In the edge plasma, an outstanding problem is the width of the H-mode pedestal, which has an enormous effect on the overall plasma confinement. Kinetic codes, valid in the long mean-free-path regime of the edge and scrape off layer remain to be developed. Anomalous transport in stellarators is only beginning to be addressed. These are only a few of myriad tantalizing examples of FSP-relevant fundamental research that will lead to the modules described in the following sections.

B. Applications Elements

The applications elements are key system components. They integrate fundamental work, perhaps from multiple developers of the same process. These modules can be viewed as “stand alone” integrated suites of codes that address problems areas e.g. MHD, plasma microturbulence, and external sources. Each applications element must be developed to be compatible with other elements so that it is possible to join these elements together seamlessly to assemble the comprehensive simulation suite. Software engineering/standards and collaborative tools are included in this category. Applications elements will be built to deal with the broad concepts outlined below.

Element i. Turbulence and Transport

Plasma transport or confinement will be a major component of the integrated simulation project. We envision a time when reliable calculations of transport fluxes, informed by theory, and validated of experimental comparisons, will “inter-operate” with the other components of the computation. Loss of plasma particles and energy across field lines results from at least three categories of phenomena: diffusion and convection based on individual orbits and collisions (classical, neoclassical), anomalous diffusion and convection from turbulent microinstabilities (usually thought to be dominant), and phenomena that are instantaneous and nonlocal.

1) Neoclassical codes for both 2- and 3-dimensional configurations are available subject to certain approximations. Additional work will be required to fully implement the existing theories and to account for additional effects in the inter-operative environment, particularly in 3-D configurations (stellarators) and in tokamaks with transport barriers.
2) Micro-turbulence-driven anomalous transport will be dealt with on three levels: a) fine-scale stand-alone gyrokinetic simulations of core plasma turbulence will continue to be developed, interpreted by theory, and compared with experiment to firmly validate the fundamental theory and benchmark the other descriptions; b) reduced simulations will be coupled directly to the transport equation solvers. In some cases, it may be possible to directly couple the full turbulence simulations with the transport equation solvers; and c) algebraic models of transport will continue to be developed, again informed by theory, experiment, and the just-described simulations. When supported by turbulence simulations for selected cases, they will provide the most rapid parameter scans.
3) Work will continue on development of models of observed rapid and nonlocal phenomena (e.g. avalanches, radiative transport, or global magnetic interactions) that do not fit into the diffusive-convective approach. The architecture must include provision for these from the outset, so they can become incorporated when available.

A measure of success for these efforts and their validation will be the ability to predict and model a transport barrier, a region of steep gradients where turbulence is suppressed.

Element ii. Extended MHD

Modern fusion plasmas are subject to low frequency, long wavelength, fully three-dimensional hydromagnetic phenomena that can degrade confinement, and in some cases lead to major disruptions. The only computationally tractable model to describe these dynamics is based on fluid equations, which are derived from velocity moments of the more fundamental kinetic equation. These equations are solved simultaneously with the low frequency Maxwell equations. The resulting model is local in space but requires additional closure relations to obtain a self-contained system of equations and take account of kinetic effects. Models of magnetized plasmas based on this approach are collectively called (eXtended) MagnetoHydroDynamics (X-MHD).

There are two approaches to developing an appropriate system of closed Extended MHD equations. One approach is to calculate analytic expressions for the highest order moments of the distribution function for use in the fluid equations. Another approach is to solve the kinetic equations numerically to obtain the distribution function, and then evaluate its moments to obtain the required contributions to the fluid equations. The result of an X-MHD calculation is often that an initial equilibrium that has crossed a stability threshold will exhibit unstable behavior and then relax to a saturated state in a few Alfvén wave transit times. This is the case, for example, in a sawtooth oscillation. For an integrated plasma model, the effects of this MHD profile relaxation must be encapsulated into the description of the plasma evolution on the even longer transport time scale.

Element iii. External Sources

External systems that add mass, momentum, or energy to a plasma have been essential tools in the successful efforts to obtain good performance in present experiments and are sure to be a necessary part of plasma control in any future experiments and reactors. At present, the external sources include beams of neutral atoms that can carry energy, particles, and angular momentum across magnetic fields; radio frequency waves (RF) whose interactions with a plasma can be used for heating, current drive or flow drive; high-speed pellets of frozen fuel gas that can deliver particles deep into the plasma core; and gas fueling which supplies particles to the plasma edge.

The computational capabilities related to neutral beam injection are very well developed and are presently integrated into many codes. The work could be easily ported to codes developed in new initiatives. Wave-plasma interactions at RF frequencies (from ion to electron cyclotron frequencies) are the subject of intense ongoing research including fusion SciDAC activity. However, the scope of needed work, and the ability to provide interactive coupling with other plasma codes, extend far beyond the SciDAC activity. This area includes many distinct problems and will be an essential element of future plasma prediction, interpretation, and control schemes. Work on the ablation and subsequent transport and deposition of fuel from injected pellets is in a relatively early phase of development but certainly amenable to computation. However the physics of fueling in general is not in a satisfactory state at present and would benefit from basic theory studies of particle transport.

Element iv. Physics of the Plasma Edge and Connection to the Core and Wall

Edge plasma, which bridges the hot plasma core and the material wall, plays a crucial role in both overall plasma confinement and plasma-wall interactions. Our current understanding of the physics of edge plasma and the tools to model it are rather sketchy. We know that the physics of edge plasma is very complex and ranges from turbulent plasma transport to atomic physics and radiation, and to surface and condensed matter physics. Moreover, edge plasma turbulence is highly intermittent with a strong contribution to particle and energy fluxes from large but rare events, e.g. the so-called edge-localized modes (ELMs). Therefore, the conventional separation of spatio-temporal scales for the description of turbulence and transport is questionable. New approaches should be developed for both turbulence and transport phenomena that relax this ordering. Additional complications result from a strong variation of the plasma parameters from highly collisional to collisionless regimes. Therefore, the simpler fluid description is not always adequate and should be replaced by a much more complex hybrid or kinetic one. Because of the open field lines, such a code will have different boundary conditions from those of the core. Thus, the understanding and modeling of edge plasma and its coupling to the core from first principles are a real challenge for both theory and computing.

With large-scale efforts in this area, it is realistic to anticipate a number of advances. These include crucial improvement (e.g., adding neutral effects, some kinetic features, impurity transport, atomic physics, and geometry) of fluid edge turbulence codes to the level required to do more detailed modeling of the pedestal physics as well as to study macroscopic transport phenomena (e.g., heat loading, plasma-wall interaction, and tritium retention). Ultimately, edge plasma turbulence gyrokinetic codes should be advanced to a level adequate for the study of core-edge synergy effects.

Element v. Computational Science Framework

Advancing simulation capabilities in each constituent module of fusion simulation, and developing the ability to couple codes from multiple modules to create integrated simulations, will require development of new computational science research and methodologies in at least three areas.

1) Fusion simulations present a unique characteristic when compared to other PDE applications – the different physics modeled by different codes are often overlapping in space, instead of being decomposed into physical sub-domains. This implies tight coupling between modules, necessarily large communication to computation ratios, and close collaboration among physicists, applied mathematicians, and computational scientists.
2) Building software infrastructure and middleware for creating multi-physics simulations enabling dynamic interoperability of codes from different researchers and sites. Business and industrial computing now use software component architectures for such integration, but it is still a major challenge to connect large, distributed, and parallel physics codes.
3) Data management and sharing technologies. The challenges range from developing self-describing and portable file formats, to full-fledged data and meta-data frameworks such as MDS-plus which is already in extensive use by the fusion community. New scientific data systems can greatly ease the sharing of results between experiments and simulations and form a necessary first step towards code inter-operability for different regimes. Storage systems are now reliably supporting large scale (petabyte) data. Providing users with the ability to navigate, search through, and manage the large distributed data sets that will be generated and used in an integrated simulation is another major research problem.

The FSP software architecture will provide exciting new challenges for mathematicians and computer scientists, and can leverage the research from other programs, such as DOE SciDAC projects now developing numerical methods and computational infrastructure for large distributed simulations and models being developed within the ongoing theory program within OFES. Basic computational infrastructure has recently been deployed that will help: reliable authentication mechanisms for security, tools for wide-area scientific collaborations, software component systems supporting efficient data transfers, large-scale distributed data management systems, and capabilities that provide end-user access to these facilities. The FSP will, moreover, provide valuable mission-driven impetus for the development of user-friendly modules, infrastructure, and training, which will then be provided to code teams beyond the FSP.

Element vi. Interpretation and Visualization Tools

An integrated simulation will only be beneficial to our community if we can understand what it is telling us. To this end, it is imperative that the FSP have built-in a powerful diagnostic and analysis capability from the beginning.

There are several categories of diagnostics that are needed:

1) The ability to query the calculation regarding virtually any combination of internal variables, be they physical or numerical in origin, and including integral and differential operations.
2) The ability to easily graphically display any of the results of a calculation together with similar results from previous simulations, theoretical models, or experimental results.
3) Capabilities that facilitate experimental comparisons. Thus, we envision a number of software packages that provide a signal that can be directly compared with an experimental diagnostic on a given machine.

C. FSP Integration

As discussed in Sect.V of this report, MFE physics simulation presently includes primarily two categories of codes: 1) detailed simulations of a particular physical process (e.g. micro-turbulence, macroscopic MHD, RF-plasma interactions), and 2) transport codes that use reduced descriptions of the details to follow a significant portion of the plasma (e.g. the core or the edge) in reduced dimensionality (1 dimension for core, 2 for edge) over long timescales.

Our approach to integration is to develop an architecture that will:

- promote the development of the physics modules and their validation through experimental comparison, beginning in the near term;
- facilitate study of mutual physics interactions presently modeled in separate codes as such interconnections become appropriate; and
- increase significantly the depth and breadth of physics compared to today's transport codes, incrementally as better modules become available.

Two fundamental issues are common to many fusion physics integration areas: coupling of phenomena at disparate time and spatial scales, and coupling models of different dimensionality. To solve these generic problems and achieve the integration we are seeking, strong collaboration and advances in physics, applied mathematics, and computer science will be required. This disciplinary integration will be an essential element of the program.

To succeed, a central feature of this initiative must also be an intensive and continual close coupling between the calculations and experiments. The phenomena in magnetic fusion devices, the equations describing them, and the interactions among the various critical phenomena are sufficiently complex that developing the most effective approximations and establishing when the models have the desired accuracy can only be accomplished by continual iteration and testing of the models against experimental data. Hence, a continual process of testing and iteration is required to advance both modeling and the characterization of experimental results. From these objectives flow a number of requirements that the integration framework must satisfy:

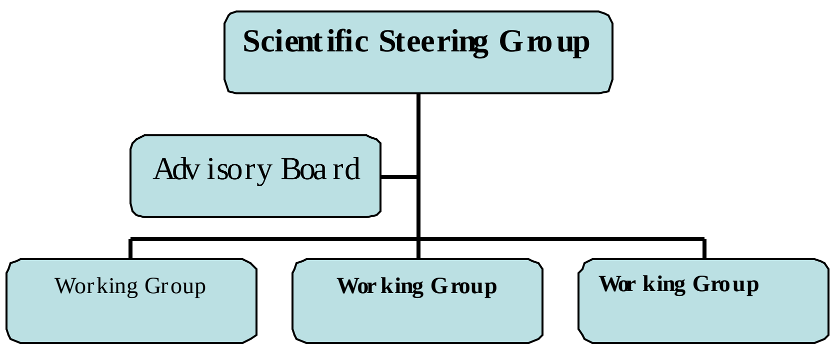
- It must be extensible.
  - Easy connections can be made early in the project while more difficult ones, for example those involving very disparate time-scales, can be added when appropriate.
  - Its architecture must permit continuous improvements and additions.
- It must be flexible.
  - Only the particular physics modules required for a given study need be interconnected.
  - It must be robust to changes in physics paradigms. For example a traditional diffusive transport model will be inadequate if non-local effects turn out to be essential.
  - It must be interpretive as well as predictive. That is it must be possible to make use of both experimental information such as profiles, and predicted information such as source rates, to interpret other needed quantities such as transport coefficients.
  - It must support choice in appropriate level of description for any of the modules in the particular study. It must allow for 3D effects but also be capable of lower level 1D and 2D models where appropriate.
- It must support collaborative research.
  - It should interface well with experimental databases and provide appropriate tools such as synthetic diagnostics to facilitate understanding its output.
  - It must include protocols for effective communication among geographically and scientifically diverse physics participants and code developers.
- It must complement existing research.
  - The facility must provide value to the individual involved in basic physics research, who may himself be doing large-scale computation.
  - It must not impose a significant overhead (computational or human) on the use and development of the separate physics modules. It must provide needed services so as to be of value even to a single module.

At this stage it is not necessary to specify how these connections are to be made. That will be a major part of the research program and will require the involvement of applied mathematicians and computer scientists to define. In fact, to satisfy the above requirements it is likely that several integration schemes will be necessary.

IV. Project Governance

The FSP initiative should be focused, highly interdisciplinary, and involve a significant number of people. For these reasons it is extremely important that careful attention be given to governance of the project. The governance structure needs to effectively balance the professional needs of the creative and individualistic people who will carry out the work with the programmatic needs for focus and timely delivery of results. In addition the structure needs to work effectively with the two programs offices (OASCR and OFES) that will support and manage the initiative. A sketch of a proposed governance structure is provided below. It is recognized that extensive discussions with the relevant communities are needed to assure buy-in of this or any other structure.

An analogous set of issues has been addressed by the Community Climate Systems Model activity (see http://www.ccsm.ucar.edu). While there are significant differences between the nature of the science involved in the CCSM and the initiative discussed here, there nonetheless are sufficient similarities that the CCSM activity can help provide the needed structure. Three critical elements are needed: a scientific steering group, a series of working groups including one which addresses software management issues, and an external advisory board. The organizational chart for these groups is:



The functions of these groups are:

Scientific Steering Group: This group provides the overall scientific direction and vision for the project. It provides oversight and coordination of scientific activities. It is the key group for assuring the integration described above is effected. It coordinates with program offices on resource allocation issues.
Working Groups: Each working group is focused on one of the applied modules (see above) as well as a software engineering group. A working group oversees the scientific direction of the module development including determination of required fundamental work. It assures integration of components within the modules and compatibility of the module with the rest of the system. This is where the real work gets done.

Advisory Board: This group is made up of people with scientific breadth that are not directly engaged in the initiative. The group will provide scientific and management advice to both the Steering Group and the program offices.

V. Fusion Simulation Capabilities Status

This section summarizes the current status of integrated computational modeling and simulation of toroidal confinement fusion systems. The intent in this section in the present document is to provide a general perspective of the status of this very active and mature field. This section responds to the explicit request in the subcommittee's charge letter to report on the status of fusion simulation capabilities. These capabilities form a significant part of the critical underpinning of the FSP.

There are over 50 major toroidal physics design and analysis codes being maintained by the magnetic fusion community. The major multi-user codes are depicted in Figure 1, which shows how they divide into groups, and indicates with arrows the flow of information from one code group to another.

The axisymmetric free boundary equilibrium codes solve the force balance equation by calculating the poloidal magnetic flux in cylindrical coordinates for given pressure and current profile parameterizations. These can be used to define the boundary for the inverse equilibrium codes. There are also two major fully 3-D equilibrium codes in use: VMEC, which assumes the existence of good magnetic surfaces *a priori*, and works in a coordinate system based on these, and PIES, which calculates the existence of surfaces as part of the solution, if they exist.

The collection of linear macroscopic stability codes maintained by the MFE community is quite mature and can assess the stability properties of a given equilibrium with respect to both ideal and non-ideal (resistive) MHD, including the effects of an energetic particle component.

The nonlinear codes fall into four major groupings. In descending order of the frequencies addressed, these are the: 1) RF Heating and Current Drive codes, 2) the Nonlinear Gyrokinetic codes, 3) 3-D Nonlinear Extended MHD codes, and 4) the 2-D Transport codes.

The RF Heating and Current Drive codes calculate the propagation of electromagnetic waves of a given frequency through a prescribed background plasma, including reflection and absorption. The codes are of two major types: ray-tracing (or geometrical optics), and full wave (global solution). There are also depicted antenna and Fokker-Planck codes, which are closely coupled with the RF codes, and provide boundary conditions and background distribution functions. The RF codes are designed to calculate the instantaneous heating and current-drive profiles for a given plasma equilibrium subject to a given RF oscillator source and antenna.

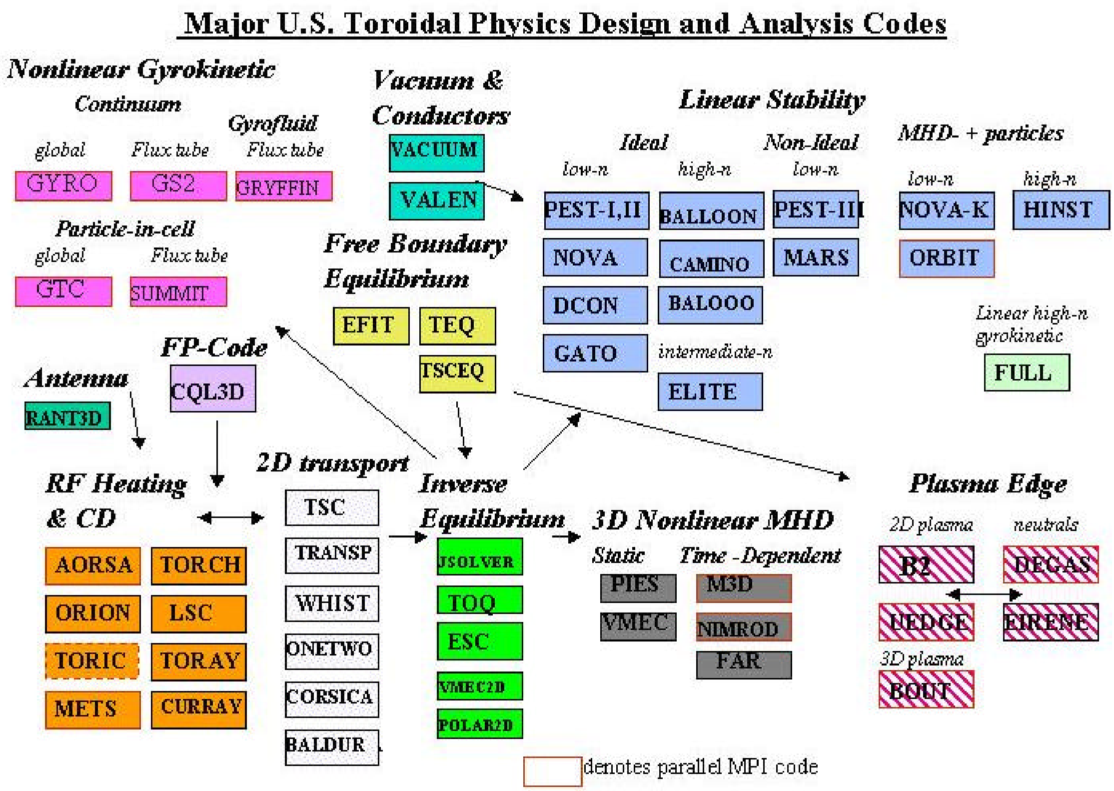


FIG. 1. Major U.S. toroidal physics design and analysis codes used by the plasma physics community.

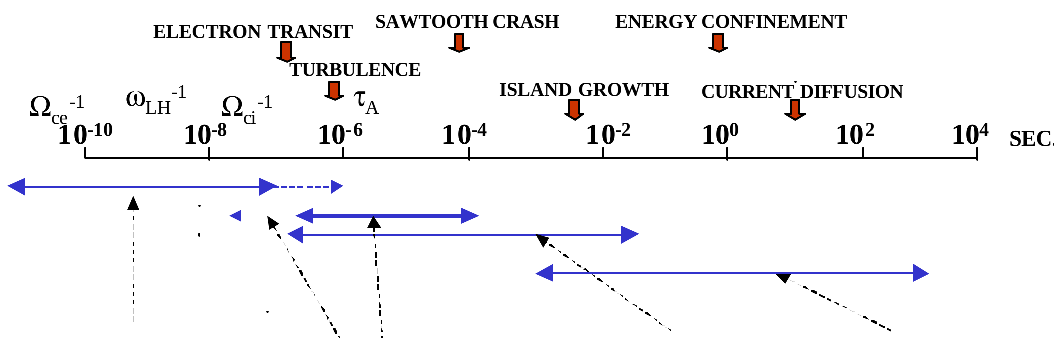
The gyrokinetic codes are based on an analytic reduction of the full 6-dimensional plus time plasma distribution function obtained by averaging over the rapid gyro-motion of ions in a strong magnetic field, and by neglecting the displacement current in Maxwell's equations to remove "light waves" from the system. These codes are appropriate for studying 3-D turbulent transport in a background system with fixed profiles.

The 3-D nonlinear Extended MHD codes are based on taking velocity moments of the Boltzmann equation to yield 3-D magneto-fluid equations for the evolution of the average plasma velocity, density, and pressure, along with a closure procedure. These codes are appropriate for describing global stability phenomena such as sawteeth oscillations, magnetic island evolution, and plasma disruptions.

The 2-D transport codes presently form the core capability in our community for integrated modeling. There are six major codes, with considerable overlap, that exist largely for historical reasons. These codes are all based on the Grad-Hogan evolving equilibrium description where the inertial terms in the momentum equation are neglected and the remaining MHD equations are averaged over the flux surfaces, where they exist.

The 2-D transport codes are all very modular. They are each a collection of equilibrium modules, transport modules, solvers, and source and sink modules representing Neutral Beam Injection (NBI) and RF heating, pellet and gas injection, impurity radiation, and the effects of saturated MHD activity such as sawteeth and islands. These codes have recently benefited from the National Transport Code Collaboration (NTCC), which has formed a modules library so that modules taken from individual codes can be exchanged and shared (see, e.g., w3.pppl.gov/NTCC for more details on this). While these codes address integrated modeling, the individual modules represent simplified reduced descriptions of the full three-dimensional physical phenomena being modeled.

Typical Time Scales in a next step experiment with B = 10 T, R = 2 m, $n_e = 10^{14}$ cm^{-3}, T = 10 keV



Single frequency and prescribed plasma background	Neglect displacement current, average over gyroangle, (some) with electrons	Neglect displacement current, integrate over velocity space, neglect electron inertia	Neglect displacement current, integrate over velocity space, average over surfaces, neglect ion & electron inertia
RF Codes	Gyrokinetics Codes	Extended MHD Codes	Transport Codes
wave-heating and current-drive	turbulent transport	device scale stability	discharge time-scale

FIG.2. Summary of the four major code groups and the timescales being addressed.

A summary of these four major code groups and the timescales being addressed by them is given in Figure 2. The RF codes address frequencies of order the ion cyclotron frequency, Ω_{ci} , and above, up to the electron cyclotron frequency Ω_{ce}. The gyrokinetics codes typically take time steps about 10 times longer than the ion cyclotron frequency, whose motion is analytically averaged over, and are normally run for 10^3 to 10^4 time steps to calculate stationary turbulent fluctuation levels. Recent additions to these codes to include some electron timescale phenomena bring in the electron transit time, which lowers the maximum timestep. The Extended MHD codes need to resolve phenomena occurring on the Alfvén transit time, τ_A, although most codes are at least partially implicit to avoid a strict restriction on the timestep based on this. These codes can normally run 10^4 to 10^5 time steps to address MHD phenomena such as sawteeth and island growth.

The 2-D transport codes are very efficient and can take many long timesteps to model the entire discharge. However, the 2-D edge transport codes need to resolve the parallel dynamics and use a time-step based on the parallel sound-wave propagation near the edge region.

The calculations now being performed with the gyrokinetics codes, the Extended MHD codes, and the RF codes, are straining the limits of the existing computing capabilities and capacities. For example, recent attempts by the core-turbulence gyrokinetics codes to include both electron and ion dynamics in a self-consistent simulation require upwards of 10^4 processor-hours (over one processor-year) on the IBM SP3 at NERSC to generate one result for a set of fixed background profiles. Similar times are required by the Extended MHD codes to calculate the growth and self-consistent saturation of a neoclassical tearing mode. Thus, we can take solace in the fact that the capability is mostly in place, but must deal with the fact that the computational requirements for a fully integrated 3D comprehensive simulation capability are truly daunting.

Examples of fundamentally important experimental phenomena which involve 3D physical processes that cross theoretical boundaries and thus cannot adequately be addressed by the present suite of above-described codes include:

- *Pedestal physics* – A description of the transport barrier that forms in the region of the plasma between the core and the edge, and of the associated edge localized relaxation events;
- *Long time scale profile evolution* – A way to self-consistently evolve the global profiles of plasma temperature and density on the energy-confinement time scale from turbulent transport and in the presence of magnetic islands and other MHD phenomena.
- *Edge transport*: A description of long-mean-free-path particle and heat transport outside the closed magnetic flux surfaces, on the open field lines that impact the first wall or divertor and involve multi-phase physics
- *Self-consistent heating and current drive*: A fundamental model of the interaction of Radio Frequency (RF) waves with plasma in the presence of plasma turbulence.
- *Sawtooth phenomena* – Internal MHD-type modes in the hot core of tokamak plasmas for which fast ion and kinetic effects are clearly relevant experimentally but are only beginning to be addressed computationally.
- *Island physics*: incorporation of the effect of 3-D island formation on equilibrium evolution and turbulent transport

These are but some of the important problems to be addressed by the integrated simulation initiative.

VI. Summary

The essential goal of the Fusion Simulation Project (FSP) is to develop a computational capacity that can perform integrated simulations of toroidal magnetic confinement devices. This capability is envisioned to span fundamental dynamics of evolving plasmas, including diagnosis and control of toroidal configurations, and the coupled properties of fusion devices, in the presence of the widest expected range of plasma dynamics.

The FSP is envisioned to be comprised of three major elements that are funded approximately equally over the life of the project: fundamentals capabilities, applications modules development, and project integration. This development will be made feasible by close coupling of the integration initiative research with ongoing program activities in theory, experiment, simulation, computer science and applied math carried out under OFES and OASCR. It will be enabled fundamentally by the SciDAC efforts also presently under way in the DOE Office of Science. Taking as an example effective capabilities development from the DOE NNSA Accelerated Strategic Computing Initiative (ASCI), new funding necessary for the success of the FSP is presently estimated at approximately $20M for the first year of deployment (FY04), ramping up to a procurement and Centers' formation phase in FY05, and followed by steady, personnel-driven level of effort funding for FY06, FY07 and FY08 inclusive. To achieve the greatest productivity, this new research should be split between OFES and OASCR, with fusion scientists provided by OFES and applied mathematicians, computer scientists, and the computational toolkits provided under the auspices of OASCR. This joint undertaking represents a significant opportunity for the DOE Office of Science to create a capability that will advance the understanding of fusion energy to a level unparalleled worldwide.

VII. Acknowledgements

The FESAC ISOFS Subcommittee acknowledges helpful contributions to this report from members of the fusion and applied mathematics communities, with particular thanks to speakers at the May 23 ISOFS workshop. The Subcommittee also thanks the Theory Coordinating Committee (TCC) for their letter, and the members of the PSACI PAC for the concepts and suggestions provided in their 18 June 2002 letter to this Subcommittee, and most particularly is appreciative of their enthusiasm for the Fusion Simulation Project.

VIII. APPENDIX

February 22, 2002

Professor Richard D. Hazeltine, Chair
Fusion Energy Sciences Advisory Committee
Institute for Fusion Studies
University of Texas at Austin
Austin, TX 78712

Dear Professor Hazeltine:

This letter provides a charge to the Fusion Energy Sciences Advisory Committee (FESAC) to assist the Office of Fusion Energy Sciences (OFES) in preparing a roadmap for a joint initiative with the Office of Advanced Scientific Computing Research (OASCR). Recent reports, such as the FESAC report "Priorities and Balance within the Fusion Energy Sciences Program," the "Report of the Integrated Program Planning Activity" (IPPA), and the NRC report "An Assessment of the Department of Energy's Fusion Energy Sciences Program," have identified a predictive understanding as a measure of the quality of the science and the maturity of the knowledge base of a field. The IPPA report lists several challenging10-year objectives for the fusion program, including "develop fully integrated capability for predicting the performance of externally-controlled systems including turbulent transport, macroscopic stability, wave-particle physics, and multi-phase interfaces." This objective, as well as several other IPPA objectives related to innovative confinement configurations, will require significantly enhanced simulation and modeling capability. Therefore, the goal of this initiative should be to develop an improved capacity for **Integrated Simulation and Optimization of Fusion Systems**.

The initiative should be planned as a 5-6 year program, which would build on the improved computational models of fundamental processes in plasmas that are being developed in the base theory program and in the SciDAC program. Rough estimates are that an integrated simulation initiative would require a total funding level of about $20 million per year, with funding for the plasma scientists provided by OFES and funding for the applied mathematicians, computer scientists, and computational resources provided by OASCR. Thus, the roadmap should include not only human resources but also computer and network resources.

Please carry out the preparation of the roadmap using experts outside of FESAC membership, as necessary, including experts recommended by the Advanced Scientific Computing Advisory Committee. The sub-panel of experts should obtain community input through a series of workshops covering at least the following questions:

- What is the current status of integrated computational modeling and simulation?
- What should be the vision for integrated simulation of toroidal confinement fusion systems?

- What new theory and applied mathematics are required for simulation and optimization of fusion systems?
- What computer science is required for simulation and optimization of fusion systems?
- What are the computational infrastructure needs for integrated simulation of fusion systems?
- How should integrated simulation codes be validated, and how can they best be used to enable new scientific insights?

The ultimate product should be a roadmap document similar to the one developed for the Genomes to Life Initiative (http://www.doegenomestolife.org/roadmap/index.html). Please conduct a workshop on the first two questions above and provide a summary document with overall program goals and objectives, major program deliverables, and a brief description of the OFES and OASCR funded elements of the program by July 15, 2002, so that OFES would be able to include a description of the program in the FY 2004 OMB budget request. Please complete work on the final roadmap by December 1, 2002, in order to provide the detailed information needed by OFES and OASCR to develop detailed program plans, program announcements and grant solicitations.

I appreciate the time and energy that members of FESAC and FESAC sub-panels have provided to the continuing efforts to develop program plans and roadmaps for the OFES program. I am confident that the Committee's recommendations on a roadmap for **Integrated Simulation and Optimization of Fusion Systems** will form a sound basis for beginning a joint OFES/OASCR program.

Sincerely,

James F. Decker
Acting Director
Office of Science