Report of the Fusion Simulation Program Advisory Committee (FSPAC) Review of Fusion Simulation Program on March 30-April 1, 2011

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May 8, 2011

Charge to the Panel From Stewart Prager, PPPL Director

(1) FSP Science Goals -- Regarding the proposed Integrated Science Applications (ISA's) and associated science development road-maps, please comment and advise on:

(a) the vision for the code capabilities that can be expected in nearer-term (within 5 years) and longer term time frames;

(b) an outline of the key prioritized issues faced in carrying out such an ISA program – highlighting roadmaps for advanced components and software integration/engineering;

(c) the plan for cross-disciplinary integration of ASCR computer science and applied math elements into the FSP Plan; and

(d) the plans/roadmaps for V&V & UQ and collaborative development environments.

(2) FSP Management & Governance – In line with the DoE RFP guidance, please comment and advise on:

(a) the organizational structure; and

(b) the approach for dealing with the distributed project nature of the FSP.

(3) DRAFT FSP Plan – In line with the DoE RFP guidance, please comment and advise on the current content of the DRAFT FSP Plan, including the targeted user community and potential impact of the FSP.

Executive Summary

Based on the demonstrated progress, the Fusion Simulation Program (FSP) planning team has made toward developing a plan for the FSP, the Fusion Simulation Program Advisory Committee (FSPAC) strongly endorses both the concept and the potential of the Fusion Simulation Program. The FSPAC judges that:

1) the FSP will enable significant advances in fusion science,
2) the FSP will substantially increase the value of ITER to the US,
3) the FSP will make major contributions to build the knowledge base required for DEMO,
4) the FSP provides one of the few opportunities available for the US to provide recognized leadership in the international fusion science community, and
5) a Fusion Simulation Program of the type proposed by the FSP team provides the most credible path forward for the integrated whole device model that will be highly important for the realization of fusion energy.

The FSP planning team has made substantial progress since the last review held on September 23 and 24, 2010. The concept for Integrated Science Applications (ISA) has been refined and prioritized. In particular, two ISA's, whole device and plasma-edge models, have

been identified for an initial focus. There has been substantial progress in defining multi-disciplinary roles within the program. The FSP planning team has achieved a good level of consensus on FSP goals and vision within the fusion community─a significant accomplishment. The FSP planning team has enhanced the working relationship with the applied math community, a relationship that will be highly important for developing the necessary degree of scalability to exploit the next generation of computing platforms and achieve the scientific results that are the goal of the program. The team has fleshed out an initial validation plan with the experimental community for the two ISA's. It has identified the major Verification, Validation and Uncertainty Quantification (V & V and UQ) issues for the ISA's and outlined approaches for addressing them. The team has identified the major collaboration issues and begun development of a plan to address them. It has developed an outline for the first 5 and 10 years of the program and started to tackle the difficult issue of defining tasks, resource levels, and schedules. Finally, the team has developed a preliminary draft plan that documents the activities and conclusions of the FSP planning team. It provides a good starting point for the final plan to be submitted to the Department of Energy (DOE) in mid-summer.

Responses to the Specific Charges

The FSPAC based its responses on the presentations to the FSPAC during the March 30-April 1, 2001, review (agenda attachment 1), the draft plan provided to the FSPAC before the review, additional documents provided to the FSPAC through the FSP website, participation by some FSPAC members in FSP planning workshops, and the prior FSPAC meetings (September 17-18, 2009; March 25-26, 2010, and September 23-24, 2010, http://www.pppl.gov/fsp/FSP_PAC_MTGS.html).

(1) FSP Science Goals -- Regarding the proposed Integrated Science Applications (ISA's) and associated science development road-maps, please comment and advise on:

1(a) the vision for the code capabilities that can be expected in nearer-term (within 5 years) and longer term time frames;

The FSP team has made significant progress in defining the software vision for the first few years of the FSP. They have met extensively with the plasma simulation community to determine what code capabilities are required for the initial ISA's. A top level resource analysis has made it clear that all the planned ISA's cannot be developed simultaneously given the 25M dollar per year funding envelope envisioned for the FSP. As a result the team has down-selected to two ISA's. These two, a model for the whole plasma (Whole Device Modeling, WDM) and a model that provides an integrated treatment of the boundary and the pedestal region, are very central to future ITER performance. The PAC endorses this choice. Later on, other ISA's may be initiated.

For Whole Device Modeling, the team gives priority (correctly in our view) to developing simulation capability that can be used to optimize future discharge experiments. For example, if it were possible to predict stability boundaries and then develop simplified models of the discharge process, it would then be possible to develop control strategies which would optimize performance. The approach is to develop a modular simulation capability that can employ a hierarchy of physics models from validated, reduced models to high fidelity models

that require large high performance computing resources. This suite of models provides the ability to address issues that require a high level of detail while more quotidian resources could be deployed for scoping studies prior to an experiment. A good whole device modeling capability is missing from the international fusion program and the FSP is a very credible way to provide that capability.

The development strategy for WDM is to adapt existing components into an FSP framework, develop a 2.5 dimensional WDM capability coupled with a transport solver that initially uses a fast transport model, and then to evolve these components to more accurately deal with more complex issues like RF heating and turbulence. Eventually this work would presumably couple to the results of the first ISA on wall/plasma interactions.

As presented by Martin Greenwald, there are several scientific issues that must be resolved to develop a predictive model of the pedestal/boundary region. These include prediction of the heat and particle loads on the boundary both in steady state and during an ELM event, the edge turbulence and its reduction by an edge transport barrier, tritium absorption by internal components, atomic and molecular and surface interactions at the wall and the generation of impurities. As correctly indicated, this is, in all respects, a three-dimensional multi-physics, kinetic, multi-scale problem which must be addressed if we are to understand ITER performance.

The strategy calls for developing the needed capability incrementally as a sequence of simulation levels, similar to the hierarchial modular approach planned for the Whole Device Model. Level 1 is the use of linear modeling of the pedestal with later addition of quasi-linear gyrokinetic models. Level 2 will calculate the dynamic evolution of the boundary and pedestal by coupling 3D fluid or reduced kinetic simulations to 2D transport codes. Finally, Level 3 targets full multi-scale kinetic simulations. A set of tasks has been laid out that establish a high level path to a full simulation capability. For each task, supporting work has also been identified with specific requirements for integration as well as solver development. This was achieved through a process of outreach to the community to identify the needed physics as well as to develop initial resource estimates (FTE's etc.) required to perform the tasks.

While the high level planning is of great value, it is less clear to the FSPAC what actual code capabilities will be delivered in the initial years for either ISA. This is to some extent understandable because it has not yet been made clear to the FSP team whether they will in fact be the executors of the FSP. Thus it is difficult to develop truly concrete plans. Nevertheless, it would be useful to complete this exercise by the end of the FSP definition phase. The PAC recommends that the team develop a more complete short-term code vision covering perhaps the first two years of the FSP program. In particular, it would be compelling in the program plan to specify how FSP "Release 1.0" will actually be implemented. In this regard the following questions should be answered:

1. What codes or code capabilities will be delivered in the initial phases?
2. What development work is required to bring each of these codes to a level at which they will have integrated treatments of the relevant physics effects. ?
3. What type of integration or integration framework is envisioned?
4. What capabilities will FSP Release 1.0 provide that are beyond what can be done with existing codes (showing that the integrated whole is more capable than the sum of its parts)?
5. Perhaps just as important – what capabilities won't be provided in Release 1.0?

It is understandable that not all aspects of the development can be decided at this point. In such cases it would be useful to outline the choices among components and the criteria that will be used to choose which capability is ultimately employed.

As an example of the above, X. Tang's presentation proposed work was described on components such as:

1. Free boundary Grad-Shafranov equilibrium code,
2. Local turbulence-based transport models,
3. Pedestal and SOL equilibrium model, etc.

While it is clearly essential to identify these components, it is difficult to see in the program plan or in the final reports which codes are being described and what further efforts will be needed to integrate them into an initial cut of the FSP.

The team must also determine (with DOE OFES guidance) the ultimate objective of this planning phase. Was the goal to define FSP capabilities and then to identify the components that would make up an early version of the FSP software as constructed by this team or was the goal to lay down a set of requirements that other groups (including the present team) might propose to fulfill by building software? In either case the development of a concrete target for "Release 1.0" of the FSP would be an important step.

Charge 1 (b): an outline of the key prioritized issues faced in carrying out such an ISA program –highlighting roadmaps for advanced components and software integration/engineering.

The PAC supports the FSP's overall intentions to organize the plan around the two initial ISAs. At the time of the FSPAC meeting more work was needed to flesh out the plan with the right balance of succinctness and detail. The information that constitutes the plan is too scattered, making it difficult to find the relevant information for most issues. Rather than roadmaps, the information presented was composed primarily of lists. Viewgraph 27 of Xianzhu Tang's presentation is a good starting point but needs to be supported by a description of codes, timelines, FTE levels and skill set requirements. Timelines need to be elucidated especially for the first two years, with critical tasks and deliverables. The critical components of the initial ISAs need to be identified.

The FSP draft plan contains parts that focus on bringing existing or simplified simulation capabilities into a single integrated framework, but it also has parts that will develop new simulation capabilities that do not yet adequately exist. The relative balance between these two parts needs careful consideration. For example, regarding the boundary/pedestal ISA, there is mention in the planning document of developing quasilinear models of transport for the evolution of profiles in the boundary region. While this is the fastest approach and works fairly well in the core region (such as the TGLF transport model), it may be of limited usefulness (unless novel extensions are found) in the edge region where turbulence spreading and sub-critical turbulence are important. What is needed eventually is the development of a new capability to do comprehensive gyrokinetic turbulence simulations of the edge region. While the FSP planning document discusses plans to eventually develop such a capability, one might consider investing even more resources into this part of the project, given the importance of this problem and the major computational initiative that the FSP represents.

In the Whole Device Modeling (WDM) ISA section, consideration should be given to accelerating the capability of including "first-principles turbulent transport tools", which at present is not implemented until years 5-8 (p.76). The TRINITY (GS2 / Barnes) and TGYRO

(GYRO / Candy) codes have already demonstrated the feasibility of multi-scale coupling between short-time gyrokinetic turbulence codes (for the main plasma core region) and a long-time transport code, so there does not seem to be a reason to delay this capability for so long. While one will want to implement a reduced, fast transport model (like TGLF) for most simulations, the capability to turn on full 5-D gyrokinetic turbulence simulations will be an effective way to showcase petascale computing capability at an early stage of the FSP, and will stimulate an active campaign to carry out validation test comparing the FSP code with various tokamak experiments around the world.

1 (c) the plan for cross-disciplinary integration of ASCR computer science and applied math elements into the FSP Plan; and

With respect to cross-disciplinary integration of computer science (CS) and applied math (AM), the FSP Planning team correctly stressed the importance of incorporating a broad range of talents and interests, a characteristic of successful development teams. The team's February 2011 workshop held at General Atomics provided an excellent start. The FSP Planning team was able to recruit leading researchers from the solver, software integration, data management, mathematical/numerical formulation, and uncertainty quantification communities to participate and contribute their expertise. The FSP team presented the needs, fusion simulation practitioners described present approaches, and there were frank discussions of the challenges and the state of research in the relevant CS and AM areas. Discussion leaders from the breakout sessions contributed to a final report on the workshop that summarizes important findings. The report is available at: http://www.pppl.gov/fsp/documents/FSP%20Workshop_Summary_Feb2011.pdf. Involvement of fusion experimentalists and discussion of validation was the other important aspect of the workshop. The information has been further processed to estimate whether needs are adequately met by currently used CS/AM technology and where development is required, whether it is expected to require near-, mid-, or long-term research efforts. The edge/pedestal ISA, the whole-device/disruption ISA, and advanced components have been considered separately.

These organizational and outreach efforts will help the actual FSP activity when it begins. However, the FSPAC noted that there are three levels at which CS/AM involvement is needed, and the plan should consider each. The first is the application of current best practices for solvers, visualization, data analysis, etc. Here, fusion simulation practice is mixed, being adept in some areas and relatively ignorant of others. Critical assistance may not require new CS/AM research in all areas. The second level is fully engaging CS/AM research within the FSP effort. The planning presented to the FSPAC emphasizes this level. The third level is to encapsulate and communicate unsolved computational problems to stimulate new thinking and independent research—engaging the AM/CS community as active partners in fostering new science.

1 (d) The plans for V&V and UQ and collaborative development environment.

Validation refers to the process of establishing the adequacy of a code for modeling a physical process with some stated goal of matching experimental results. Typically this involves understanding how adequate a model is for solving a specific problem. This is colloquially stated as "solving the right equations" as opposed to verification which is "solving the equations right".

Associated with both of these is the study of Uncertainty Quantification (UQ) which attempts to assess uncertainties coming both from epistemic sources (uncertain parameters in models) as opposed to aleatory sources (experimental error, numerical noise, etc.). Over the years it has been appreciated that these are important components of all computational investigations. The FSP team has, in the view of the FSPAC, clearly understood and adopted the requirements for state of the art verification, validation and uncertainty quantification.

The FSP team has provided appropriate emphasis on validation. This effort is an important element of the Fusion Simulation Program aimed at improving the physics and computational models. The key participants that will be engaged in validation (ISA teams, analysts, and experimentalists) were identified and their roles and responsibilities developed with discussions involving the broader community. The plan for validation is well thought out, and the final personnel resources presented in response to the FSPAC questions are reasonable. While it is true that codes that have not been validated will typically not be useful for prediction in regions where no experimental data exist, it is not necessarily the case that validated codes are in fact predictive. True validation of a theory requires ongoing comparisons with experiment and assessment of the regions of validity of various models.

The FSP team has also appropriately identified the importance of systematic treatment of the quantification of uncertainties in developing predictive simulation capability toward advancing fusion energy. A work flow and tools for verification and Uncertainty Quantification has been developed, the participants identified, and their responsibilities delineated. This plan seems appropriate, but with limited budgets, the specified resources may not be available due to the need to address higher priorities. While important, a formal UQ process is not an urgent priority for the FSP in the initial phases as compared to the development of the initial code capabilities. It will, however, be very important in the later phases.

The PAC recommends that, with limited funding, the FSP must develop clear task priorities with the goal of an experimentally validated predictive simulation capability, and provide clear logic and justification for the resources individually allocated to verification, validation, and uncertainty quantification, especially in the early phases of the FSP. In this regard, the FSP team should give some thought to the level of UQ that will be achieved at least initially and should also think about the use of existing methodologies. For example, the DAKOTA tool kit provides many UQ methodologies and further developments have been made by the ASC PSAAP centers. It would be useful to overview these capabilities and develop a plan for their utilization in the early mid and later terms of FSP development. Some of these decisions will have an impact on the nature of the framework design in future years.

Finally, the PAC recommends that the FSP team consider how the early engagement with experiments to generate validation data will proceed; including a more definitive work plan with specific experiments, facility, and planning with the experimental group.

(2) FSP Management & Governance– In line with the DOE RFP guidance, please comment and advise on:
2 (a) the organizational structure; and

At the September 25-26, 2010, FSPAC meeting, a draft organizational chart structure was presented, and the overall structure appeared generally well suited to the fully implemented FSP. This effort was a major step forward for the FSP. In contrast, there was little mention of this organizational structure in the presentations to this PAC or in the written report. Despite

uncertainties in the overall management of the FSP, the underlying organizational structure is still a good starting point. The written report would greatly benefit from a figure/schematic of the program organization and matrix structure, and additional schematics of each of the sub-elements of the organization, including the FTEs required, when they are needed, and their skills and responsibilities for each organization element.

Additionally, it is unclear how the results (successes and failures) of the proto-FSPs have been folded into the overall FSP plan, or if/how this feeds back into the FSP organizational structure and the approaches taken. There was very little discussion of this during the PAC presentations or in the report. We recommend the plan describe clearly the lessons learned from the proto-FSPs, and clearly discuss how these lessons have influenced the organizational structure.

The PAC notes that the FSP cannot be fully funded from day zero and will inevitably have a staged approach to its goals and milestones, funding, staffing, and therefore its organization structure. Given that the revised plan initially involves a reduced set of targets, we recommend the FSP team define a modified reduced-scope organizational structure that is optimized for the initial funding level. Similarly, the trigger-points and processes for growing the FSP organization and modifying its structure toward the full FSP should be described.

Finally, the PAC notes and applauds the down-selection to two highest priority ISAs. In the FSP planning document, the goals of these ISAs should be front and center and appear much earlier in the report, since they define the early deliverables of the FSP.

2(b) the approach for dealing with the distributed project nature of the FSP.

The FSP planning team clearly recognizes that there will be challenges associated with the distributed nature of the Program. The draft plan incorporates at least three approaches to dealing with these:

1) Implementation will involve some level of co-location to facilitate institutional commitments and efficient team-building. The PAC notes that the actual level of co-location is not specified or discussed in any detail in the draft. The FSPAC recommends that the anticipated levels of co-location for different major components should be fleshed out in some detail, and the trade-offs among co-location, making the best use of distributed expertise, and institutional balance, should be explicitly addressed.
2) The plan aims for significant engagement of performers and avoidance of low percentage individual participation. The PAC notes that there is a trade-off between distributing contributions broadly through the community to include a diversity of expertise and viewpoints and the risk of spreading individual efforts too thinly. The FSPAC recommends that the average FTE efforts to be a large fraction of 100% for core members of the code development teams.
3) The plan mentions optimal utilization of modern collaborative tools, including video conferences, teleconferences, and wikis. The PAC notes that these are important elements of the plan. The plan needs to address monitoring of work performance at distributed sites, as well as the mechanisms that will be used to choose teams and team members.

(3) DRAFT FSP Plan– In line with the DoE RFP guidance, please comment and advise on the current content of the DRAFT FSP Plan, including the targeted user community and potential impact of the FSP.

The present draft plan is a history of the planning activity rather than a plan. Given the short time between the September 25-26, 2010 FSPAC review and the need to address the important issues and prioritize the tasks, it is understandable that the plan is not complete at this stage. The draft plan provides a good basis for developing the plan to be submitted to DOE in mid-summer of 2011. The FSP Planning Team needs to produce a plan that describes the FSP purpose and scope of work and lays out the high-level technical tasks, along with the operational strategy and a schedule for accomplishing them. The FSPAC recommends that the FSP plan contain an executive summary followed by a ~25 page implementation plan. All the supporting information and history of the planning process should be put in appendices or a separate report. The executive summary should contain a clear set of statements about the problem (fusion program capability gaps), the FSP vision for filling the gaps, the impact of filling the gaps, and the credibility of the FSP for realizing the vision. It should briefly describe what is going to be done, when the tasks will be done, the required resources, and the decision points. The plan should address these areas in more detail including the codes and how they will be integrated, the expected customers for the codes, the impact that the integrated applications will make, the challenges, the risks, and how the team will meet the challenges and deal with risks. The plan should also describe the necessary skill mix and a schedule for ramping up the initial program funding level to the asymptotic funding level. Typical large software programs start at funding levels of 30 to 40% and build up to 100% over three to four years.

A short ("one pager") succinct, compelling summary of the FSP needs to be developed for describing the FSP to high-level stakeholders.

A number of detailed comments on the draft plan and recommendations for the format of the final plan are given in Appendix 2 of this report.

Final Comments

The President's FY2012 Budget Submission to Congress calls for a "pause" in the FSP. As stated at the beginning of this report the FSPAC strongly endorses the concept and potential of the FSP. The FSPAC judges that the preparation of a compelling vision and plan for the FSP for consideration by DOE is the best approach for restarting the FSP after the pause. The FSP planning team has done an excellent job of engaging the entire US fusion community in developing a concept and vision for the FSP, and in assessing the issues and developing tasks to produce concrete deliverables for the FSP in the short and medium term while identifying key research topics that need to be addressed and resolved for the FSP to achieve its ultimate objectives.

Signed: May 8, 2011

Dr. Douglass Post, Chair, Fusion Simulation Program Advisory Committee

For the members of the Fusion Simulation Program Advisory Committee:
Allen Boozer, Leslie Greengard, Brian Gross, Gregory Hammett, Wayne Houlberg,
Earl Marmar, Daniel Meiron, Jonathan Menard, Michael Norman, Douglass Post, Carl Sovinec,
Tony Taylor, and James Van Dam.

Appendix 1

FSP PROGRAM ADVISORY COMMITTEE MEETING AGENDA
March 30 – April 1, 2011 Room LSB-318, PPPL

WEDNESDAY, March 30, 2011

8:00 AM – 8:45 AM: PAC CLOSED SESSION (I) PAC Chair (D. Post)
8:45 AM – 9:00 AM: Welcome & PAC Charge (S. Prager)
9:00 AM – 10:15 AM: FSP Progress Overview & Management Plans (W. Tang)
10:30 AM – 12:00 PM – Plans for ISA Code Capabilities in Near and Longer Term (M. Greenwald)
12:00 PM -- 2:00 PM WORKING LUNCH -- PAC CLOSED SESSION (II) in DCR (Director's Conference Room)
2:00 PM – 2:45 PM – Prioritized Goals & Roadmap for Advanced Components (X. Tang)
2:45 PM – 3:30 PM – Prioritized Goals & Roadmap for Software Integration/Engineering (J. Cary)
3:45 PM – 4:30 PM – Prioritized Goals & Roadmaps for Experimental Validation (V. Chan)
4:30 PM – 5:00 PM – Prioritized Goals & Roadmaps for Verification & UQ (J. Hittinger)
5:00 PM – 6:00 PM -- PAC CLOSED SESSION – (III)

THURSDAY, March 31, 2011

9:00 AM – 10:00 AM – Plan for Cross-Disciplinary Integration of ASCR Computer Science & Applied Math (A. Siegel)
10:00 AM – 10:30 AM – FSP Targeted User Community & Plan for Support (D. McCune)
10:45 AM – NOON – FSP Plan Outline with Highlights of Content and Vision for Potential FSP Impact (W. Tang & M. Greenwald)
NOON – 2:00 PM – WORKING LUNCH in DCR -- PAC CLOSED SESSION (IV)
2:00 PM – 2:30 PM – CLARIFYING QUESTIONS FROM PAC TO FSP TEAM
2:30 PM – 4:00 PM – PAC CLOSED SESSION (V)
FSP TEAM PREPARES ANSWERS
4:00 PM – 6:00 PM -- RESPONSE OF FSP TEAM TO PAC QUESTIONS & ASSOCIATED DISCUSSIONS

FRIDAY, April 1, 2011

9:00 AM – 1:00 PM – PAC FINAL CLOSED SESSION (VI) in DCR to DRAFT REPORT
1:00 – 2:00 PM -- PAC Outbrief
2:00 PM – PAC Meeting Adjournment

Appendix 2

Detailed comments and recommendations for the final report and on the draft report

To reiterate the points made in the main body of the FSPAC report, the present draft plan is mainly a description of the FSP planning activity rather than a plan. It needs to be reorganized and be made into a plan. The draft plan needs to address software development approaches, release strategies, and software engineering practices. It should include recommendations for activities during the pause that would allow an orderly program initiation when the pause is over. In particular, the best strategy for ensuring that a restart will occur is to deliver a compelling FSP plan to the DOE. In addition, the FSP Planning Team should develop a compelling presentation for DOE and other senior stakeholders and encourage support for other scientific initiatives in the fusion program that will develop some of the capabilities needed by the FSP.

The FSPAC has a number of detailed comments and observations on the draft plan that should be considered as the final plan is completed. The structure of the written report does not do a good job of describing the overall FSP plan. For instance the deliverables are in the back of the report in table 14, and the physics deliverables are vague. The most specific goals of the first two years are described in X. Tang's presentation on slide 27 and need to be in the plan. It would be valuable to look at successful proposals for large scale code development projects (e.g. ASCI U of Chicago Flash Project and other proposals). Andrew Siegel should have access to that proposal. The FSPAC endorses the concept that the initial ISAs should be the organizing principle, i.e. that the initial ISAs should define the requirements and that everything should flow from the initial ISAs. The plan needs pictures/figures. They add credibility and illustrate the points in the text.

Chapter 4 of the draft report is very dense and difficult to read. The organization of the chapter could be improved. The goals of the two highest priority ISAs are not articulated until late in the report, in section 5.4 on "Experimental Validation". The goals of these ISAs should be up-front and be organizing principles for the report, since they encapsulate the work and deliverables of the first few years.

The draft report document is largely silent on the issue of the distributed nature of the project/program. References to it, and proposed ways of dealing with it, are scattered through the report. They appear wholly focused on technologies to overcome distance. Consistent with the comment above, the Draft Plan must address not only distance, but also techniques for unifying teams with members with different organizational approaches and expertise.

In addition, the plan should state that the FSP is aware of and will address the legal issues that arise during software development, including retention of ownership, control of distribution, foreign collaboration, and export. In addition, the plan should address computer security issues, networks, code storage, distribution, information assurance, backup, code support, and the other issues associated with the mechanics involved in developing and deploying large codes to external users.