

Fusion Simulation Project:

Integrated Simulation & Optimization of Fusion Systems

Final Report of the FESAC ISOFS Subcommittee • December 1, 2002



$$\frac{\partial f_a}{\partial t} + \mathbf{v} \cdot \nabla f_a + \frac{q_a}{m_a} [\mathbf{E} + \mathbf{v} \times \mathbf{B}] \cdot \nabla f_a = C(f_a)$$

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EXECUTIVE SUMMARY

Fusion is potentially an inexhaustible energy source whose exploitation requires a basic understanding of high-temperature plasmas. The development of a science-based predictive capability for fusion-relevant plasmas is a challenge central to fusion energy science, in which numerical modeling has played a vital role for more than four decades. A combination of the very wide range in temporal and spatial scales, extreme anisotropy, the importance of geometric detail, and the requirement of causality which makes it impossible to parallelize over time, makes this problem one of the most challenging in computational physics. Sophisticated computational models are under development for many individual features of magnetically confined plasmas and increases in the scope and reliability of feasible simulations have been enabled by increased scientific understanding and improvements in computer technology. However, full predictive modeling of fusion plasmas will require qualitative improvements and innovations to enable cross coupling of a wider variety of physical processes and to allow solution over a larger range of space and time scales. The exponential growth of computer speed, coupled with the high cost of large-scale experimental facilities, makes an integrated fusion simulation initiative a timely and cost-effective opportunity.

Worldwide progress in laboratory fusion 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). Such an experiment, at the frontier of the physics of complex systems, would be a huge step in establishing the potential of magnetic fusion energy to contribute to the world's energy security. An integrated simulation capability would dramatically enhance the utilization of such a facility and lead to optimization of toroidal fusion plasmas in general. This science-based predictive capability, which was cited in the FESAC integrated planning document (IPPA, 2000), represents a significant opportunity for the DOE Office of Science to further 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 reliably the behavior of plasma discharges in a toroidal magnetic fusion device on all relevant time and space scales. By its very nature in enabling more comprehensive modeling, the FSP will lead to a wealth of insights not realizable previously, with new understanding in areas as diverse as wall interaction phenomena, the effects of turbulence on long time confinement, and implications of plasma self heating in advanced tokamak operating regimes. The long-term goal 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. Since confidence in the ability to predict is ultimately based on code performance against experimental data, a vigorous and ongoing validation regime must also be a critical element of this project.

The characteristics of fusion plasmas make the goal extremely challenging. These characteristics include the presence of multiple time scales, ranging over fourteen orders of magnitude, and multiple spatial scales, ranging over eight orders of magnitude. The linear algebraic systems that must be solved are often ill-conditioned. The computational domains are geometrically complex, and the solutions severely anisotropic. In many cases, the physics approximations are not completely understood, and hence the simulation equations are unclear. The underlying physics is coupled with essential nonlinearities. Taken in isolation, approaches have been developed or are under investigation for each of these challenges. However, an integrated simulation for fusion plasmas will present *all* of these features simultaneously.

Success of this project will require coordinated and focused advances in *fusion physics* (to further develop the underlying models and elucidate their mathematical basis), *applied mathematics* (to further develop suitable algorithms for solving the mathematical models on the appropriate computer architecture, and to define frameworks within which these algorithms may be easily assembled and tested), and *computer science* (to provide an architecture for integrated code development and use, and to provide analysis and communication tools appropriate for remote collaboration). Strong collaborations, forged across these disciplines and among fusion scientists working in different topical areas, will be an essential element of the program. In addition, the Fusion Simulation Project will require significant improvements in computational and network infrastructure, including enhancements to shared resources as well as to local or topical computing centers. Because of the complexity of the FSP, the planning process should continue into CY2003. We recommend a staged approach: beginning with clarification of the physics issues, accompanied by efforts to address algorithmic issues and followed by clarification of architectural issues.

The necessary core expertise for the FSP is resident in several units within the DOE Office of Science. Primary among these are the ongoing fusion experimental and theoretical research and development activities within the Office of Fusion Energy Sciences, the applied mathematics development activities within the Office of Advanced Scientific Computing, the recently developed SciDAC initiative, and materials science research in the Office of Basic Energy Sciences.

To achieve its goals, the FSP is envisioned as proceeding through three five-year phases in which successively more complex and disparate phenomena will be integrated. During the first five years, the project will concentrate on specific physics integration issues that are expected to deliver significant scientific insights in their own right, but are also prototypical of the integration issues faced by the whole initiative. Each Focused Integration Initiative (FII) will concentrate on developing a predictive modeling capability for a specific programmatically important scientific problem and will begin to develop and gain experience with relevant mathematical tools, new algorithms, and computational frameworks. During the second five-year period the project will undertake larger and more comprehensive integration activities and take them to the next level of development. During the final five-year period, the focus will be on comprehensive integration. There will be links among all the physics components of the project. To provide a tradeoff between computational efficiency and physical fidelity there will be multiple levels of description of many of the physical processes.

Verification and validation are critical components of the FSP. To succeed, an integral feature of this initiative must be an intensive and continual close coupling between the simulation efforts 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 that the models have the required accuracy can only be accomplished by continual iteration and testing against experimental data.

Funding for the FSP must be at a level adequate to accomplish the project goals. The successful NNSA Accelerated Strategic Computing Initiative (ASCI) Level 1 University Centers Program, funded at \$25M/yr, provides an appropriate example of the level of resources required. A preliminary assessment of the challenges and complexity of possible FIIs indicates that they would be comparable to that of each of the five ASCI University Level 1 Center Programs. We further estimate that four-five such FIIs will be required to cover all the critical science areas which must eventually go into the final integrated simulation code. Further refinement of the costs and timelines will be carried out as the FSP is developed. Through the course of the project, we envision that funding would be approximately equally allocated between the DOE OFES and OASCR research elements. Because this initiative rests entirely on a progressing science base, and will for successful execution attract and retain junior researchers committed to the goals of fusion energy sciences, it is paramount that FSP funding be new rather than redirected from present critical areas.