

Discussion of the Final Version of the FESAC Panel Review of Theory and Computing

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Panel Chair

Oak Ridge National Laboratory and
the JIEE at the University of Tennessee.

At the Princeton Plasma Physics Laboratory

August 1, 2001.

Incorporation of comments from the last FESAC meeting

- Useful comments, both oral and written were made by FESAC members,
Dave Baldwin, Steve Dean, Rob Goldston, Adil Hassam, Stan Milora, and Miklos Porkolab
- We particularly appreciate the written suggestions for improving the report and have incorporated much of what was proposed.
- The report was adjusted a number of times.
- I thank the Panel members, FESAC members, and other people who gave input for all of their contributions.

Report of the FESAC Panel Reviewing the Theory and Computing Program

July 11, 2001.

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Executive Summary

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, good.

- 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 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 peer review not necessarily based on the NSF model) 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.