Computational Fusion Energy Research:
The Need for New Levels of Supercomputing

The fusion research program has long been at the forefront of large-scale scientific computing, dating even before establishment of the National Magnetic Fusion Computer Center, the forerunner of the present NERSC. Computation and simulation are critical to progress in fusion research both to enable scientific understanding, and to design and interpret new experimental devices containing burning, reactor grade plasmas. These machines can be in the $1B to several $B class. To achieve program goals we must push models into the new physics parameter regimes required to study burning fusion plasmas, including higher spatial resolution, dimensionless parameters characteristic of higher temperature plasma, longer simulation times, and higher model dimensionality. It is also essential to begin integrating these models together to treat non-linear interactions of different phenomena. Various estimates indicate that factors of 10^3 to 10^5 increases in combined computational power are needed. These increases will require advancing computer technology, algorithmic development, and improved theoretical formulation. The U.S. fusion program has traditionally lead the world in fusion theory and in application of this theory by state of the art numerical computation. With the appearance of the Earth Simulator computer in Japan the ability of the U.S. to maintain this leadership role is certainly challenged.

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Plasmas comprise over 99% of the visible universe and are rich in complex, collective phenomena. A major component of research in this area is the quest for harnessing fusion energy, the power source of the sun and other stars, which occurs when forms of the lightest atom, hydrogen, combine to make helium in a very hot (100 million degrees centigrade) ionized gas or "plasma." The development of a secure and reliable energy system that is environmentally and economically sustainable is a truly formidable scientific and technological challenge facing the world in the twenty-first century. This demands basic scientific understanding that can enable the innovations to make fusion energy practical. Fusion energy science deals with vast ranges of scale in space and time, in some cases spanning over ten decades; extreme plasma anisotropy; the interaction between large-scale fluid-like (macroscopic) physics and fine-scale kinetic (microscopic) physics; and the need to account for geometric detail.

There has been great progress during the past decade in developing a fundamental understanding of key individual phenomena in plasmas for fusion, space physics and industrial plasma applications that was enabled to a great extent by supercomputer based simulation and modeling. In fusion, important new knowledge has been obtained in microturbulence and transport driven by ion temperature gradients, macroscopic equilibrium and stability properties in magnetically confined systems, the physics of laser-plasma interaction in inertial confinement experiments, and the physics of intense particle beams as inertial fusion drivers. Excellent progress has also been made in understanding magnetic reconnection dynamics, which is a central scientific issue for fusion energy, as well as for allied fields including space and solar physics. For inertial confinement, the DOE NNSA has embraced simulation as a key element in science-based stockpile stewardship. However, accelerated development of computational tools and techniques are vitally needed to develop predictive models which can prove superior to empirical scaling. For example, this will have a major impact on the fusion community's ability to effectively utilize a Burning Plasma Experiment (BPX) as endorsed by the recent Snowmass Fusion Summer Workshop (July 2002). The probability that a BPX (with an estimated cost upwards of $1B) will achieve its goals can be significantly enhanced by our capability to numerically simulate the plasma behavior under realistic conditions. The challenge to unravel the mystery of the complex behavior of strongly nonlinear, non-equilibrium plasma systems, including interactions with their external environments is clearly the next frontier of computational fusion research..

Modern magnetic fusion experiments are typically not quiescent, but exhibit macroscopic motions that can affect their performance, and in some cases can lead to catastrophic termination of the discharge. The modeling of such dynamics for realistic experimental parameters requires an integration of fluid and kinetic physics in complex magnetic geometry as described by the Extended MHD equations. The key challenge in performing computations relevant to the hot plasmas of modern fusion experiments is to increase the dimensionless parameter characterizing inverse plasma collisionality, the Lundquist number, S. Present Extended MHD calculations have achieved 18 Gflop/sec (GF) on 384 processors of an IBM SP3. This performance limits both the accessible Lundquist number ($\sim 10^7$) and the problem time (~1 msec). These values are several orders of magnitude less than are required to accurately simulate present fusion experiments. We estimate that a 1000-fold increase to 20 Tflop/sec (TF) sustained performance could allow values of S approaching 10^9 and the problem time to approach a tenth of a second or more, enabling validation of the mathematical models and comparison with present experiments. Further extensions into the 100s of TF regime would likely be needed to treat some key problems for burning plasma devices.

The confinement of energy and particles in fusion plasmas is often significantly degraded by turbulence associated with small spatial-scale plasma instabilities driven by gradients in the plasma pressure. The detailed physics of the growth and saturation of these instabilities, their impact on plasma confinement, and the understanding of how such turbulence might be controlled remain unsolved problems for which we have only glimpses of understanding. At the present time roughly 10^{-3} s of a turbulent discharge can be modeled at minimal spatial grid resolution with 120 hours on 128 processors on the NERSC IBM SP (115 MF sustained performance → 1.5 TF hours). This time needs to be increased by a factor of 10-100 to address transport time scales. Furthermore additional physics associated with kinetic electrons (which necessitates an increase in computing resources ~50 to 100) and electromagnetic coupling must be included in the models in order to allow a quantitative understanding. Codes in the SciDAC Plasma Microturbulence Project have recently added this physics capability, but presently there are insufficient computer resources to carry out the scientific studies. We estimate that 10^3 to 10^4 TF hours are required to include kinetic electron dynamics for transport time scales.

The edge plasma region connects the hot plasma core to the material wall, and plays a crucial role in both overall plasma confinement and plasma-wall interactions. The physics of edge plasma is very complex and ranges from turbulent plasma transport to atomic physics and radiation, and to surface physics. Although there are many computationally challenging problems in edge physics; one that is particularly hardware-limited is edge turbulence. In contrast to the core, edge turbulence fluctuations can be of order of the background (average) levels and their spatial scale can be comparable to the smallest equilibrium gradient lengths, which in turn are not much larger than a gyroradius. On the other hand, many orders of magnitude in time scale and several in spatial scales must be spanned. Furthermore, the collisionality varies from highly collisional to collisionless. These considerations require the inclusion of kinetic effects in the codes. Present state-of-the-art codes are fluid-based and are a challenge for current computers. A gyrokinetic edge code simulation would require a capability in the 20 TF (sustained performance) range to simulate up to nominal background relaxation timescales. Full-shot simulation, or simulations requiring coupling to the largest spatial scales (e.g. for edge-localized modes) would require at least an additional order of magnitude.

The scientific issues of magnetic fusion encompass a wide range of disciplines including those mentioned above, as well as others. However the dynamics of high temperature plasma does not respect these categorizations, and the understanding of overall plasma performance requires integrating all of these issues in an integrated simulation that includes interactions between phenomena which were previously studied as essentially separate disciplines. To achieve the ultimate goal of such integration, we must follow the evolution of the global profiles of plasma temperature, density, current and magnetic field on the energy-confinement time scale and we must include the relevant physics on all important time scales. While this is a long term goal, the program now stands ready to begin such cross-disciplinary studies and to increase the physics content of existing integrated codes, a major requirement being access to significantly increased computing power. To accelerate this process the fusion community is already engaged in a study laying the groundwork for a major initiative, referred to as the Fusion Simulation Project (FSP), for 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 enables the models to work together. Such integration of code modules, many of which are individually at the limits of computational resources, clearly will benefit from substantial increases in computer power.

Progress in all key physics areas of Inertial Fusion Energy (IFE), including the "drivers" which impart the energy to the fusion fuel, the targets, and also an advanced concept known as fast ignition, would be dramatically accelerated by an Earth Simulator-class resource. The principal IFE driver approach supported in the Office of Science consists of beams of heavy ions produced by linear induction accelerators. These intense beams are non-neutral plasmas that exhibit collective behaviors dominated by space-charge forces; demanding a self-consistent, integrated treatment from the source to the target for a full understanding. Such a calculation is estimated to require of order 100 hours (at a sustained 20 TFLOPS) through the driver, and a comparable amount through the fusion chamber and onto the target. Similarly, target calculations, which are beginning to employ codes run on the ASCI computers, stand to benefit from an Earth Simulator-class machine. In the heavy-ion targets currently being simulated, X-rays generated by the beams implode the fuel capsule "indirectly;" a similar concept is used in targets planned for the National Ignition Facility. For laser-based IFE, direct illumination of the capsule by the driving beams is envisioned. Indeed, a 3-D simulation of such a target is cited as a demonstration of the Earth Simulator’s power (with 12.5 TFLOPS sustained, 39% of peak). Finally, there is broad international interest in fast ignition, which uses a separate short-pulse laser to ignite the compressed fuel, reducing the total required input energy. Because of the wide range of time and space scales, and strong anisotropy, it will be necessary to employ coupled models even with Earth Simulator-level capabilities.

An increase of 50-100 in computing power, along with a modest increase in human resources to support partnerships between fusion physicists, applied mathematicians and computer scientists, will enable fusion researchers to make a major advance in resolving the spatial and temporal complexity in simulations of individual phenomena as well as to begin to develop fully integrated simulations of fusion systems. Such an integrated simulation capability would dramatically enhance the utilization of a burning fusion device in particular and the optimization of fusion energy development in general, and would serve as an intellectual integrator of physics phenomena ranging from advanced tokamaks to innovative confinement concepts. The Fusion Energy Science program very clearly needs and is also well poised to benefit from access to powerful new computational hardware in the class of the Earth Simulator Computer (ESC).