A Comprehensive Computing Initiative for MFE

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A Comprehensive Computing Initiative for MFE

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Summary:

We propose that a national initiative be launched to develop a comprehensive simulation facility for MFE. The facility would consist of physics codes developed by the national MFE community tightly but flexibly coupled through a programmable shell, enabling effectively simultaneous solution of the models in the various codes. The word "facility" is chosen to convey the notion that this is where one would go to conduct numerical experiments, using a full set of modules to describe an entire device, a coupled subset to describe particular aspects of a device, or a combination of the facility's modules plus the user's own physics.

Introduction: the need

The scientific base of magnetic fusion research comprises three capabilities: experimental research, theoretical understanding and computational modeling, with modeling providing the necessary link between the other two. The past decade has seen dramatic advances in all three areas, particularly in the first two where the larger emphasis has been placed. As a result, the MFE experimental program during this period has continued to advance performance despite the absence of major new experimental facilities, a feat which can be attributed at least in part to increased understanding enabled by the theory and computing efforts.

In parallel have been near-revolutionary advances in computer hardware and software. These have been continuously exploited by the MFE program, but the promise of further dramatic increases in computing capability offers an opportunity for a qualitative increase in the role of modeling within MFE.

The U.S. now faces a budget climate that will preclude the construction of major new MFE facilities and limit MFE experimental operations. In response, DOE is restructuring the program to have as its major focus the stewardship of fusion science. The situation is rather analogous to the one experienced by the DOE Defense Programs (DP), in which continued viability of the nuclear stockpile must be ensured despite the prohibition of underground experimental tests. DP is meeting this challenge, in part, by launching the Accelerated Strategic Computing Initiative (ASCI) to bring advanced algorithms and new hardware to bear on the problems of science-based stockpile stewardship (SBSS). ASCI has as its goal the establishment of a "virtual testing" capability, and it is expected to drive scientific software and hardware development through the next decade.

We argue that a similar effort is warranted for the MFE program, that is, a national initiative aimed at developing a comprehensive simulation facility for MFE, with the goal of enabling "virtual experiments." It would play a role for MFE analogous to that played by present-day and future (ASCI) codes for nuclear weapons design and by LASNEX for ICF, and provide a powerful augmentation to constrained experimental programs.

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Developing a comprehensive simulation facility could provide an organizing theme for a restructured science-based MFE program. The code would become a central vehicle for integrating the accumulating science base. In time, it would lead to a fundamental shift in the relationship between computing and experimentation within MFE. Currently, as in the past, experimental facilities are regarded as the primary vehicle for exploration. Theory and computing are invoked to confirm experiments through analysis and understanding of their results, to provide the rationale for some of the new experiments on existing facilities, and to contribute to the design bases for conservatively extrapolated new experimental facilities. In the context we propose, the relationship could ultimately be reversed: computer simulation would become a primary vehicle for exploration, with experiments providing the necessary confirmatory evidence (or guidance for code improvements). This shift would allow much more aggressive steps to be taken in the experimental program, as well as more efficient and extended use of existing facilities. It would also allow a more vigorous assessment of alternatives to the tokamak. The net result would be a more cost-effective program.

Note that achievement of this role for the project is a long-range goal; implementation of the project in no way eliminates the need for either experiments or theory. There are important areas of magnetic fusion physics where our understanding is far from complete, and where repeated cycles of code prediction, experimental tests, theoretical analysis, and improvement to the code will be required to develop a reliable predictive capability and build the confidence which enables this role.

Comprehensive simulation requires self-consistent simultaneous solution of the equations describing many distinct physical processes in a magnetic-fusion device. These physical processes operate on often disparate spatial and temporal scales. Hence our vision of the comprehensive simulation facility is a tightly coupled suite of physics codes in which the code models are effectively solved simultaneously. This is a more challenging undertaking than simply having sequential calculations by various codes which read and write a common file format. It is nevertheless required for truly self-consistent simulation. It is also a technique which has been successfully employed in other complex projects, such as ICF (the LASNEX code) and global climate and weather modeling.

In addition to the challenge of global simulation, there is growing recognition that simultaneous solution of nominally distinct physics ingredients is required for the qualitative and quantitative understanding of important physics phenomena in MFE. Examples are given Appendix 1. The development of algorithms and structure for the tight coupling described above will enable exploration of such phenomena as an added benefit. Indeed, running subsets of the full suite to explore the interaction of particular physics building blocks may turn out to be the most common use of the facility.

Another side benefit of this project is that it would provide the national theory program with a visible set of deliverables (and the overall MFE program with additional deliverables) in an era where this consideration may well be critical to survival.

Feasibility: Now is the time to start

The concept of a comprehensive simulation capability for MFE is not new and has been proposed before. The question always has been "When is the understanding base sufficiently well founded to start developing a large-scale integration?" Given that development might take several years, we argue that the time is now. At a minimum, five reasons support this contention:

• The MFE theoretical base is maturing very well: The physics understanding and the implementation of computational packages in such areas as magnetohydrodynamic (MHD) equilibrium and stability and some kinds of heating and non-inductive current drive are sufficiently advanced that they could be incorporated in mature form immediately. Edge physics packages are less well developed, and turbulent transport

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and 3-D resistive MHD even less so. However, even in these least developed areas, there is growing confidence that we are solving the right equations and that with continued theoretical and computational progress we will be able to deliver good solutions. We should, therefore, assume that these efforts will be successful and begin taking steps to ensure that we can take timely advantage of the results.

- Even a facility based on the physics packages available today would be valuable, and the physics base will be even more mature by the time the first version is ready: The experience with LASNEX and the fledgling but growing experience of the MFE community with prototype efforts such as LLNL's CORSICA (see below) indicate that extremely useful codes can be generated today even in the absence of fully matured physics packages in all areas. Early versions of the new facility would contain the best prevailing packages, a combination of good theory where available, careful empiricism where theory-based solutions are unavailable, and competing physics models where that makes sense. Later, because its architecture will be made sufficiently flexible, improved packages can be included as they are developed. Thus, the MFE comprehensive simulation facility should be viewed as an evolving entity that is constantly being modernized and improved, much as is the case with LASNEX.
- Computer hardware and computational algorithms are progressing at a pace that computations that are unthinkable now will be straightforward in a decade or less. This further enhances the likelihood that the weak areas in our physics base will be successfully strengthened on a timescale comparable to that of the development of the overall project.
- Developing a comprehensive simulation facility fits well with the new program priorities adapted following the recommendations of the Fusion Energy Advisory Committee (FEAC). This point will be elaborated upon in the next section.
- We now have a demonstration of at least one prototype for such an endeavor, CORSICA. The project, funded by LLNL's Laboratory-Directed Research and Development program, has demonstrated the feasibility of coupling together relevant disparate-scale physics modules to make a comprehensive simulation, and the first released version is in routine use today by ITER and DIII-D scientists. This is discussed in more detail below; and
- Starting now would permit MFE to leverage off of the much larger DP investment in ASCI. Many of the algorithms, software and hardware advances made by ASCI could directly benefit the MFE effort.

A Good Fit to the New (FEAC) Program Strategy

Development of a comprehensive computing facility for MFE meshes well with the new program strategy recommended by the FEAC and adopted by OFE. The key ingredients of this strategy are development of fusion science, advancement of plasma science, increased focus on concept innovation and alternative approaches to fusion, and pursuit of fusion energy through international collaboration. We comment here on the role this initiative could play in each area.

• Fusion science: The comprehensive simulation facility would be a target vehicle for theoretical and computational advances in fusion physics. The necessity of fixing weak links would provide incentive for science advances. Once the facility becomes operational, there will begin cycles of prediction of experimental results, comparison with experiments, corrections to the theoretical models, and updates to the facility.

This cycle should invigorate the science in all parts of the magnetic-fusion physics program: experimental, computational, and theoretical. In addition, the facility will enable the study of theoretical physics ingredients in the self-consistent environment of the rest of the fusion device (or some portion of the rest of the device), which should create new possibilities for scientific advancement. Stated another way, the facility will allow exploration of the way the building blocks of fusion science interact with one another. Finally, the facility would allow integrated evaluation of fusion concept improvements.

- Plasma science: The MFE experimental facilities are useful for performing basic plasma experiments as well as fusion experiments, and these could be modeled with the facility. Additionally, the modules in the facility can be combined to model plasma phenomena not realizable in MFE devices, and, because of the programmable shell structure, specialized modules for a specific basic plasma science concept can be readily combined with pre-existing general purpose modules to model a wide range of phenomena not directly treatable with the basic MFE modules. Finally, the existence of this facility could open up a new line of research in the coupling of complex nonlinear models of plasmas.
- Alternative approaches/concept innovation: the comprehensive computational facility should facilitate the integrated study of alternate concepts, permitting a more knowledgeable assessment of new configurations. Configurations close to the traditional tokamak will be addressable by the suite of tokamak physics modules with little modification. Others would be addressed by combining new specialized modules with ones already existing in the facility; as noted in the preceding paragraph, this process is greatly facilitated by the flexible, programmable shell.
- Fusion energy through international collaboration: the comprehensive computational facility will be valuable for projecting the performance of future international machines and modeling experiments on existing facilities. Hence, the facility could be a major U.S. contribution to the world fusion effort.

The Facility

In brief, our vision is as follows: the computational facility will consist of code modules describing all important aspects of toroidal magnetic fusion physics (and some engineering), linked by a common programmable framework. When the modules are executed on the same CPU or on multiple CPU's sharing the same memory, this framework will allow the modules to communicate with each other rapidly via a sharedmemory database. Tight coupling of the modules as in the shared-memory database approach allows simultaneous and self-consistent solution of all of the equations being solved. The CORSICA project has demonstrated that coupling algorithms can be developed to make such a tight coupling work efficiently. A comprehensive simulation of a tokamak or an alternate configuration (or a partial simulation of one of these devices) is created by combining the appropriate modules for each case. Slower alternatives, available when such frequent communication is not required, are interprocess communication or, even more slowly, via shared self-describing disk files. (The latter is of value mainly for occasional exchange of data with codes not integrated into the facility.)

We emphasize that the framework should be interactively programmable and extensible. A programmable system allows the user to experiment with individual modules or combinations of modules, without recompilation, and to perform tasks that were not envisioned by the module authors. Furthermore, interactive extensibility allows the facility to be designed with a layered "onion-skin" structure: a menu of modules of varying complexity can be available for modeling particular physical processes. This menu would provide quick-running options, executable on work stations, for parameter surveys and other fast-look applications, and more comprehensive slower-running options, requiring supercomputers or massively parallel platforms, for more detailed studies. This layered structure ensures that the facility will be usable at an earlier date and be continuously usable, even as more complete layers are being developed.

Furthermore, the menu can also include competing modules, perhaps developed with different physical approximations or different numerical techniques. This would allow module developers and users to test and compare modules in a common environment, and to easily experiment with the effect that the models have in a fully self-consistent simulation. Because input and output is handled by the framework, the physicist needs only to code up the physics; and even significant pieces of physics (the less computationally intensive parts) can be added via scripts for the programmable framework, obviating even the need for recompilation. The compared models also have access to the same diagnostics and the same input format. Thus the facility provides added value for testing models even if they are not coupled to other physics.

We describe the object of this initiative as a "facility" in order to convey the notion that this is where one would go to conduct numerical experiments, using a full set of modules to describe an entire device, a coupled subset to describe particular aspects of a device, or a combination of the facility's modules plus the user's own physics. The latter could be added either through compiled modules, or without recompilation via interpreted scripts as noted above.

Important aspects of such an endeavor are that it be accessible to the broad community of experimentalists and theorists, that the codes be sufficiently robust and the user interface be sufficiently intuitive that non-developers will be able to easily use it, that the constituent modules be validated against experiments, other computational models, and theories, and that both the code framework and project management structure encourage participation from code developers around the community. These aspects would be assured by having integrated teams of computational physicists, theorists, computer scientists, and experimentalists, by incorporating user- and developer-friendly tools in the framework, and by having project managers committed to these goals.

A Prototype

The MFE Program at Lawrence Livermore National Laboratory has been developing CORSICA, a prototype for such a coupled suite, under Laboratory-Directed Research and Development (LDRD) funding. The project has developed efficient coupling algorithms and successfully applied these algorithms to several of the important coupling problems that must be addressed in a comprehensive simulation facility. These include: (1) coupling a module describing the macroscopic transport of heat, particles and current to a module that solves for the magnetic geometry (MHD equilibrium) in response to these profiles and to currents in external circuits; (2) the coupling of macroscopic transport to calculations of the microscopic turbulence that drives the transport; and (3) the coupling of transport in the core and edge regions, where the characteristic time and space scales are vastly disparate and the basic dimensionality also differs. The CORSICA project has also demonstrated the utility of structuring the facility as a suite of modules connected by a programmable shell: The developers find that they can do considerable algorithm development at the interactive shell level, and that they can easily add or substitute modules. The users (including experimentalists) find that they can easily set up problems, define new diagnostics, and even define new classes of numerical experiments, without direct involvement of the development team. As a "comprehensive tokamak simulation," the project is far from complete; nevertheless, the released version (core transport plus axisymmetric MHD and circuit equations) is being frequently used by members of the DIII-D experimental team and by the ITER designers, was an active contributor to the Tokamak Physics Experiment (TPX) design effort, and is being utilized for studies of the

spheromak, an alternative to the tokamak. Throughout, the CORSICA effort has been managed as a project with time lines, milestones, etc. We believe that this should be the case for the proposed initiative, as well, in order to assure a clearly focused effort, timely development of deliverables, and a high degree of accountability for the investment.

Relationship to Numerical Tokamak Project

The Numerical Tokamak Project (NTP) was formed by a consortium of Laboratories and universities in 1992, with the long term vision of developing "a physics-based model of an entire large fusion device." It was recognized that the most difficult aspect of such an endeavor is the calculation of the plasma turbulence that governs the confinement of particles and heat. Hence the NTP is focusing exclusively on this problem under partial sponsorship of the High Performance Computing and Communications Program. The initiative being proposed here has as its objective the achievement of the NTP's long-term vision. It assumes future success of the NTP's turbulence mission, by developing a structure into which the NTP output can be inserted along with models for the rest of the device. Until such a time as the NTP results are available in appropriate form, the new simulation facility can progress by utilizing provisional models of the turbulent fluxes, it would offer a series of increasingly realistic modeling tools as short and intermediate-term deliverables.

Leveraging ASCI

There is an opportunity to obtain significant leverage from the Defense Programs investment in ASCI, particularly if a major role in the MFE initiative were to be assigned to LLNL, as LLNL is one of the three major ASCI participants (with an especially relevant ASCI program) as well as a significant participant in MFE. This leverage would come in several ways: (1) the computer hardware and associated computer science developed by and for ASCI will facilitate the MFE initiative. ASCI will be a major driver of supercomputer advances for the next decade. All large-scale computational efforts in the next several years will benefit. By having close contacts (such as, but not limited to, shared personnel) we can gain early access to ASCI-developed computer science advances and perhaps some access to ASCI computational platforms. (2) the ASCI applications program at LLNL will have two components which have considerable intellectual overlap with needs of the MFE initiative. The high-energy density (HED3D) component is envisioned as a closely coupled suite of complicated codes with a programmable framework, much as we propose for the MFE initiative; and there are a number of physics ingredients, particularly in the intended application of HED3D to inertial-confinement fusion problems, which are common with MFE. The ASCI turbulence component will have spin-off benefit to the calculation of plasma turbulence and, even more directly, to the calculation of neutral-fluid turbulence in the divertor region. Through collaboration with ASCI personnel, we could, for example, share the cost of the program development system (the "programmable shell") and wind up with a much better product; we could also gain better access to ASCI-sponsored computational physics advances, and possibly (as in the neutral turbulence example) gain access to entire codes with value for MFE. Finally, (3) the ASCI and MFE initiatives would share some common personnel (technical and management), a common Laboratory heritage in large code construction, and a common commitment to project-oriented science.

The physics expertise needed for success of the MFE comprehensive computing facility is distributed over a large number of institutions; hence the initiative must be a truly national project. The connection to ASCI through LLNL, as outlined above, would provide substantial benefit to the national community of developers and users.

Appendix 1: Examples of magnetic-fusion physics problems which require tight coupling of modules

Aside from the goal of whole-device self-consistent simulation, there are important physics motivations for the development of a facility and algorithms that enable tight coupling of modules. There are numerous examples where a loose coupling, for example by reading and writing common disk files, will suffice. This is adequate if one code postprocesses the result of another, or if only occasional two-way communication is required. However there are also a number of problems in magnetic-fusion physics where a much tighter communication is required; these occur in problems where one in effect needs to solve the equations in multiple codes simultaneously as opposed to sequentially. Examples are the following:

Efficient modeling of plasma control and shaping systems and calculation of voltsecond consumption requires tight coupling of core transport, MHD equilibrium, and external circuits.

Modeling of plasma evolution through a "soft beta limit" requires tight coupling of core transport, MHD equilibrium, and MHD stability (with enhanced transport coefficients related to the degree of instability).

Proper treatment of core gas-puff fueling requires self-consistent coupling of core transport to 2-D (at least) plasma edge transport and neutrals packages in order to quantitatively assess the attenuation of neutrals in the edge.

Quantitative assessment of radiative divertor plasma detachment requires coupling of core and edge transport with impurity transport and radiation packages, in order to account for the radiation inside the last closed flux surface as well as contamination of the core.

Modeling of disruption effects in a reactor requires coupling core transport, edge plasma transport, MHD, external circuits, radiation transport, plasma-wall interactions, impurity transport and neutral transport, at least.

Quantitative modeling of the L-H transition and its effects on core and SOL properties will require a self-consistent core-edge-SOL coupling and transport coefficients with adequate physics. If the currently popular paradigm (Diamond et al) of suppression of edge turbulence by sheared $\mathbf{E} \times \mathbf{B}$ flow coupled with turbulent generation of flows is correct, then the narrowing of the SOL that accompanies the transition to H mode will impact core and edge transport and the transition itself. Likewise, conditions in the core affect the other regions. Similarly, modeling of ELMs and their effects requires close coupling of the core, the edge, and an MHD instability model.

Calculation of turbulence with self-consistent profiles for the driving equilibrium fields (temperatures, density, flow velocity, ...): Particularly if the turbulence is non-local (e.g. because of correlation lengths non-negligible compared to equilibrium scale lengths, or coherent structures which make sizable radial excursions), simple parameterizations of the turbulent fluxes in terms of equilibrium quantities may not be possible, and a numerical approach becomes necessary. It is best done with coupled turbulence and transport codes, because of the large disparity in equilibrium and fluctuation time scales. Such coupled simulations should be useful in addressing such fundamental questions as how gyrobohm-like turbulence could give Bohm-like transport scaling in a tokamak.

Appendix 2: Status and needs of ingredients for a comprehensive simulation

The ingredients required for a comprehensive simulation suite include codes for freeboundary ideal magnetohydrodynamic (MHD) equilibrium (including interaction with coils and external circuits), plasma turbulence, core (one-dimensional, averaged over flux surface) transport, edge (two-dimensional) transport, ideal MHD stability, non-ideal, nonlinear time-dependent 3-D MHD, alpha particle confinement (orbits and instability effects), neutral beam deposition and other fueling processes, heating and current drive, neutral gas interaction with the edge plasma, plasma-surface interactions, and impurity radiation (as well as impurity transport, which may or may not be part of the main-plasma core and edge transport packages). Also required is the shell in which these will be tied together, as well as the coupling algorithms and a scripting feature which allows one to program the shell and its interaction with the modules.

A complete status report on these codes would constitute a review of the entire fusion computations program. We highlight here several modules which are central to the proposed project.

Ideal MHD equilibrium: although there are many MHD equilibrium codes in the community, most of these are "fixed boundary" (specified outer flux surface shape); there are only a few which are set up to interface with coils and external circuits. These include LLNL's TEQ, the DINA code from Triniti, Russia and Princeton's TSC. Future development required is minimal for coupling to core transport, but additional work is required to accommodate currents in the boundary plasma in a way that is consistent with the 2-D edge transport models.

Core transport: Many choices exist. One was developed for the CORSICA project which already includes the possibility of obtaining its transport fluxes from another code, such as a turbulence code, and its time-stepping accommodates CORSICA iterative schemes for coupling to turbulence. Further development required for the codes themselves is minimal, though key pieces of physics input -- such as turbulent transport -remain the subjects of major research efforts.

Core turbulent fluxes: This is the focus area of the national Numerical Tokamak Project. Two main computational lines have emerged: gyrokinetic codes (PPPL, LLNL, UCLA), which follow particles in self-consistent (usually electrostatic) fields but average over the fast gyro motion of the particles, and gyrofluid codes (PPPL, U. Texas, GA, NERSC, ORNL), which follow multi-species fluid equations in which models for kinetic effects have been incorporated. Both have made major strides in the past five years, to the point where simulations for realistic parameters of large tokamaks are now routinely done and compared with experiment. These large-tokamak simulations are done mainly with "flux-tube codes," which follow the local neighborhood of a field line around the torus. Some progress has been made in parameterizing the results of these simulations, offering the hope of a simple way of incorporating the results into transport codes. However, there are indications that such parameterizations may not be adequate under all circumstances. (For example, the turbulence appears some times to be non-local, responding to remote changes in background profiles more rapidly than local transport models would predict.) Hence, a capability for direct coupling of transport and turbulence codes is a desirable option. For this purpose a global turbulence code is highly desirable, both because it allows for non-local turbulence effects and because it makes more efficient use of the computational grid than multiple copies of a local code. With the exception of a specialpurpose code at ORNL, there are no existing global gyrofluid codes. There are global gyrokinetic codes (PPPL, UCLA), but they are more expensive to run than a comparable fluid code would be, and the adequacy of the resolution in present versions has been questioned. Hence, a global turbulence code, preferably gyrofluid, remains an important unfulfilled need. Other needs include improved treatments of collisions, fluctuating magnetic fields, and kinetic electrons.

Edge transport: the two principal codes in the U.S. are UEDGE (LLNL/INEL/MIT/ ORNL) and B2/B2.5/B3 (NYU/PPPL and European collaborators). These are both 2-D fluid codes, with similar physics; both are the result of a substantial development effort. These codes are heavily employed in modeling edge and divertor performance in tokamaks. The underlying fluid approximation is at best marginally satisfied, making incorporation of kinetic effects a high priority for future work. Another area requiring future attention is incorporation of improved models of edge turbulent transport; this subject is much less well developed for the boundary plasma than for the core.

Three-dimensional non-ideal magnetohydrodynamics (MHD) to model the evolution during a disruption, sawtooth crash, ELM, etc. A 3-D resistive code has been developed over the past several years by Park at PPPL, and has been extended to include fast alphas from a gyrokinetic code. Also, OFE has launched an MHD computing initiative (NIMROD) aimed at developing a new 3-D non-ideal MHD code with equilibrium flows and arbitrary cross-section shapes.

Other modules that are less central to the basic concept of a "numerical tokamak" but still important for a comprehensive simulation include neutral beam deposition, other fueling, R.F. heating and current drive of various types, orbital loss of and instabilities driven by alphas or other energetic particles, neutral gas penetration, radiation transport, atomic physics and plasma-surface interactions.

Coupling algorithms: If two codes are to be tightly coupled with frequent two-way flow of information, then it is essential to find ways of exchanging this information that does not slow down progress of the codes. For example, if one of the codes is a diffusion equation solver, which depends on fluxes generated by another code, then the flux provided must be at the advanced time step in order to not impose a time step constraint on the diffusion code. Such coupling algorithms have been formulated and demonstrated, as part of the CORSICA project, for coupling core transport to axisymmetric MHD and external circuits, core transport to turbulence, and core transport (1-D) to edge transport (2-D). The limits of applicability of these algorithms are still being explored, and optimization and improvement remain outstanding challenges.

Programmable shell: We propose that the shell which binds the modules be fitted with an interpreted scripting language. This allows the user or developer to set up "on the fly" complex problems that use the compiled modules as building blocks. A fairly trivial example is that the programmable shell can be used to instantaneously add a new diagnostic. A less trivial example is that one can construct, without recompilation, an optimization procedure that optimizes over the output of one or more of the modules. CORSICA was written under Basis, an LLNL-developed code framework, which was the best available at the time the CORSICA project began. Basis continues to serve us well; However, some newer products are becoming available that are more compatible with object-oriented programming languages and methodology, and with massively parallel and distributed computing.

Appendix 3: Synopsis of Proposed Project

The objective of the project is to assemble a suite of codes from which a set can be selected to simulate a shot in an entire magnetic fusion device, or alternatively a portion of device operation can be simulated (potentially, in more detail) by selecting a smaller set. Some of the codes in the smaller set may not be ones that one would run in the larger set. For example, one might want to study turbulent transport using a gyrokinetic code coupled to an MHD equilibrium code, in a year where it is not (yet) feasible to use the gyrokinetic code as part of a comprehensive simulation. Thus the project must proceed in several directions simultaneously:

1. Continue the development and refinement of the coupled prototype suite begun under the CORSICA project. This includes additions to CORSICA core-edge coupling to include evolving MHD, impurities, and the rotation profile, extending coreturbulence coupling to global gyrofluid and gyrokinetic codes with a full set of coupled variables coupled to toroidal transport, and implementing edge turbulence models. The project may need to assume responsibility for developing the global turbulence codes if these are not forthcoming from the Numerical Tokamak consortium.

- 2. Add modules to the suite to make it (a) "comprehensive" as well as (b) "layered". Item (a) includes 3-D resistive MHD, R.F. heating and current drive, coupling to dynamic neutrals models, etc., as well as modules needed to describe specific alternate concepts. Some of these, such as 3-D resistive MHD, are themselves ongoing major computational physics projects. Item (b) includes, for example, adding a menu of transport models ranging from simple phenomenological ones, through models like the IFS-PPPL model or GA's quasilinear model that require running a linear stability code, to full turbulence simulations. One might also include under (b) interpolation from a look-up table that summarizes the results of simulations.
- 3. Add modules that might never be used in the comprehensive suite but that might be used, in conjunction with modules from the comprehensive suite, to study in more detail a piece of overall device performance; for example, gyrokinetic codes coupled to MHD for turbulence studies, or a Fokker-Planck code coupled to electron-cyclotron or lower-hybrid ray tracing to study current drive.
- 4. Support module improvements, particularly with regard to robustness and portability. Physics improvements to individual modules are the responsibility of the core MFE theory/computations program, which should be expanded to support this effort.
- 5. Establish and maintain a program of ongoing validation for individual modules and the coupled combinations, with validation to be provided by bench-marking with experiments, theory, and other codes.
- 6. Adapt and implement a more modern application framework as a replacement for Basis, with the object of providing increased portability, increased user and developer friendliness, increased compatibility with new programming paradigms such as object-oriented programming, and increased ease of accommodating massively parallel and distributed applications. This should include development and upgrading of a graphical user interface.
- 7. Add "advisor" features to the suite to monitor initial conditions and the progress of the simulation and warn users about potential pitfalls---for example, the suite is entering into a regime where it needs to rely on a model outside its established regime of validity---and suggest alternatives.
- 8. Foster development of physics modules and new computational algorithms that will add important functionality to the suite or improve the existing functionality.
- 9. Provide support for users and developers. User support should include collaborations to set up and interpret applications, as well as diagnostic development.
- 10. Internal documentation: provide users' manuals in hard-copy and on-line form.
- 11. External documentation: write articles on algorithm and scientific research results for publication in the appropriate journals; prepare periodic progress reports and meeting presentations.

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