

Integrated Simulation of Fusion Plasmas

Magnetically confined plasmas, with their many coupled phenomena, pose great difficulties to computer modelers. Several initiatives worldwide are working to meet the challenges.

Donald B. Batchelor

For some 50 years, scientists have been studying magnetically confined plasmas with an eye toward producing fusion energy. But understanding the behavior of such plasmas has proved to be a scientific challenge of the highest order. (For a review of the basics, see boxes 1 and 2.) A perhaps provocative comparison with biological organisms or Earth's climate system might shed light on why. All three systems are delicate and heterogeneous, maintained by a myriad of nonlinearly coupled processes in a self-organized state very far from statistical equilibrium. Moreover, those processes occur over a vast range of time and space scales.

Just as biology has developed subfields such as neurology, physiology, and cardiology, and just as climate science has developed independent models for the atmosphere, sea ice, and land mass, fusion science has developed subfields like plasma microturbulence theory, magnetohydrodynamics (MHD), and transport theory to study phenomena that take place in restricted time or space scales. Physicists, enabled by modern computers, have made enormous progress in the theoretical understanding of those fusion subfields. But, as with systems biology or climatology, the science of the whole of what takes place in a fusion plasma is far richer than the science of the pieces, and one doesn't understand the organism, the evolution of climate, or the plasma until the couplings between the various contributing phenomena are understood. Given the impressive strides that plasma physicists have made in theory and in the experimental diagnostic techniques for validation of theory, and in anticipation of rapid improvements in computer power, now is the time to begin developing such an integrated understanding.

The need for an integrated picture is all the more pressing because the fusion community is about to begin a major new phase of research on so-called burning plasmas with ITER, an international prototype fusion energy reactor (for more on ITER, see box 3). The dominant energy source in ITER will be internal fusion reactions rather than external systems. Thus the plasma state will be self-organized, rather than externally controlled, to a much greater extent than in previous experiments. One might expect that the interactions between phenomena on different scales will be stronger and that new phenomena and new interactions may appear as fusion reactions come to dominate. Already, experiments that are preparing the way for ITER are seeing effects that cannot be understood

by microturbulence theory, MHD, or transport theory alone.

Large-scale numerical simulation has always been a part of magnetic-fusion research. Fusion devices such as the tokamaks and stellarators described in box 2 have complicated shapes, and the behavior of the magnetized plasma inside—the rate of en-

ergy and particle leakage or the maximum plasma pressure that can be stably confined, for example—is surprisingly sensitive to those shapes. The plasmas are very far from thermal equilibrium, and many different reservoirs of available energy can drive unstable motions. Therefore, by the time effects are experimentally observable, a plasma is often in a highly nonlinear state. If a simulation is to accurately resolve rapid-time-scale and short-wavelength phenomena, then dealing with slow-time-scale and longer, device-scale-length phenomena will require special mathematical and computational methods. Otherwise the computation will face impossibly large numbers of short time steps and densely packed spatial grid points.

Simulations not only help plasma physicists understand basic theories, they also provide important support for fusion experiments. Run time on large fusion devices is expensive and highly prioritized. Operating costs for ITER could amount to \$1 million per day. Scientists need detailed simulations so they have a clear idea of what effects to expect in an experiment and whether those effects can be observed with the diagnostic systems available. They also require simulations to help them determine if the plasma conditions needed for a given experiment can actually be produced with the heating, fueling, and control systems available, and how they must operate those systems to achieve the desired plasma state. Proposed experiments, especially with today's large devices, are thoroughly reviewed and planned months to years in advance. The review process relies extensively on simulations to enable scientists to get the most from precious machine resources. At a more fundamental level, the development of new and improved devices for plasma confinement requires modeling of all aspects of plasma performance.

Fusion time scales

An ideal toroidal system can, in principle, confine independent charged particles forever. Practical fusion energy production, though, requires such high density and energy that the confined particles do not behave independently, but act collectively as a plasma that can modify the imposed field. Real-life fusion plasmas, which typically contain electrons and ions of hydrogen, deuterium, and tritium along with other ions and impurities, vary with time for three fundamental reasons. First, the particles collide to produce thermal fluctuations. The result is a slow transport of energy and particles across the flux surfaces defined by magnetic field lines. Second, the plasma is affected by the outside world through its interactions with the confining boundary and externally produced particles, energy, and momentum. Third, the pressure gradients,

Don Batchelor is the leader of the fusion theory program at Oak Ridge National Laboratory in Tennessee.

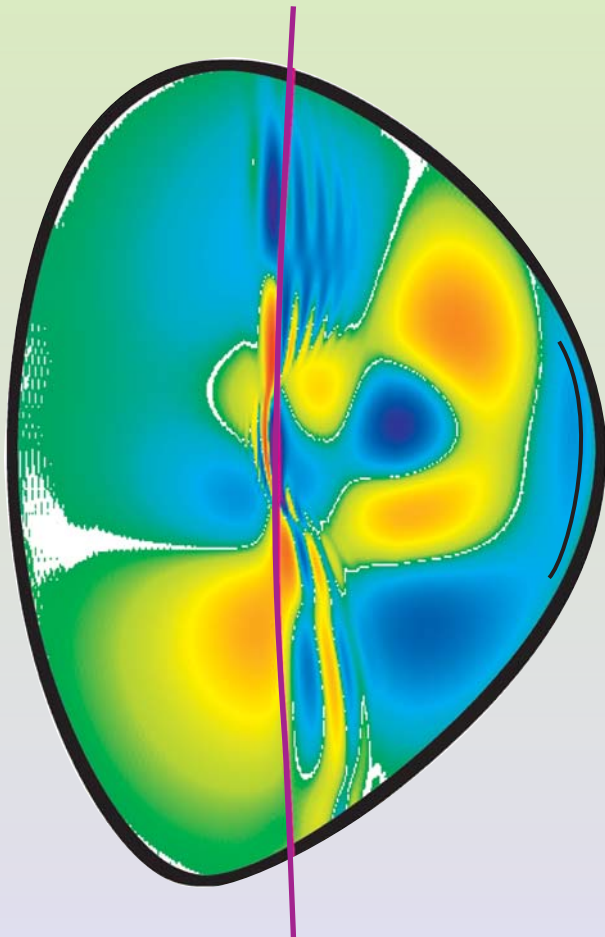


Figure 1. In mode conversion, plasma wavelengths change dramatically. In this simulation, plasma waves introduced by the antenna (visible to the right just inside the conducting boundary) are converted into shorter-wavelength modes near the surface indicated by the purple line. (The part of the nominal surface beyond the conducting boundary is to guide the eye.) Colors indicate the amplitude of an electric-field component: Warm colors are positive, cool colors are negative. The simulated region is about 0.4 m across. (Adapted from E. F. Jaeger et al., *Phys. Rev. Lett.* **90**, 195001, 2003. See also E. Nelson-Melby et al., *Phys. Rev. Lett.* **90**, 155004, 2003.)

electric currents, plasma flows, and velocity distributions, when they are far from thermal, are sources of available energy that can couple to the electromagnetic field in very complicated ways and can relax as a result of that coupling. The time scales of plasma interactions span some 15 orders of magnitude, from the 10^{-11} second period of electromagnetic waves that heat plasma electrons to the hours over which escaping particles come to equilibrium with confining walls.

The theory of hot magnetized plasmas starts with the kinetic equation, a form of the Boltzmann equation that describes the time evolution of the phase-space number density f of plasma particles with charge q and mass m :

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \frac{q}{m} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla f = C(f). \quad (1)$$

The second term on the left side describes convection in position space, the third term describes convection in velocity space due to electromagnetic forces on the charged particles, and the term on the right describes the redistri-

bution of particles in velocity space due to collisions. The electric field $\mathbf{E}$ and magnetic field $\mathbf{B}$ are determined by Maxwell's equations. Each particle species in the plasma is subject to its own kinetic equation; the different kinetic equations are nonlinearly coupled through the contributions of the various species to the electromagnetic field and through interspecies collisions.

Wave-plasma interactions

The high-power RF waves that are injected into fusion plasmas to heat them are quite versatile: They can drive plasma flow or localized electric current and can be used to create energetic or anisotropic populations of particles. RF waves can also be spontaneously generated inside a plasma. Experimental work has successfully used RF waves to improve plasma confinement and stability, but a detailed understanding of those improvements remains elusive. A related challenge—one that computer simulations might help physicists meet—is to realize the potential that RF waves have to exert control over plasmas for optimum fusion performance.

Computations of RF wave behavior in plasmas are simple in the sense that a plasma can be regarded as essentially stationary on the short time scale of the waves. The slower evolution of the plasma can be calculated separately. Still, the computations are complicated because electromagnetic waves in plasmas can have much shorter wavelengths, and therefore much slower velocities, than they would have in vacuum. Electrons, and even the much slower ions, can have thermal velocities comparable to the wave speeds and so can have resonant interactions with the waves. As a result, the plasma current induced by the wave at a given time and position depends not just on the wave field at that time and position, but on a weighted integral over earlier times: The wave equations that must be solved in computations are partial-differential-integral equations.

Figure 1 shows a simulation of a mode conversion in which RF waves are launched into a tokamak plasma that contains hydrogen and deuterium ions. In the mode conversion process, two different kinds of plasma waves that normally have very different wavelengths can couple in a thin region where their wavelengths become comparable. Such simulations are challenging because they include modes with wavelengths that can become much shorter than the Larmor radius before they are absorbed and modes with wavelengths comparable to the size of the tokamak. Mode conversion can be of practical importance for plasma control because in some situations short waves can drive electric current or plasma flow much more efficiently than long waves can.

Drift waves, another important class of waves, arise from gradients in density or temperature in magnetized plasmas. They tend to have short wavelengths perpendicular to the magnetic field but are nearly constant along the magnetic field. They don't result in large-scale motion of the whole plasma. Rather, they produce a state called microturbulence, which has a broad spectrum of small-scale turbulent eddies.

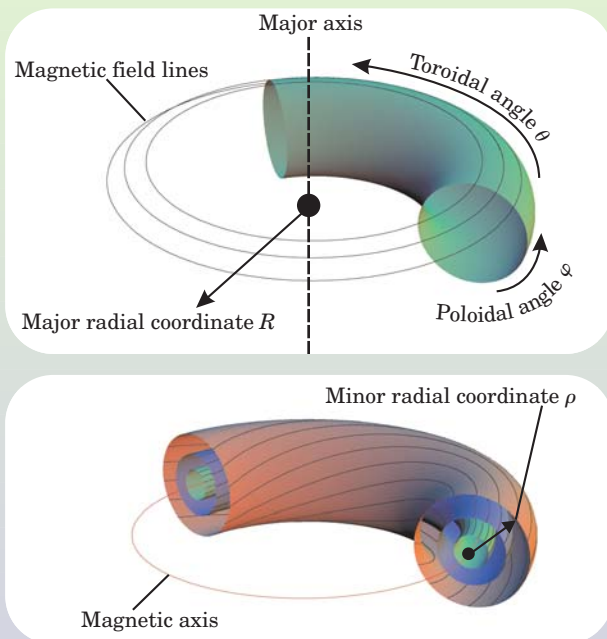
Usually, the chaotic flows around microturbulent eddies dominate the transport of energy and particles across flux surfaces, so understanding and controlling the instabilities of the microturbulent state is a pressing problem for fusion physics. The frequencies of the unstable drift waves are low enough that one can average over particles' motion around magnetic field lines and consider the particles as moving rapidly along the magnetic field lines while drifting slowly across them. When one performs the average, the kinetic equation reduces to the so-called

Box 1. Magnetic Confinement of Plasmas

The basic concept of magnetic plasma confinement relies on simple properties of charged-particle orbits in strong magnetic fields. In a plane perpendicular to the field, the particle is confined to a circular orbit with a so-called Larmor radius proportional to the velocity component perpendicular to the magnetic field. (For additional detail, see the article by Richard Hazeltine and Stewart Prager in *PHYSICS TODAY*, July 2002, page 30.) For a field typical of a large fusion experiment and a perpendicular energy of 10 keV, that radius is about 0.05 mm for electrons and approximately 0.4 cm for deuterium ions. Both radii are much smaller than the size of the plasma. The motion along the magnetic field is almost free; the velocity parallel to the field varies slowly and decreases as the field strength increases along the field line.

Toroidal geometries allow magnetically confined particles to move great distances along the field without leaving the confining volume. Locations in such geometries may be simply specified in terms of the coordinates R , θ , and φ defined in the upper figure. The major radial coordinate R is the distance to the major axis of the torus; θ is the toroidal angle, which varies the long way around the torus; and φ , the poloidal angle, varies the short way around. Sometimes it is convenient to introduce the minor radial coordinate ρ , which, as illustrated in the lower figure, is the distance to the torus's magnetic axis.

Unfortunately, a simple toroidal magnetic field as produced by a doughnut-shaped solenoid does not confine particles for long. The variation of magnetic field strength intrinsic to toroidal geometries causes a particle's motion to not quite close on itself; the particle drifts slowly across the field lines in the vertical direction. For a large fusion experiment,



a typical ion would drift completely out of the machine in about 2 ms. The problem is solved by adding a poloidal component to the magnetic field so that the magnetic field lines wind around to form a set of nested, closed toroidal “flux surfaces,” as seen in the lower figure.

gyrokinetic equation. Figure 2 shows a simulation of drift-wave microturbulence in a tokamak, obtained by solving the gyrokinetic equation.

Microturbulence forcefully illustrates the multiscale challenges of fusion simulations. The particle and energy transport resulting from the turbulent fluctuations causes the radial derivative of the average pressure to slowly evolve, typically on a time scale of about one second. But the pressure gradient is the source of the available energy that is actually driving the high-frequency instability. A self-consistent simulation that directly treats the interaction between turbulence and transport would thus require a solution of the gyrokinetic and Maxwell's equations for some 10^8 wave periods and over a spatial domain spanning the plasma cross section—an area of about 10^5 square turbulence wavelengths. Today's supercomputers can affordably simulate about one millisecond of microturbulence. Though far short of the time required to predict long-term plasma evolution, that's enough time to estimate the instantaneous transport rate of particles, energy, and so forth for comparison with experiment.

Magnetohydrodynamics

The strong, externally applied magnetic fields in toroidal fusion devices give a plasma considerable rigidity. High-frequency fluctuations notwithstanding, the large-scale motion of the plasma is well described by fluid-like equations that can be obtained by taking velocity-space moments of equation 1. The resulting equations are not a closed system; one must include additional assumptions—for example, an external model for the pressure.

A plasma of the quality needed for fusion experiments has extremely high electrical and thermal conductivities in the direction of the magnetic field and a nearly

Maxwellian phase-space distribution f . Those properties allow for a number of well-justified simplifications. The most basic model, ideal MHD, treats the plasma as a single, perfectly conducting fluid with an isotropic pressure p related to the density ρ by a simple adiabatic law, $p\rho^{-\gamma} = \text{constant}$, where the exponent γ is model dependent. Furthermore, ideal MHD limits consideration to long time scales so that the displacement current in Maxwell's equations can be neglected. In the idealized model, the plasma fluid is frozen to the magnetic field lines and the two move together. Those field lines can stretch, bend, and compress, but they can never break or reconnect; in particular, they never change topology. Ideal MHD is a very successful model that has applications beyond fusion plasmas: Its reach encompasses, for example, astrophysics and dynamo engineering. The mathematical simplicity of ideal MHD allows for computationally feasible application to quite complicated shapes.

A fundamental question with implications for plasma confinement is, What magnetic field structures and distributions of pressure and current are in force balance? That is, what are the equilibrium structures and distributions that can hold plasma for an extended period of time? For a steady state, ideal MHD reduces to two deceptively simple equations:

$$\begin{aligned}\mathbf{j} \times \mathbf{B} &= \nabla p \\ \nabla \times \mathbf{B} &= \mu_0 \mathbf{j},\end{aligned}\tag{2}$$

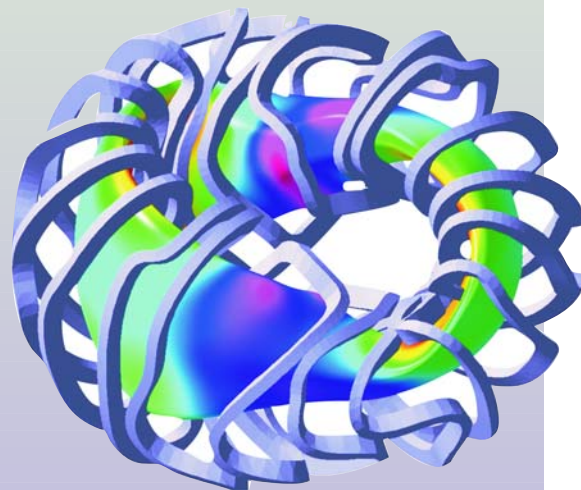
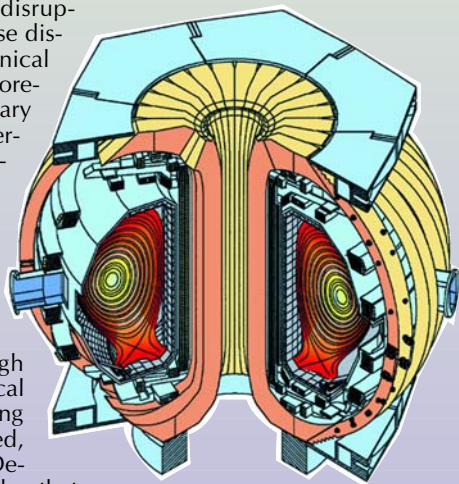
where $\mathbf{j}$ is the current density and μ_0 is the vacuum magnetic permeability.

Those coupled, nonlinear, partial-differential equilibrium equations are a challenge to solve, particularly in three dimensions as would be required for an application

Box 2. Approaches to Toroidal Confinement

The method by which the poloidal magnetic field is produced defines the various approaches to toroidal magnetic plasma confinement. One can generate a poloidal field component by driving a large electrical current through the plasma in the toroidal direction, as is done in tokamak devices such as that depicted on the left below. Tokamaks can confine particles and energy for a long time and can also stably hold high plasma pressure. However, the very large internal current that they require poses problems. It constitutes an available energy reservoir able to drive instabilities that, in turn, can degrade plasma confinement or produce violent plasma disruptions. In extreme cases, those disruptions can cause mechanical damage to the device. Moreover, the necessity of auxiliary systems to control and externally drive much of the current for steady-state operation adds complication and expense.

A steady-state magnetic field having a poloidal component can be produced entirely with external currents, although the coils must have a helical twist such that the resulting plasma has a complicated, nonaxisymmetric shape. Devices called stellarators take that ap-



to stellarators. The pressure's spatial distribution depends on the shapes of the magnetic flux surfaces, which are not known until the equations are solved. The magnetic field is a combination of external fields generated by coils and the internal field generated by plasma current. The current, in turn, must satisfy the equations, which involve the pressure and magnetic field. In an experiment, the pressure profile will change due to heating and transport, and the current distribution will change in response to the pressure and to external controls. Therefore, calculating the evolution of flux surfaces typically requires many solutions of the equations. As a consequence, calculational algorithms must be fast, accurate, and robust.

Some MHD equilibria are stable, but others can be driven to instability by gradients in pressure or current. The consequences of instability can range from negligible, if the growth saturates at a low level, to very serious, if the perturbation grows sufficiently to degrade or destroy plasma confinement. Plasma stability depends very sensitively on such details of the equilibrium as the shape of the flux surfaces and the distributions of pressure and current across different flux surfaces. With the help of computer codes to calculate sequences of equilibria and to simulate their stability properties, plasma physicists can design, and controllably produce in experiments, plasma states with sufficient pressure to be feasible for fusion reactors and stable to the modes described by ideal MHD. The principal remaining challenge is to understand the slowly growing modes that arise from physics left out of the ideal MHD model—most importantly, finite electrical conductivity and kinetic effects such as nonvanishing flow along the magnetic field and anisotropic pressure.

When such nonideal effects are included, the model is called extended MHD. Although the new modes introduced in extended MHD grow slowly, the effects that produce

them usually introduce time- and space-scale separations that make calculations difficult. For example, in hot plasmas the electrical resistance is so small that the time scale for global changes in current distribution or magnetic field structure is hundreds of seconds in a device the size of ITER. But the local effects of MHD modes are communicated across the plasma in microseconds, and extended MHD must deal with the full range of time scales.

Nowadays, plasma physicists can carry out realistic simulations of extended-MHD phenomena for relatively small experiments in which the scale separation is not too large. Figure 3 shows two time slices from a simulation of a sawtooth crash in a tokamak-like device called a spherical torus. The sawtooth is a relaxation-type oscillation in which the electron temperature slowly builds up and then suddenly crashes down. The crash is accompanied by a redistribution of plasma current and, to some extent, a change in the magnetic topology in the plasma interior. The sawteeth themselves can limit plasma performance, or the magnetic perturbations associated with them can trigger other instabilities, including sudden, potentially damaging events called plasma disruptions.

Long time-scale evolution

Most of the time, appropriate macroscopic parameters averaged over flux surfaces and rapid-time-scale variations are themselves slowly varying quantities. Such parameters, which include the magnetic field structure, plasma current, and the radial density profile, temperature, and flow of the various particle species, are quantities with which researchers can hope to understand what the plasma is doing and that one can measure experimentally. A description in terms of averaged macroscopic parameters serves as the starting point for a simulation of the always-present rapid-time-scale phenomena of heat-

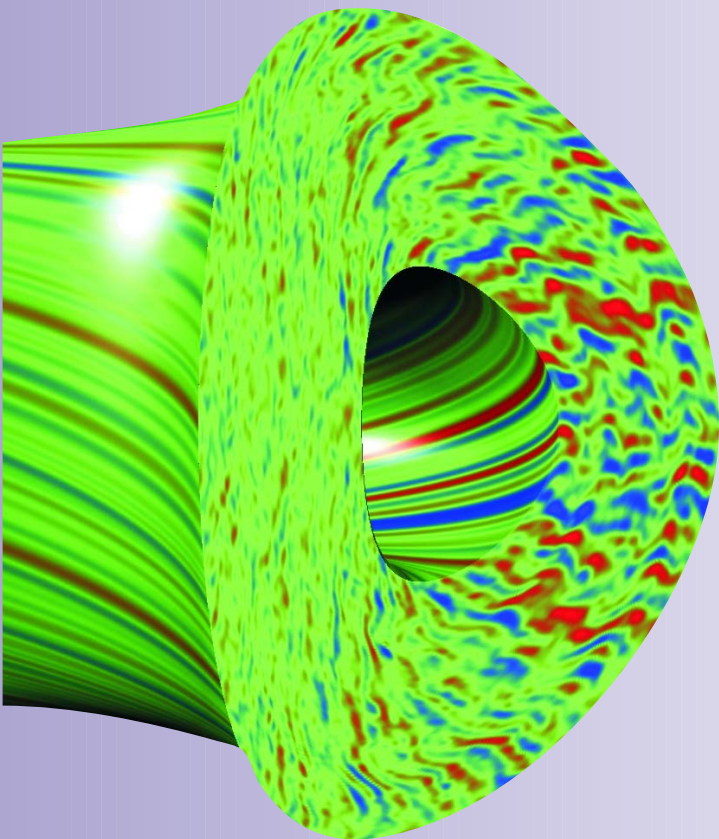


Figure 2. Microturbulence in a tokamak is associated with turbulent eddies that are extended along the helical magnetic field lines but have fine-scale variation perpendicular to the field. In this simulation, colors indicate deviations from the average plasma density: Red regions are overdense; blue, underdense. The hollow central region is an artifact of the simulation. (Courtesy of Jeff Candy, General Atomics.)

ing, microstability, and MHD.

Although physicists cannot self-consistently incorporate the short-time and short-wavelength phenomena, they can use reduced models to simulate evolution occurring over long time scales. The models relate the time evolution of averaged parameters to appropriate sources and sinks. The physics of transport and of the sources and sinks depends on the geometry of the flux surfaces, which shift around in space as the pressure, current, and external fields evolve. Therefore, the one-dimensional transport equations must be coupled to two- or three-dimensional MHD models in what are called 1.5D transport models.

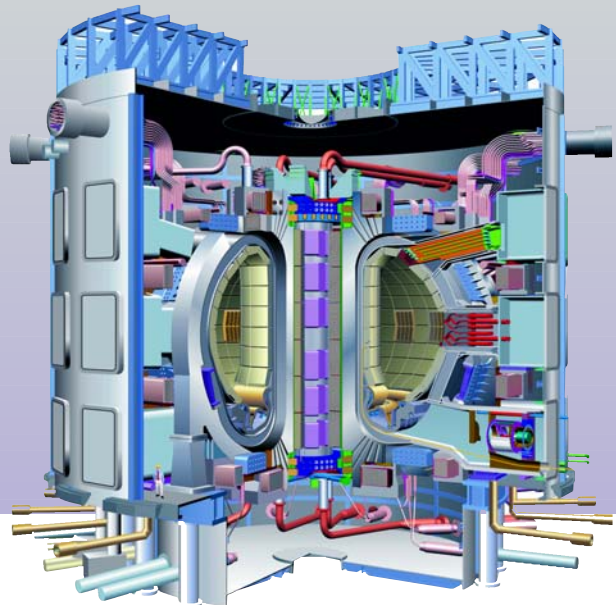
A plasma simulated in a 1.5D transport model can evolve to be susceptible to a sawtooth event. At that point, one can stop the simulation, redistribute pressure and current across flux surfaces in a way that models the effects of a sawtooth crash, and restart the simulation. Simulations employing that technique mimic the fast effects of MHD and are essential tools for the support of experiments.

Toward an integrated fusion model

In 2002, the US Department of Energy's Office of Science charged its Fusion Energy Sciences Advisory Committee with defining a major new initiative in fusion simulation. That project, called the fusion simulation project (FSP), is now conceived to be made up of three elements: a research

Box 3. ITER

At a nominal construction cost of \$5 billion, ITER, the international fusion energy reactor, will be among the most ambitious single research devices ever constructed. (See the illustration below, based on an image provided by the ITER collaboration.) Its goal is to demonstrate both the scientific and technological feasibility of fusion energy. A basic design for ITER has been developed, and intergovernmental negotiations are under way to discuss site selection (see *PHYSICS TODAY*, August 2004, page 28) and the roles of project partners in construction and operation. After having dropped out of the project for four years, the US has recently rejoined negotiations with the European Union, Japan, Russia, Korea, and China. The reactor will be a very large superconducting tokamak capable of producing some 400 MW of fusion power. About 80 MW from energetic fusion alpha particles will remain in the plasma for self-heating, and some 40 MW of external wave and beam power will serve for heating and control.



and small-scale integration component, a large-scale integration and production component, and an infrastructure consisting of software, a database system, and collaboration tools, all available to the other two components as well. The FSP will advance theoretical research and existing experiments in the near term and develop the fusion simulation program on a time scale compatible with the need to support ITER.

Several obstacles inhibit a simple gluing together of a set of existing codes to make an integrated model. New algorithms and perhaps new physics formulations may be necessary, particularly if the coupling of multiple phenomena introduces intermediate scales where previously there was wide separation. The research component of the FSP will develop solutions in several parallel initiatives. Any given initiative will not attempt a comprehensive simulation, but instead will focus on a small number of issues by coupling two, or perhaps a few, physics models.

Those focused integration initiatives will be structured to address critical near-term issues that are cross disciplinary. For example, we in the plasma physics community need to understand how MHD stability is affected by plasma currents that can be driven by both transport processes and external sources such as waves. We need to

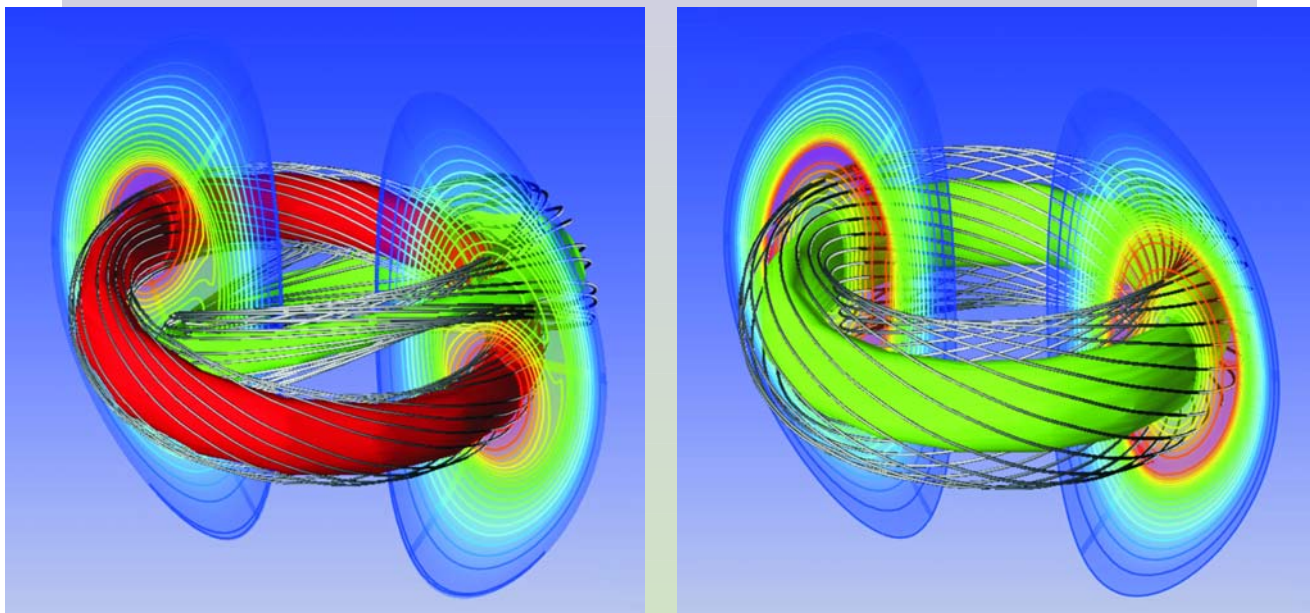


Figure 3. In a sawtooth oscillation, the electron temperature slowly rises, then abruptly falls. In this simulation, the bean-shaped surfaces are toroidal cuts and the circular shapes on those cuts indicate magnetic flux surfaces. The colors of the contours give the plasma temperature: Red indicates hot plasma and blue signifies cool. (a) Previously nested surfaces have broken to form two separate nested regions, or magnetic islands; the panel shows two interlocked flux surfaces. (b) In time, the cooler region moves inward (that is, toward the magnetic axis of the torus) while the hot region moves out. The magnetic surfaces eventually reconnect into a nested configuration with low-temperature plasma on the inside. (Adapted from W. Park et al., *Nucl. Fusion* **43**, 483, 2003.)

understand the interaction between microturbulence and the global structure of density, temperature, and plasma flow. And we especially need to understand the physics of the plasma-edge region, where large- and small-scale stability and transport are all complicated by a number of factors: Those include proximity to the material containment walls, magnetic field structures that no longer form closed flux surfaces but make contact with solid material, and fluxes of neutral particles that are unaffected by the magnetic field. Conditions at the plasma edge, as experiments have confirmed, have an enormous effect on plasma confinement.

The production component will provide publicly released simulation tools that will include a collection of experimentally validated models of limited scope as developed in the research component. (For the importance of validation, see the article by Doug Post and Lawrence Votta, *PHYSICS TODAY*, January 2005, page 35.) It will also create an evolving, comprehensive model called the integrated plasma simulator (IPS). That task will present daunting challenges of design and software engineering. The software architecture will have to be very general and extensible, not tied to a particular computer architecture, and it must offer an easy-to-use interface. Furthermore, such flexibility cannot impose a significant cost. Initially, the IPS will integrate reduced physics models much in the spirit of today's 1.5D transport codes, but in time it will incorporate the improved models and advanced methods for dealing with multiscale issues as they are developed in the focused integration initiatives.

The importance of integrated simulation is recognized throughout the world fusion community. Japan's burning plasma simulation initiative (BPSI) is a collaborative project among universities and government laboratories. To

date, the project has held several workshops and is developing a core integrated modeling code with goals similar to those of the IPS in the US plan. Because stellarators are of great importance in the Japanese fusion program, the BPSI simulator will support nonaxisymmetric systems, not just tokamaks and ITER. Since the middle of 2003, Europe's Integrated Tokamak Modeling Task Force has been working toward providing a comprehensive integrated simulation package for ITER. Their present concept closely resembles the FSP, although the US initiative is more ambitious than its Japanese and European counterparts. The US approach should meet head-on the mathematical and computational challenges of including all plasma-physics interactions at all relevant scales. To that end, the FSP will include a balanced mix of mathematicians, computer scientists, and fusion physicists from many institutions.

The challenge of coordinating many institutions and disciplines has been successfully met by DOE's SciDAC (scientific discovery through advanced computation) program. The fusion SciDAC projects are providing advanced codes that can be valuable building blocks for the FSP, and the computer science and math SciDAC projects are contributing to the needed algorithmic and software infrastructure. With the help of such programs and the constant improvement of supercomputers, the FSP will enable the US to play a major scientific role in ITER and the further development of fusion energy.

Further Reading

- M. Wakatani, *Stellarator and Heliotron Devices*, Oxford U. Press, New York (1998).
- J. Wesson, *Tokamaks*, 3rd ed., Oxford U. Press, New York (2004).
- J. Dahlburg et al., *J. Fusion Energy* **20**, 135 (2001).
- The ITER website, <http://www.iter.org>. ■