

Fusion Energy Sciences Advisory Committee (FESAC)

# Review of the Fusion Theory and Computing Program

August 2001



U.S. Department of Energy  
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# **Report of the FESAC Panel Reviewing the Theory and Computing Program**

**August 6, 2001.**

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## Executive Summary

This Panel was set up by the Fusion Energy Sciences Advisory Committee (FESAC) at its November 2000 meeting, for the purpose of addressing questions from the Department of Energy concerning the theory and computing/simulation (T/C) program of the Office of Fusion Energy Sciences.

There have been recent deliberations by FESAC (at its Knoxville 1999 meeting) and by the Integrated Program Planning Activity (IPPA, 2000) concerning theory and computing plans. The report of the Panel extends these deliberations to include findings and recommendations about program structure, balance, community governance, and management.

Although the Panel primarily addressed programmatic questions, it acknowledges that the theory and computing in fusion energy sciences has a stellar record of research successes. (A recent FESAC report entitled “Opportunities in the Fusion Energy Sciences Program” listed a number of theory and computing research highlights.) Last year the National Research Council performed an assessment of the quality of the fusion energy sciences program—including theory and computing—and concluded that the quality of its research is on a par with that of other leading areas of contemporary physical science.

In the remainder of this Executive Summary, we give a summary of the key points of our response to the DOE questions about theory, computing/simulation. The detailed questions are in Appendix A, and our response is given in more detail in section 2.

**The Panel received oral and written input from 27 persons, representing 20 different institutions. Overall, this input did not indicate any great deficiencies with the theory and computing/simulation program content and management. The Panel agrees with this sentiment. Hence our primary finding is that the quality, structure, balance, and management of the OFES theory and computing program are, on the whole, functioning well.**

The Panel also commends the T/C program for having several notable successes in self-governing certain community efforts e.g., JIFT, TTF, NIMROD, and PSACI.

Nevertheless, there were a number of important points made about ways in which the conduct of the program might be improved. Many of these points were related to whether a more formal management approach is needed in the program. Not surprisingly, views ranged from a belief that a theory/computing program should be relatively unconstrained, to a belief that a more systematic approach is needed to ensure that key T/C needs are met and that the roles of the various players are well defined. The T/C program should have both focused and free-ranging elements.

The sense of the Panel is that a more systematic approach is needed because:

- It is not completely clear how the program priorities are set.
- It is not clear how the T/C needs of each experimental program and design effort are met;
- It appears that a more systematic approach to code development and retention is needed; and,

- It is not clear how the efforts of the various types of institution and T/C groups (large, medium, and small) are connected to the broader goals of the program in terms of leadership and support.

The panel therefore makes the following recommendations:

- The T/C program should be focussed on achievement of the FESAC goals through T/C community and Theory Coordinating Committee input to an updated Integrated Program Planning Activity (IPPA) report. Also, a vision statement and regularly updated list of key issues and challenges should be published.
- The Theory Coordinating Committee could respond to specific charges from OFES or call to the attention of OFES, FESAC, and the T/C community overarching issues that require timely resolution.
- A systematic approach to providing theory and computing support should be developed for experiments and design studies, and should be considered in the review of proposals.
- Multi-user code projects should be initiated only on the basis of compelling usefulness, but then should receive adequate support. Code duplication should be minimized and resources should be concentrated (through a peer review process which is cognizant of the overall program goals) on fewer codes. The support of legacy codes and production codes should be put on a business- like basis.
- OFES should develop an understanding of how the T/C needs of a particular program are to be met, and of the responsibilities for leadership and support of the various institutions involved (e.g., by means of memoranda of understanding, program advisory committees etc).

The balance among theory and computing topical areas is reasonable on the whole. However, as might be expected given the successes in the T/C program, the panel sees areas that would benefit from an increase in the T/C budget. Of course, it is also the case that most of the elements in the fusion energy sciences program are under-funded. Nevertheless, two T/C areas stand out as needing attention.

- Adequate theory and computing support should be included directly in proposals for experiments, or in companion proposals focussed on the theory and computational aspects, and considered in their review. The underlying theory should be supported, consistent with the program needs.
- Recent OFES initiatives to strengthen advanced computing should continue to be pursued vigorously. Efforts in advanced computing should be strengthened.

A small minority view in the Panel is that there was insufficient testimony and discussion to support a recommendation that would result in any significant shift in resources or priorities in these two areas.

Theory and computing research is reasonably well distributed across national laboratory, university, and industrial groups, in a healthy mix. However, the research efforts of some individual scientists have become highly fragmented and OFES, T/C groups, and individual scientists should be sensitive to this concern. The connectivity to adjacent scientific fields is relatively weak, in spite of apparent applicability. Hence connectivity with non-fusion science fields should be enhanced. The proposed new interdisciplinary centers and the recent involvement of fluid dynamicists in the “reconnection” contract are steps in the right direction.

Theory, modeling, and simulation are fairly well integrated in the current program. Separation of theory, computing, and modeling should be resisted. Modeling requires specialized skills and knowledge; hence modelers need to be aware of current developments in computing science. Outreach, involvement, and visibility in the broader computational science community should be enhanced.

The new OFES peer-review process is commendable. Further improvements would be to provide more timely feedback; be transparent and similar for all institutions; allow review of program sub-elements; provide rewards for collaborations with experiment and involvement in cross-institutional teams; and incorporate relevance to the US program and stature in the international program as criteria. A detailed description of the review procedures should be posted on the OFES web page.

There is an urgent need to attract and retain younger scientists. OFES might consider setting up a task force to study the problem of how to strengthen their graduate programs.

# 1. Introduction

At the November 14-15, 2000, meeting of the Fusion Energy Sciences Advisory Committee, a Panel was set up to address questions about the Theory and Computing program, posed in a charge from the Office of Fusion Energy Sciences (see Appendix A).

This area of theory and computing/simulations had been considered in the FESAC Knoxville meeting of 1999 and in the deliberations of the Integrated Program Planning Activity (IPPA) in 2000. A National Research Council committee provided a detailed review of the scientific quality of the fusion energy sciences program, including theory and computing, in 2000.

The FESAC Knoxville report said:

- “The dramatic advances in the predictive power of modern theory and simulation make these tools essential elements of a cost-effective program.”
- “Strengthen theory and computation as very cost effective means to advance fusion and plasma science, taking advantage of advances in computation science and technology.”

The Integrated Program Planning Activity report represented the central elements of the fusion energy sciences plans in terms of four MFE and two IFE programmatic goals, as follows.

## **Magnetic Fusion Energy Sciences Program ( MFE) Goals**

1. Advance the fundamental understanding of plasma, the fourth state of matter, and enhance predictive capabilities, through the comparison of well-diagnosed experiments, theory and simulation.
2. Resolve outstanding scientific issues and establish reduced-cost paths to more attractive fusion energy systems by investigating a broad range of innovative magnetic confinement configurations.
3. Advance understanding and innovation in high-performance plasmas, optimizing for projected power-plant requirements, and participate in a burning plasma experiment.
4. Develop enabling technologies to advance fusion science; pursue innovative technologies and materials to improve the vision for fusion energy; and apply systems analysis to optimize fusion development.

## **Inertial Fusion Energy (IFE) Sciences Program Goals**

1. Advance the fundamental understanding and predictability of high energy density plasmas for IFE, leveraging from the ICF target physics work sponsored by the National Nuclear Security Agency’s Office of Defense Programs.
2. Develop the science and technology of attractive rep-rated IFE power systems, again leveraging from the work sponsored by DOE in the DP ICF Program.

The knowledge base for next step decisions in the development of fusion energy will be based upon these six key program goals. These goals are the guiding basis for the Integrated Program. More details on the IPPA goals and objectives may be found in Appendix B.



The report of the National Research Council's committee to assess Fusion Energy Sciences concluded that "the quality of the science funded by the US fusion research program in pursuit of a practical fusion power source (the fusion energy goal) is easily on a par with other leading areas of contemporary physical sciences." It also noted that the US has played a dominant role in plasma theory, in the context of the international fusion energy effort; that theory and modeling are now able to provide useful insight into instabilities and to guide experiments; and that many of the major experimental and theoretical tools that have been developed are now converging to produce a qualitative change in the approach to scientific discovery in the program."

The report of the present Panel extends the previous FESAC and IPPA deliberations on plans for Theory and Computing by including findings and recommendations on overall content, plans, structure, and governance. In agreement with the NRC report, the Panel recognizes the stellar record of successes in the program. A recent discussion of the successes may be found in "Opportunities in the Fusion Energy Sciences Program", prepared by FESAC for the Office of Science of DOE, June, 1999.

[http://www.foe.er.doe.gov/more\\_html/FESAC/FES\\_all.pdf](http://www.foe.er.doe.gov/more_html/FESAC/FES_all.pdf)

The Panel met twice, at UCLA January 31/ February 1, and at PPPL March 29/30, 2001. The meeting agendas, identifying those who gave oral and/or written input to the Panel, are in Appendix C.

## **2. Findings and Recommendations**

Please note that the questions in the original DOE charge letter include some duplication! We have chosen to structure our answers around the questions. Consequently, this duplication is reflected in our answers.

### **Question A.1. What is the appropriate role of theory and computation in the OFES program?**

The capabilities of the OFES theory and computation program continue to grow in interpreting and designing experiments, and are highly valued by experimentalists. This enhanced capability is a result of advances in theory, increased computing capabilities, and more complete and detailed diagnostic data. These advances indicate the need for continued basic theory as well as the development of comprehensive simulation capabilities to explain new experimental phenomena and support innovation and new concepts. The Panel applauds and encourages this close coupling of experiment, theory, and simulation.

The OFES theory and computation program has the ultimate goal to achieve a predictive scientific understanding of the behavior of high-temperature plasmas. The program has dual objectives:

--Advancing plasma science; and

--Assisting and guiding efforts to realize practical applications of fusion energy.

These objectives are complementary and reinforcing.

The theory and computation program contains both long-range efforts, as well as those that dynamically respond to nearer term challenges and opportunities. These are often best carried out in a synergistic manner, rather than being compartmentalized. More specific objectives that define the appropriate role of the theory and computation are the following:

- Advancing the understanding of complex basic fusion plasma physics;
- Formulating analytical models and developing advanced simulation tools to interpret experiments;
- Discovering innovative approaches to improve confinement system performance; and
- Predicting plasma performance to guide experimental plans and system studies.

**Is the current balance between theory and computing and the rest of the fusion program reasonable?**

In FY01 the theory and computation research budget increased by 10% to \$27.2M. Theory and computation comprise 11 to 13% of the overall OFES funding. The higher value includes an estimate of the support funded by experimental research programs. Overall, OFES resources for FY01 have been allocated as 55% for science and 45% for the operation of major facilities, enabling R&D, and equipment. Theory and computation therefore comprise approximately 23% of the science research in OFES, with the remaining science funds supporting experimental research, diagnostic instrumentation, data analysis, as well as construction and operation of small innovative concept experiments.

While the Panel finds this balance to be reasonable, there remain strong arguments for increasing the support for theory and computation. The advanced computations area is a particular opportunity, when coupled with a strong underpinning of basic theory. Although the Panel has not reviewed the total, fusion energy sciences program, it is aware of similar severe funding limitations in the overall OFES program. Therefore, any changes should take into account the important complementary needs for other program elements such as experimental operating time, diagnostic development and data analysis.

The most compelling arguments to increase the effort in theory and computation include the following:

- Theory and computation provide exceptionally high leverage to increase scientific understanding;
- Increased effort would enable the U.S. to maintain areas of international excellence, while providing valuable and unique contributions to both the U.S. and international programs;
- Some small experimental programs are severely lacking in theoretical and computational support, and generally there is an inconsistent approach to providing T/C support to experimental programs;
- Today's experiments are increasingly more sophisticated and require more detailed analysis;
- Advanced computational science tools are now available to be exploited for more complex and comprehensive simulations;
- Theory and computation provide excellent avenues to attract high quality students and new researchers; and

--Increased local computing capabilities (e.g., Beowolf clusters) would enable the theory and computation community to make significant advances in terascale computing and would complement capabilities at NERSC.

The Panel sees advanced computing as an especially high-leverage growth opportunity, in view of current computational capabilities and fusion energy sciences needs. The OFES program would benefit significantly from an increase in computational activities, as has occurred in other areas of science. Recent OFES initiatives to strengthen advanced computing should continue to be pursued vigorously.

**Question A.2. Is the current structure and balance between the elements of the theory/computing program appropriate? What changes, if any, are needed in program content?**

The Panel finds that the present balance between topical science areas (approximately 38% transport; 37% MHD; 13% wave-particle interactions; and 12% boundary physics issues) is approximately correct. The emphasis on transport and MHD helps to sustain U.S. international excellence in these topical areas, which are critical for innovative concepts exploration. Many researchers actively reach across these topical scientific areas. Cross-coupling and integrated research should be highly valued in ranking research proposals. The Panel prefers describing the OFES program in terms of these scientific topical elements, rather than by confinement concept or discipline (e.g., theory and computing). Nevertheless, these descriptions also provide additional valuable measures of balance in overall program content.

OFES experimental research on non-tokamak concepts is supported at a level comparable to tokamak experimental research. Yet the level of theory research applied to the many non-tokamak concepts is much less. This has occurred because of the much more detailed data available from U.S. and international tokamaks, and the important role for mature, high-performance tokamaks as a test bed for generic plasma studies. Nevertheless, with an increasing U.S. emphasis on these other confinement concepts, a more effective theory effort is essential, to guide and extract the underlying science from them. OFES should consider theory and computation as an essential element of scientific experimental research on all experiments, and include them as a review element. The underlying theory should be supported.

One decade ago, the U.S. fusion energy sciences program was arguably the leader in scientific computation and simulation. With recent cutbacks in fusion funding, the OFES's computation effort has fallen behind, and has not taken adequate advantage of advanced computing capabilities. The Panel's views in this regard are discussed in more detail later in this report.

In summary, the majority of the Panel recommends that increased efforts be directed toward theory and computing support of the non-tokamak confinement concepts and toward strengthening advanced computational activities. A minority view in the Panel is that there was insufficient testimony and discussion to support a recommendation that would result in any significant shift in resources or priorities in these two areas. Some specific suggestions for ensuring a more balanced funding between the various concepts are outlined below in response to the question A.4.

Many aspects of the OFES theory and computation effort could be applied to adjacent scientific fields, yet the existing connectivity is relatively weak. There should be an increased effort to strengthen outreach and interaction with other scientific fields, including such areas as space and astrophysical plasmas, fluid dynamics, and high-intensity accelerators. Researchers should be encouraged to make these connections, and these connections should be an important aspect of evaluating and ranking proposals to OFES. Scientists should, moreover, make efforts to learn from other fields, in order to know current developments, be able to describe fusion science in their vocabulary, and also import and adapt new ideas.

To some degree, the above imbalances arose due to the absence of a detailed community theory and computation plan. Various theory and computation groups have detailed institutional plans, as do individual principal investigators. Portions of an overall theory and computation plan are embedded within various program documents, such as FESAC reports, the Snowmass proceedings and the IPPA report. Nevertheless, there is no national theory and computing plan that is clearly documented. Therefore, there is no sense that deliberate choices have been made in constituting the current program, nor that a clear vision has been articulated concerning critical challenges and opportunities for future research. The theory and computing/simulation program should be focussed on the goals of FESAC, as elaborated in the Integrated Program Planning Activity report. An IPPA report, updated through T/C input, would demonstrate the key role of T/C in the overall, fusion energy sciences program and would integrate it with the experimental activities. A national theory and computation plan would describe the program content in a clear and compelling way, as part of the overall program plan. Needless to say, such a plan is not a substitute for simultaneously stimulating innovations, supporting scientific excellence, and encouraging creative scientists to interact with related areas and other scientific fields.

The Panel also recommends that there be a vision statement and that a regularly updated list be published summarizing key scientific issues in theory and computing/simulation. A possible model could be the Opportunities and Challenges reports issued by the Theory Coordinating Committee, the most recent of which was published in March 1999. These five-page documents, which listed near- and long-term challenges were particularly useful. In hindsight, it is impressive to realize the outstanding progress that has been made in addressing both the near-term and the long-term challenges. A body such as the Theory Coordinating Committee might undertake this activity. Additional discussion of this issue is given in the answer to questions B1 and B3.

**Question A.3. Several groups and numerous individual investigators at many institutions carry out theory/computing research. Is the distribution of research among these research performers appropriate?**

Theory and computation research is conducted by national laboratories (48% in FY00), universities (37% in FY00), and industries (15% in FY00). In FY01, the theory and computation budget increased by 10% to \$27.2M, with allocations determined on the basis of proposals reviewed by OFES. There are seven theory and computation groups with annual funding over \$1M (PPPL, Texas IFS, ORNL, GA, LLNL, MIT, and LANL), four groups with annual funding

between \$0.5M to \$1M (NYU, Lodestar, UCSD, Maryland), and approximately 30 smaller theory grants funded by OFES. Approximately 30% of OFES theory and computation funding is provided in grants of less than \$0.5M. The OFES theory and computation community consists of nearly 200 individuals.

The Panel heard presentations from several research groups and from principal investigators at a number of institutions, and concluded that the balance of research activities is reasonably well distributed. Opinions ranged from the view that the research is too thinly spread, to that it be more widely distributed. Most importantly, the common view is that the research should be distributed according to scientific and technical merit. The Panel strongly endorses the new peer review process being implemented by OFES that provides for comparative ratings based on scientific excellence. In these reviews, however, technical relevance to the OFES mission and to the international fusion program should be incorporated into the ranking of proposals.

This diverse distribution of participants, with its very healthy mix of institutions and individual investigators, is a strength of the US theory and computation program, in that it provides valuable cross checks and stimulates innovation. Despite this distribution, there is the perception that fusion plasma science is not as widely represented in university physics and engineering departments, in the younger age bracket, relative to other fields of physics. On the other hand, OFES has an ultimate energy application goal, which calls for a greater degree of focused scientific research, as well as the integration and synthesis of scientific issues, which is facilitated by larger research teams. In practice, such categorizations are blurred, as one can find healthy examples of small university groups that provide design support to large projects, and large laboratory groups that develop seminal basic theory and support university efforts.

Still, there is an issue regarding the poor definition of the roles of the different types of institution and of their T/C groups. It is not clear in many cases how the different institutions and T/C groups, ranging from large groups to individual contributors, are used systematically to provide support and leadership to the various program activities involving theory and computing/simulation. This was seen in the case of a number of small experimental groups, but is also the case in larger program activities. Do large theory groups associated with major experiments have a responsibility for the general scientific development of the concept, or is their primary role to provide for the local experiment? Are the sizes of the various groups appropriate for their responsibilities? There does not appear to be a systematic approach to providing T/C support and program leadership. In order for each program element to have the necessary T/C content funding must be adequate, and the roles and responsibilities of all the participants defined. For example, a definition of the role of the large T/C groups in supporting a local experiment and the more general scientific development of the concept needs to be clarified. The Panel recommends that OFES consider these factors in establishing and reviewing programs, and ensure that there are adequate memoranda of understanding and program advisory committees to make the programs function effectively.

There is a significant community concern about the fragmentation of the time of some individual researchers in theory and computation. Fragmentation occurs by scientific topical area, and also by confinement concept, by project, and by institution. Many individuals inefficiently multiplex their research time in 10-20% allocations. This fragmentation can be inflicted by the individual

on him/herself, by the institutions, or by OFES. This is a very important area of concern, which should be addressed by OFES, by institutions, and by individual theory and computation investigators. The proposed new interdisciplinary centers and the recent involvement of fluid dynamicists in the “reconnection” contract are steps in the right direction.

**Are there structural changes that would make the program stronger?**

Many fusion researchers tend to spend their entire career at one institution. On-site collaborations among the staff at the various institutions should be strongly encouraged e.g., by means of sabbatical leaves and extended visits. Many long-range collaborations have been very successful, aided by electronic communications, conferences and workshops, video-conferences, and frequent visits. Greater advantage should be taken of the distribution of research among the many institutions involved in fusion research by encouraging interdisciplinary research with scientists in other fields. Universities and laboratory research groups have natural opportunities for doing this.

As a scientific endeavor, the theory and computation community should take a more proactive role in community governance. Possibilities include enhancement of the Theory Coordinating Committee, or greater reliance on groups like the Transport Task Force to build on or as role models to emulate. This process would cultivate community spokespersons to advocate theory and computation priorities, and to reach out to other important fields of scientific research.

**Question A.4. In many areas of physics "modeling/simulation" studies are now viewed as a third discipline, distinct from both experimental and theoretical studies. How effectively are the modeling/simulation and theory communities working together to support the needs of the rest of the fusion program?**

While recognizing that computational physics requires a highly specialized set of knowledge and skills, there is a strong consensus in the community and on the panel to resist any fragmentation between theory and computation. The two approaches are intrinsically linked in fusion science. Both theory and experiment provide the necessary underpinnings and interpretation for simulations. Decoupled from basic theory, computation would be a sterile exercise. At the same time, progress in theory without computation would be severely limited by the complex, nonlinear nature of plasma physics. Any attempt to separate these sectors of our community through funding or management practices could cause harm to both, leading each to develop their own priorities, to stress narrow, ever more specialized problems and to engender conflicts over turf.

Some have suggested that integrated modeling be viewed as a fourth discipline, distinguished from first-principles simulations as well as from experiments and formal theory. For the reasons cited above, the Panel disagrees with this suggestion, but recognizes that this type of modeling has an important, but challenging role to play in the fusion energy sciences program. On the one hand, it must serve as an honest broker, calculating the consequences of theory as it applies to actual experiments. On the other hand, it is used as a tool for predicting the performance of future machines and for developing operational scenarios for current ones. In the first role, much

can be learned from difficulties and discrepancies between the model and experiments. The second role requires fulfilling the promise of accurate prediction.

It is a finding of the panel that theory and computation are well integrated in the current program. In general, work is carried forward by small teams containing both formal theorists and computational specialists or by individuals with expertise in both areas. The Panel also finds that separating the theory, computation, and modeling communities into distinct disciplines would lead to detrimental fragmentation of the effort.

Modelers do need to stay current with the latest developments in computer science. We should explore ways to improve our outreach into the broader computational science community and to recruit talented computer scientists into our research teams. This would allow us to take advantage of developments in other fields as well as increase our visibility and reduce isolation. Although there is a need for "quality assurance" of complex codes through a rigorous regime of validation and verification, real engagement of the theory and computing must go far beyond mere benchmarking exercises.

At the same time we want to encourage strong collaboration and co-development between theory/computation on the one hand, and experiments on the other. There is general recognition that the coupling between these communities has steadily increased and has been responsible, in large measure, for the remarkable progress in fusion science. Nevertheless, there is still ample room for improvement. We need theory support and collaboration on a wide variety of experiments including the full range of confinement experiments as well as small science-oriented facilities.

Experiments often have specific theoretical and computational needs in direct support of their programmatic missions. The Panel notes that apparently, to some extent, experiments are funded rather than complete scientific programs. Therefore, more attention should be given to ensuring adequate theoretical and computational support. There are various approaches by which experimental groups can marshal the necessary theory and computational support - all should be encouraged:

- a. Informal collaborations based on mutual interest where the funding of the participants is independent.
- b. Experimental proposals submitted along with companion theory/computation proposals during the same budget cycle.
- c. Experimental groups putting theory/computation specialists on their staff.

However, decisions about which problems to work on and which experiments to work with, should be driven principally by scientific opportunities and intellectual excitement from the field. In a broader scientific context, we have identified specific mechanisms that could foster and reward collaborations between theory, computation, and experiments.

1. Explicitly call out such collaborations as a positive factor in the merit criteria for proposals. This could encourage proposals that seek to reach beyond narrow specializations.
2. Work with program committees of major meetings to include direct comparisons between theory, computation and experiments as one of the important criteria when invited talks are selected.
3. Exploit modern computer and communications technologies to increase the availability and ease of use of codes, to provide transparent access to experimental data and simulation outputs, and to promote the sharing of analysis and visualization tools.
4. Encourage topical physics groups (like the TTF) that are explicitly chartered to generate dialogue between the sectors of our community. To be effective, the dialogue must be reflected in programmatic and institutional priorities.

Finally, while recognizing the importance of the confinement-concept orientation which has been the main organizing principle for the program historically, the panel sees an important need to encourage cross-cuts based on common science. The physics common to the concepts is generally greater than that which distinguishes them. Therefore, the free flow of ideas, results and intellectual capital should not be impeded by organizational or administrative constraints.

**Question A.5. How should the modeling/simulations efforts be conducted to increase their contribution to the overall program, considering issues such as code proliferation, legacy codes that are expensive to maintain and difficult to upgrade, introduction of modern computational techniques, and formation and functioning of multi-institutional modeling/simulation teams?**

A balanced approach between computational problem solving and multi-user code development is required. Small one- or two-person research codes function best with informal procedures and minimal oversight. Small projects can efficiently develop massively parallel codes with little structure, but even for them, modern code development practices will be helpful. Larger efforts, which include both large code efforts and smaller codes that have many users, require more formal processes, resources and planning. There is a need for the larger efforts to use the more modern code development tools and practices (e.g. project planning, internal and external coding reviews, modern version control, adequate documentation, modularity, risk management, regression testing, formal verification and validation program, good user interface). The fusion energy sciences program needs to modernize its procedures for the multi-user codes to be more effective. This will require more resources. Computer scientists will need to be integrated members of the code development teams, especially if the codes are to be able to exploit the full potential of massively parallel platforms.

Theory and computing represent an opportunity for the US fusion program to sustain excellence in plasma physics and fusion science in both the national and international arenas. The US, with NERSC, has world class computer facilities. Advances in computing capability offer an opportunity to improve current solution methods and to attack new problems that were previously intractable. Increased computing power has brought theory to the point where it plays an essential role in the planning and interpretation of experiments. An excellent computing and



theory program provides the US fusion sciences community with necessary tools for increasing plasma understanding, and offers an effective route for collaborative research with foreign experiments.

The Scientific Discovery through Advanced Computing (SCIDAC) initiatives provide an important means of sustaining a leading role for computational physics and theory for the US fusion program, both nationally and internationally. Within the fusion program, the Plasma Science Advanced Computing Initiative (PSACI) has as its goals the development and deployment of better mathematical models and computational methods for optimal utilization of modern supercomputing resources. However, the level of funding increase envisaged for PSACI (~\$3M) is marginal to take full advantage of the opportunities that advanced simulations offer. By comparison, in ASCI, a large scale computing effort typically involves 20 FTEs (about 40 people) and around \$5M a year. The SCIDAC process and the general view that simulation is an important method for scientific research offer a significant growth opportunity for the fusion theory and computation program.

There are a number of promising multi-institutional code development efforts. An advantage of multi-institutional efforts is that they lead to community owned codes that may be more widely used, thus eliminating duplication. Furthermore, group-developed codes may be, of necessity, modular and easier to upgrade. Benchmarking and documentation of these codes is essential. The community needs to know what equations are being solved, what algorithms are being used, and what benchmark tests have been performed.

That multi-institutional efforts and codes exist and are useful bears testimony to the professional competence and dedication of the team members. However, almost none of these projects is well enough supported to be really competitive with other large-scale computational physics projects in the US and international scientific communities. Large multi-user codes need a team composed of members from several disciplines—physicists, computer scientists, computational mathematicians, documentation specialists, testers, and others. Similarly, development and maintenance of a large multi-user code requires long-term, stable funding and support. The entire life cycle of the code including development and maintenance needs to be considered. Under-support for multi-user codes, likely, will lead to failure.

While many of the multi-institutional code development efforts have a user community, the process for identifying the need for the codes, and the potential user community is not clear. Large scale code development efforts should only be launched when there is a clear and compelling case that the program needs the capability that the code would provide, and that resources should be devoted to the code rather than other priorities.

The present fusion computational physics program is not sufficiently engaged with the national computational physics community. The panel recommends that the fusion community undertake a strong effort to participate in activities which foster interactions with this group. This includes participation in the appropriate professional societies and conferences, publishing in journals such as *Computing in Science and Engineering*, as well as other activities. If this is done, not only will fusion be viewed as part of the larger computational physics community, but also the fusion community will become more conversant with the state-of-the-art of modern massively-parallel computing.

Code proliferation is an issue that must be addressed carefully. Some duplication of research codes can serve a useful purpose. Parallel development of research codes addressing a single topic can serve to identify the best algorithms and physics approach. Cross comparison of results among codes in a new area is an essential element of verification and validation procedures. Duplication of more mature codes, however, should be minimized whenever possible. Consolidation works best for relatively mature codes and algorithms where the physics basis is stable. Examples include MHD stability, atomic physics, RF and beam heating algorithms, and data analysis. Important issues that must be addressed prior to undertaking a consolidation effort include the following: Is there duplication? Do the codes have different purposes and physics? Who are the users? How is support being provided? Are the codes modern? Are they maintainable?

Production codes need to be considered separately from research codes. For the reasons listed above, some duplication of research codes is desirable. However the development and maintenance support requirements for resources make duplication of large, multi-user production codes something to be done only when absolutely necessary. Too much duplication can lead to a number of sub-critical efforts. Code duplication should be minimized and resources should be collected and concentrated (through peer review not necessarily based on the NSF model) on fewer codes.

Legacy codes face many of the same issues as production codes. Except for a few cases, the fusion community has not explicitly provided the necessary support for external users for codes. Almost all of the codes are maintained by their original developers in their “spare time”. Issues such as porting to different platforms, updating and maintenance, documentation for users, adding user requested features, etc. get treated on an informal basis, if at all. The program should put the support of legacy and production codes on a much more business-like basis rather than the current voluntary basis. Part of this process would be for the community of users to identify the codes or code capability that is needed, then to develop a plan for modernizing the required codes (or replacing them).

**Question B.1. Are the current management practices of the program, such as program planning and merit review, sound?**

**and**

**Question B.3. What management changes would strengthen the program?**

Overall, the oral presentations and written material for the Panel did not indicate any great unhappiness with the theory and computing program content and management. The theory and computational program has an excellent track record of success. The moves toward enfranchisement of community groups within some elements of the program have been beneficial to both the program and DOE. A broadening of such efforts is clearly desirable but it must be done in the context of minimizing committees, meetings and layers of management. The concerns raised are discussed below.

The panel finds that the new, better-defined, OFES review process is a move in the right direction for the program. The strengths of this new process lie in its anonymous and comparative (i.e., involving a comparison and ranking of different proposals) review procedures

that give the benefits of constructive feedback. The constructive feedback should be automatic and timely, as well as interactive, where appropriate. Concerns and negative perceptions about this process would be best allayed by making the approach transparent and as similar as possible for all institutions. The approach, for example, could include comparative, anonymous review of specific program sub-elements (smaller programs, usually reviewed separately by a set of reviewers) while using panels, to ensure the integrated coherence of larger programs elements. Reviews should be made of the separate sub-elements of large programs. The panel recommends that a detailed description of the entire procedure should be posted on the OFES web site, as done, e.g., by the Office of Basic Energy Sciences.

The Panel recognizes that an important element in the theory program involves collaborations between theory and experiment and direct theoretical support for experimental programs. It is therefore important to foster this interaction both at the DOE level and at the programmatic level. Specifically, the panel suggests new review criteria that reward integration with experimental programs or large computational projects. A clear plan of the integration should include description of the proposed mechanisms and identification of personnel involved in the collaboration. Important programmatic goals are clearly furthered by strong, direct, theoretical support of the experimental programs. Such support must be encouraged. In the reviews, technical relevance to the OFES mission and to the international fusion program should be incorporated into the ranking of proposals.

The Panel notes that, if indeed national teams are the trend of the future, institutions should offer recognition for being a strong player, or even a leader, in a national collaboration.

A strong theory program necessarily contains a broad spectrum of elements including activities ranging from basic theory to direct experimental support. It should be made clear that every proposal does not have to satisfy all of the review criteria metrics.

While recognizing the need for some forms of programmatic categorization, the Panel feels it is important to note that in many cases a topical crosscut for categorization of theoretical projects is more representative of the program than classification by concept or facility. Additionally, the program should recognize that excellent scientific progress can be made without necessarily obtaining the final complete answers to difficult physics questions.

A standing national committee for theory and computing, with broad membership, could play a valuable role as a program advocate, in preparing a coherent program plan, in fostering outreach to the broader scientific community, and in encouraging interdisciplinary interaction. The Theory Coordinating Committee, consisting of leaders and senior members of the theory community, was formed in 1989 and has been functioning as an informal advocacy group for theory and computing/simulations. Such a group with a broadened membership to include representatives from related fields and the experimental community could take on such a role. The leadership should not be prescriptive and should represent the entire spectrum of the community. This committee could respond to specific charges from OFES or call attention to OFES and FESAC overarching issues that require timely resolution.

Within the theory program, as discussed above, a continued balanced mix of focused and broad research is important. One area of current imbalance is in the theory and computational support of the alternate concepts programs. This could be improved through general planning and by rewarding such efforts in the review process. Diversity of personnel within the program is also very important to the program's continued viability. To further this end, thought should be given to the makeup of review committees, executive committees and other organizational bodies in order to represent this diversity whenever possible,

In the T/C area, within five years, it is expected that a cadre of senior theoreticians will be retiring. Since it is anticipated that the US fusion energy sciences program will continue to broaden the range of its theoretical studies, a broad and flexible theory effort will be required to ensure the continuing viability of the field. An important consideration must be the need to *attract and retain* the next generation of plasma theorists. Plasma theory is important both from a basic-physics point-of-view and from a programmatic/societal point of view. Much of the science done by the community is intellectually stimulating and broadly relevant "basic" or applied science. This must be recognized and a better job must be done to communicate it. Encouraging outreach to the general science community as well as interdisciplinary collaboration should facilitate achieving this goal. Such encouragement could take the form of rewards at all levels, from DOE through direct support, to local leaders using annual reviews and "moral" support. The panel recommends that OFES consider setting up a task force to examine this concern.

At the introductory level, care must be taken to assure that the Post-doctoral and Graduate Fellowships are as flexible, competitive, and as well publicized as possible. We note two particular examples. The DOE Fusion Energy Post-Doctoral fellowship program should be designed to attract the best people in the field. If these positions are not competitive with other post-doctoral positions, prospective plasma theorists will accept positions elsewhere and will be lost from the field. The second example addresses the Fusion Energy Sciences Fellowship Program. It should be recognized that many graduate students start their graduate careers as a teaching assistant or unsure of exactly what sub-specialty they are interested in pursuing. After a year or two, when these students have decided on pursuing plasma theory, it is desirable that they have the ability to obtain funding. The present Fellowship program is structured so that students must apply within their first semester (or sooner). Panel members differed on whether additional flexibility in the program would remove this starting time issue and would increase the potential pool for the graduate fusion fellowship program.

A final obvious statement, which nevertheless must be an underlying principle for the program organization, is "Management should always be value added and not value subtracted".

**Question B.2. Is the role of various organizations in managing certain elements of the program reasonable (e.g., IFS coordination of the Joint Institute for Fusion Theory {with Japan} or PPPL coordination of the Plasma Science Advanced Computing Initiative)?**

There have been notable successes in the OFES Theory and Computation program in having various organizations manage elements of the program. Such efforts should be encouraged. Two

important features of such successes are strong leadership from respected leaders and a clear decoupling of programmatic and funding decisions from the institutions involved. The use of independent reviews of proposals and often a program advisory committee (PAC) are essential for ensuring credibility. The contributions of those who are providing leadership leaders for such program elements such as the US-Japan Joint Institute for Fusion Theory (JIFT), the Plasma Science Advanced Computing Initiative (PSACI), the NIMROD computational project, and Transport task Force (TTF) are highly appreciated by the Panel. This appreciation was also expressed by scientists who gave input to the Panel. Such efforts are an important part of enfranchising the fusion energy sciences community in support of OFES.

## Appendix A. Charge Letter

November 9, 2000

Professor Richard D. Hazeltine, Chair  
Fusion Energy Sciences Advisory Committee  
Institute for Fusion Studies, RLM 11.218  
University of Texas at Austin  
Austin, TX 78712

Dear Professor Hazeltine:

This letter provides a charge to review a specific element of the Office of Fusion Energy Sciences (OFES) program - the theory and computation program. Since the restructuring of the fusion program in 1996, most elements of the program have been reviewed by the Fusion Energy Sciences Advisory Committee (FESAC). The theory and computation program is the only major element remaining to be evaluated. Recent changes in the OFES review processes for the theory and computing program make this an opportune time to review the theory and computing program.

The Fusion Energy Advisory Committee report *A Restructured Fusion Energy Sciences Program* noted that "theory and modeling, in conjunction with experiment, provide the capability at the core of the scientific research endeavor." The recent draft *Assessment of the Department of Energy's Office of Fusion Energy Sciences Program* prepared by a National Academy of Sciences committee recommended that increasing scientific understanding of fusion relevant plasmas should become a central goal of the fusion program. It also recommended that the program should be open to evolution in terms of content and structure as it continues to strengthen its portfolio of research. Because the National Academy of Sciences committee has already provided a detailed review of the scientific quality of the fusion program, FESAC should focus its effort on reviewing the theory and computation program's overall content, plans, structure, and governance.

In reviewing the theory and computing program, I request that the review address at least the following questions:

1. What is the appropriate role of theory and computation in the OFES program? Is the current balance between theory/computing and the rest of the fusion program reasonable?
2. Is the current structure and balance between the elements of the theory/computing program appropriate? What changes, if any, are needed in program content?
3. Several groups and numerous individual investigators at many institutions carry out theory/computing research. Is the distribution of research among these research performers appropriate? Are there structural changes that would make the program stronger?

4. In many areas of physics “modeling/simulation” studies are now viewed as a third discipline, distinct from both experimental and theoretical studies. How effectively are the modeling/simulation and theory communities working together to support the needs of the rest of the fusion program?
5. How should the modeling/simulation efforts be conducted to increase their contribution to the overall program, considering issues such as code proliferation, legacy codes that are expensive to maintain and difficult to upgrade, introduction of modern computational techniques, and formation and functioning of multi-institutional modeling/simulation teams?

In reviewing program governance, FESAC should consider the following topics: planning and goal setting processes, merit review procedures, and coordination of international collaboration. Specific questions FESAC may wish to consider include:

1. Are the current management practices of the program, such as program planning and merit review, sound?
2. Is the role of various organizations in managing certain elements of the program reasonable (e.g., IFS coordination of the Joint Institute for Fusion Theory {with Japan} or PPPL coordination of the Plasma Science Advanced Computing Initiative)?
3. What management changes would strengthen the program?

Please carry out this review using experts outside of FESAC membership as necessary. Complete this evaluation and provide recommendations for the theory and computing program by May 1, 2001, as this advice will be important for supporting the FY 2002 budget.

I appreciate the time and energy that members of FESAC and FESAC panels have provided to these continuing efforts to evaluate and to improve the OFES program. I am confident that the Committee's findings and recommendations on the theory and computation program will also benefit the OFES program.

Sincerely,

Mildred S. Dresselhaus  
Director  
Office of Science

## Appendix B. IPPA Program Goals and Objectives

**Table B.1 The Program Goals and Objectives.**

Goals	5-Year Objectives	10-Year Objectives	15-Year Objectives
<p><b>Goal 1.</b> Advance understanding of plasma, the fourth state of matter, and enhance predictive capabilities, through comparison of well-diagnosed experiments, theory and simulation</p>	<p><b>1.1 Turbulence and Transport</b> Advance scientific understanding of turbulent transport forming the basis for a reliable predictive capability in externally controlled systems.</p> <p><b>1.2 Macroscopic Stability</b> Develop detailed predictive capability for macroscopic stability, including resistive and kinetic effects.</p> <p><b>Develop qualitative predictive capability</b> for transport and stability in self-organized systems.</p> <p><b>1.3 Wave Particle Interactions</b> Develop predictive capability for plasma heating, flow, and current drive, as well as energetic particle driven instabilities, in a variety of magnetic confinement configurations and especially for reactor-relevant regimes.</p> <p><b>1.4 Multiphase Interfaces</b> Advance the capability to predict detailed multi-phase plasma-wall interfaces at very high power-and particle-fluxes.</p> <p><b>1.5 General Science</b> Advance the forefront of non-fusion plasma science and plasma technology across a broad frontier, synergistically with the development of fusion science in MFE and IFE.</p>	<p><b>Develop fully integrated capability</b> for predicting the performance of externally-controlled systems including turbulent transport, macroscopic stability, wave particle physics and multi-phase interfaces.</p> <p><b>Advance the forefront of non-fusion plasma science and technology</b> across a broad frontier, synergistically with the development of fusion science.</p>	<p><b>Develop a fully validated comprehensive simulation capability</b> applicable to the broad range of magnetic confinement configurations.</p> <p><b>Advance the forefront of non-fusion plasma science and technology</b> across a broad frontier, synergistically with the development of fusion science.</p>



Goals	5-Year Objectives	Medium Term to 20 Years
<p><b>Goal 5:</b> Advance the fundamental understanding and predictability of high energy density (HED) plasmas for IFE, leveraging from the ICF target physics work sponsored by the National Nuclear Security Agency's Office of Defense Programs.</p>	<p><b>5.1 Beam Target Interaction and Coupling</b> Advance the understanding of driver interaction and coupling in IFE targets to a level sufficient to determine tradeoffs among driver beam focusing, absorption, x-ray production, beam-plasma instability, and target preheat.</p> <p><b>5.2 Energy Transport and Symmetry</b> Advance the understanding of energy transport to a level sufficient to determine the tradeoffs between the number of beams and chamber geometry, beam spatial profile, beam pointing accuracy and beam power balance, as well as hohlraum geometry for indirect drive.</p> <p><b>5.3 Implosion Dynamics and Equations of State (EOS) of Materials</b> Advance the understanding of implosion dynamics and EOS of fusion materials to a level sufficient to determine the pulse shape and timing requirements for IFE targets.</p> <p><b>5.4 Hydrodynamic Instability and Mix</b> Advance the understanding of hydrodynamic instability and mix sufficient to determine the tradeoffs between techniques to optimize ablation stabilization as well as other approaches to reducing instability growth, and the driver requirements on intensity, spatial uniformity and pulse shaping.</p> <p><b>5.5 Ignition and Burn Propagation</b> Advance the integrated understanding of coupling, symmetry, pulse shaping, and instability sufficient to specify the optimal assembly of fuel for ignition and burn propagation subject to tradeoffs in driver, chamber and target fabrication specifications.</p>	<p>Develop optimized target designs based on information from the IRE and NIF and other inertial fusion programs.</p>

Table B.2.. Matrix of Activities vs. Goals, for the Theory and Computation areas, from the IPPA report..

(P refers to a primary relationship and S refers to a Secondary Relationship)

	G-1	G-2	G-3	G-4	G-5	G-6
1.1. Magnetic Confinement Theory	P	P	P	S		
1.2. Inertial Fusion Theory					P	S
1.3. Plasma Simulation	P	P	P	S	P	S
1.4. Basic Plasma Theory	P	P	S		P	
Facilities, Technologies, Materials, Etc. 1.5. through 4.0.						

Report of the Integrated Planning Activity for the DOE Fusion Energy Sciences Program, DOE/SC-0028, December 2000.

## **Appendix C Panel Meetings**

### **UCLA Meeting January 31/February 1, 2001.**

#### January 31.

09.00 am Panel only.

10.00 am Input to Panel. S.Eckstrand (DOE-OFES), R.Taylor (UCLA), J.Cary (U.Colorado),  
D.Schnack (SAIC) , V.Chan (GAT).

12.30 pm Lunch.

01.30 pm Input to Panel. A.Glasser (LANL), R.Cohen (LLNL), A.Friedman (LLNL),  
J-N LeBoeuf (UCLA),

03.30 pm Break.

03.45 pm. Input to Panel. M.Tabak (LLNL), J. Van Dam (U.Texas), vugraphs R. Aamodt  
(Lodestar).

06.00 pm Adjourn.

J. Dawson (UCLA) also attended on January 31.

#### February 1 - Panel only.

08.30 am General discussion

12.00 noon Adjourn.

Written input was received from R. Hazeltine (U.Texas), W. McCurdy (LBNL), P. Peterson (UC Berkeley), W. Stacey (Georgia Tech), F. Waelbroek (U.Texas).

### **PPPL Meeting March 29/30, 2001.**

#### March 29.

9.00 am S. Eckstrand (DOE-OFES). W. McCurdy (LBNL), A. Bhattacharjee (U.Iowa).

10.30 am Break

11.00 am G. Bateman (Lehigh U.), P. Catto (MIT), W. Tang (PPPL).

1.00 pm Lunch (PPPL)

2.00 pm D. Batchelor (ORNL), N. Sauthoff (PPPL), C.Hegna (U. Wisconsin).

3.30 pm Break

4.00 pm A. Boozer (Columbia U.), E. Synakowski (PPPL), T. Antonsen (U. Maryland),  
J.Van Dam (U.Texas).

5.30 pm other

6.00 pm Adjourn

#### March 30 - Panel only

8.30 am to 4.00 pm.

Written information was also received from A. Boozer (Columbia U.) and J. Coronos (Krell Institute).