U.S. Department of Energy

Scientific Discovery through Advanced Computing: Advanced Computational Research in Fusion Science
Summary Report

Proposal Number: 82177
Center for Extended Magnetohydrodynamic Modeling

Organization Name: PPPL
Principal Investigator: Jardin, Stephen

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1. Scientific and/or technical merit of the project (01-10).

When answering this question consider the following elements:

a) The importance of the proposed project to the mission of the Office of Fusion Energy Sciences.

b) The potential of the proposed project to advance the state-of-the-art in computational modeling and simulation of plasma behavior.

c) The need for extraordinary computing resources to address problems of critical scientific importance to the fusion program and the demonstrated abilities of the applicatns to use terascale computers.

d) The likelihood that the models, algorithms, and methods, that result from this effort will have impact on science disciplines outside of the fusion research.

Reviewer 1 Comments:

This is a post festum report which has been influenced by the panel discussions but not by the written previous referee reports. I did not have the time to do justice to the extensive material provided by the PI but I have just looked at one aspect: Is there a clear scientific motivation for this proposal ? Are the problems to be attacked and the milestones leading to their solution clearly defined ? --- One declared goal is the simultaneous development of NIMROD and M3D; this is certainly part of OFES' mission. The potential for real innovation in computational modeling and plasma simulation seems however to be quite limited. The project has a need for tera-scale computers. The impact on science disciplines outside fusion might be quite limited because the project is aimed at very down-to-earth fusion problems (in the good and the bad sense).

Reviewer 2 Comments:

This is a very comprehensive proposal to improve and to utilize two mature MHD instability codes ---- the NIMROD and the M3D codes. The physics models in these codes will be extended to include a variety of dissipative and kinetic effects. In addition, the numerical techniques used in these codes will be improved and they will be interfaced to MDSplus databases. It is clear that the objective of this proposal is to obtain sophisticated physics results quickly, to compare those results with experimental data, and to address the most important unresolved issues in the field of large scale instabilities

of magnetized plasmas. This project will probably make a significant advance to the state-of-the-art in computational modeling in a practical way. The need for high performance computing was demonstrated clearly. This project will focus primarily on magnetic fusion energy problems. However, the comprehensive methods devised for solving these problems could then subsequently be applied to astrophysical applications.

Reviewer 3 Comments:
The main purpose of this proposal is to upgrade the two MHD codes M3D and NIMROD by (a) extending the physics models and (b) improving the efficiency of the two codes by new algorithms and techniques from computer science. Both (a) and (b) are essential for making progress in the modeling of macroscopic processes in plasmas. M3D is a leading code in this area since a long time, and NIMROD, that was built with more general aims, is beginning to show interesting results. Nonlinear computation of large-scale phenomena in fusion devices is very demanding in terms of computer resources. It appears likely that results from this project, in particular concerning model extensions, can have important applications in space and astrophysics

Reviewer 4 Comments:
The proposed Center aims at improved realistic modeling of macroscopic plasma stability of future fusion machines by exploiting and improving two existing XMHD codes (NIMROD and M3D). The effort builds upon existing codes and expertise. In that respect the approach is conservative, but probably the best since one must expect a lot of surprises (both pleasant and unpleasant ones) if one really starts to confront two-fluid modeling with experimental reality. The proposed extensions of present models with two-fluid and particle streaming effects are relevant, but they will also necessitate much more serious consideration of the inherent difficulties with the huge time and space scale spans that need to be taken into account. Just computing in the teraflop range will not suffice. A more extensive effort in implicit time stepping will be necessary. However, given the fusion mission, this problem is best approached starting from working codes that are gradually converted while continually confronted with experimental data, than with new tools that need much longer time to mature. From a purely scientific point of view the latter (more fundamental) approach to the computation of macroscopic plasma dynamics would be more appealing, but the constraint of fusion relevance dictates the approach taken in this project. I expect it to be the most certain road to advances in this field, even though it probably will exhibit severe shortcomings of our understanding of plasma processes on the longer time scales.

Reviewer 5 Comments:
This is a very comprehensive and impressive proposal. The main thrust is the development of two already existing and well tested codes, NIMROD and M3D, to include extended MHD. It is impressive in terms of personnel and number of institutions involved. This may pose complex management issues, although the scientists involved are certainly very reliable and capable of delivering the goods. The main drawback of this proposal is that it is not very focussed in terms of physics goals, and in that sense not particularly exciting. It is also perhaps a bit ambitious. This referee finds that addressing several, not fully understood applications in a single code may not be the best way to

proceed from a scientific standpoint.Visibility outside fusion is doubtful, given the specialization of codes to specific megnetic confinement geometrical configurations. On the other hand, advances in computation may later become useful to neighboring fields of research.

2. Appropriateness of the proposed method or approach (01-10).

When answering this question consider the following elements related to quality of planning:

a) Quality of the plan for effective collaboration among members of the center.

b) Quality of plan for ensuring communication with other advanced computation efforts.

c) Viability of plan for verifying and validating the models developed, including close coupling with experiments for ultimate validation.

d) Quality and clarity of proposed work schedule and deliverables.

Reviewer 1 Comments:

I have not been looking into the collaboration between the centers and cannot, therefore, judge its quality. I have, on the other hand, a good impression of how the PI seeks the collaboration with the computational linear algebra community (PETSc). The simultaneous development of NIMROD and M3D will allow a serious mutual validation of the codes. The collaboration and comparison with the experiment seems to be well assured. As a simple-to-formulate motivation other than extending the existing models I have only found the fact that NIMROD did not reproduce the experimental facts (page 8). Follows a list of essential ingredients of a "successful code", a kind of a check list without priorities. Unfortunately, when discussing the deliverables (page 28) they are not checked against this list. So, at the end, it is not clear what is essential for the codes and should therefore be included in this proposal and what not. Very difficult to judge ! It would be helpful if the proposal would clearly say what exactly is done, why, where and when. There should be more checkpoints and less words.

Reviewer 2 Comments:

This comprehensive plan involves two major computer codes --- NIMROD and M3D. The proposal indicates that these two codes will share modules, expertise, and access to a common database, but they will not merge into a single code. The two codes will be used to verify on each other. The extra effort needed to maintain two separate codes is a weakness of this proposal. Except for the maintenance of two separate codes, the quality of the plan looks excellent. They have established close ties with experimentalists. They have chosen the same MDSplus database that experimentalists use and they plan to develop visualization techniques that will facilitate comparison of their fully 3-D simulation results with the experimental data. They clearly plan to deliver useful results. They did not provide a detailed plan for quantitative comparisons between their simulations and experimental data.

Reviewer 3 Comments:

The chosen approach of continuing the development of two existing and (at least partly) benchmarked codes seems well advised; it improves the possibilities of benchmarking, it

broadens the range of problems that can be addressed, and it minimizes the risk of failure. The proposal includes expertise in different sub-fields, such as plasma theory, simulation, and to some extent numerical analysis, computational techniques and computer science.

The plan for collaboration is rather complex, as there are nine institutions involved and four technical leads, or PIs (for NIMROD, M3D, theory and data management). This is a potential weakness and will require very good coordination in order to keep the whole team productive and focussed. An effort that is more directly focussed towards work on M3D and NIMROD might be more cost-effective. The collaboration involving two codes improves the possibilities for validation. In addition, the team has access to other codes with which, in particular, linear results can be benchmarked. (To this reviewer, a somewhat surprising aspect of the proposal is the absence of certain researchers well versed in linear MHD computation.) As the applicants have good contacts with the major experimental facilities in the US fusion program, they have excellent possibilities of comparing computed results with experimental ones.

Reviewer 4 Comments:
The approach advocated in this proposal is appropriate, with the fusion mission as a determining factor. Gradual improvement of grid refinement, time stepping, and algorithms is a secure way of progressing. The different parts of the project appear to be in very competent hands. I have one worry though with respect to the philosophy of scaling of parameters of fusion machines from reduced parameters which is explicitly mentioned at the end of Sec. 2.3.3. Some of the less impressive features of fusion science is the endless curve fitting of transport data without progress of fundamental knowledge about the processes determining it. At this point I think the advent of the new computational tools should be used as an opportunity to finally reduce this part of the fusion effort so that the field may become attractive again for the general physicist.

Reviewer 5 Comments:
The quality of plan for ensuring effective collaboration among members of the center is not very convincing. There are provisions to meet between two and four times a year, which may be insufficient given the breadth of the proposed research program. Quality and clarity of proposed work schedule and deliverables is also not very high.

3. Competency of applicant's personnel and adequacy of proposed resources.

Reviewer 1 Comments:
This is a very impressive group of world-wide known, first-class researchers who have all the potential needed to attack problems of the kind described here.

Reviewer 2 Comments:
A rather large team of excellent physicists from 10 institutions plus additional supporting consultants have been assembled for this proposal. The team includes excellent theoreticians, who will develop improved closures for the multi-fluid equations that this group plans to use in the simulations, as well as computational physicists and a database expert. The team also includes excellent computational physicists and some numerical

analysts, who will implement state-of-the-art computational techniques in these codes.

Reviewer 3 Comments:
Generally, the competence of the listed personnel is excellent. Most of the co-PIs are very well established both nationally and internationally. However, the funding is mainly requested for unspecified new hires (post-docs and graduate students), and the proposal is not very clear concerning the involvement of the co-PIs. The proposal is very strong on theory support. Concerning solvers and grid generation, some expert support has been secured by agreements of collaboration with the TOPS and TSTT centers, but further strengthening in this area would be beneficial.

Reviewer 4 Comments:
The applicants are all quite competent in their respective fields. The PI has extensive experience coordinating an effort like the one proposed. One good aspect of this proposal is that it mainly funds new post docs, so that the tools developed will be in the hands of a future generation of plasma physicists. Since one must expect that the new era of computing has just begun with tera computing and that a long way still has to be gone before realistic simulations of 3D nonlinear plasma dynamics are feasible, one could not invest better than in the youngest generation.

Reviewer 5 Comments:
The competency of applicant's personnel is very high.

4. Reasonableness and appropriateness of the proposed budget.

Reviewer 1 Comments:
I have not been looking into these issues

Reviewer 2 Comments:
The budget appears to be too small for so many people and such a comprehensive plan. The paucity of funds is aggravated by the fact that this team will maintain two separate computer codes, rather than merging them together or concentrating on one or the other. The money will be spread very thin.

Reviewer 3 Comments:
Although I do not wish to imply that the budget is ill justified, some reduction may be necessary in view of the funding available for several proposals. The number of unspecified new hires could be reduced in favor of increased participation of the co-PIs. If such reductions are made, it would be a good strategy to make sure that the effort on further development of M3D and NIMROD is not threatened.

Reviewer 4 Comments:
The proposed budget is entirely justified by the size of the effort. (It is easier to think of meaningful extensions than of reductions of the program).

Reviewer 5 Comments:

Resources are spread a bit too thinly among nine institutions. As pointed out above, this is a very ambitious project, which would probably require more resources to be carried out in a more effective manner, so to guarantee more effective collaboration among the participating teams.

5. Summary rating.

Please use the following quide when choosing criteria ratings.

1-2 Poor
3-4 Fair
5-6 Good
7-8 Very Good
9-10 Excellent

Reviewer 1 Comments:
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Reviewer 2 Comments:
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Reviewer 3 Comments:
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Reviewer 4 Comments:
9

Reviewer 5 Comments:
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