Support of Thematic Areas

Institute Faculty and Multidisciplinary Research Thrust Areas.
The proposed institute will have an affiliated faculty who is selected based on the use of advanced computing in their research and who have, or have the potential for, external funding of their programs. These research faculty will be primarily linked to five initial research thrust areas or several areas of enabling technology and will be connected with already existing important programs of the University. The five initial research thrust areas are listed below. The thrust areas and enabling technologies will be continually evaluated for promoting expansion of the University’s research portfolio and national visibility. The plans outlined for the Institute need to build in mechanisms for flexibility since the applications of advanced computing to critical research areas will change over the next few years.

- **Climate and Environmental Modeling.** This thrust will support research at the Kellogg Biological Station, the Environmental Science and Policy Program, the Ecology, Environmental Biology and Behavior Program, the Center for Microbial Ecology and the Center for Global Change and Earth Observations, and the Laboratory for Realtime Computing and Multiscale Modeling.
- **Computational Biology: Genomics and Structural Modeling.** This thrust will support faculty associated with the Quantitative Biology Initiative; the Genetic Expression, Development and Disease Initiative; many of the plant molecular biologists; the Biomathematics group; and the Michigan Center for Structural Biology
- **Materials /Nanoscience/Energy.** This thrust will support activities in the Center for Nanostructured Biomimetic Interfaces, the Composite Materials and Structures Center, the Center for Nanomaterials Design and Assembly, the Nanoscale Interdisciplinary Research Team (NIRT) on the Structure of Nanocrystals, and the Fraunhofer USA Center for Coatings and Laser Applications
- **Computational Chemistry/Physics.** Support of this thrust area will augment research of a number of projects including the Institute for Quantum Science, the Atlas project, the D0 experiment, the Collider Detector project, the Coordinated Theoretical Experimental Project on Quantum Chromodynamics;, the computational chemistry many-body theory effort, and the Cluster Science Collaborative
- **Inverse and Multiscaled Modeling.** Supports the work of the National Superconducting Cyclotron Laboratory, the Automotive Research Experimental Station, the Computational Fluid Dynamics Project, and computational electromagnetic and acoustics and the Center for Multiscale Modeling in Hydrology.

The current enabling technology areas needed to support the research thrust areas are: Visualization, Data Modeling, Data Mining, Applications and Middleware, High End Computing, Applied Mathematics and Algorithms, and Education. Not all of these technologies are available presently at the level needed to support the activities of the Institute and development of plans to secure the needed resources will be developed over the first two to three years of the Institute. It should be noted that many of the faculty
involved in enabling technologies are also collaborating with faculty linked to one of the five thrust areas. The initial thrust areas and enabling technologies available in the Institute are depicted in Figure 1.

Resources within the center will be provided primarily to faculty associated with the Institute. The Faculty Steering Committee will identify high priority, externally funded faculty who will have preferential access to the HPCC-CPU cycles. Full membership will be decided by the Faculty Steering Committee with input from the Institute Director. Full membership will require that the faculty member has external funding of a peer reviewed project, primarily from federal agencies. Exceptions will require approval of the Director and the Executive Committee. New faculty and faculty who do not meet the requirements for full membership may apply for adjunct membership to obtain mailings of events and activities of the Institute. Access to the resources of the Institute will be preferentially allocated to faculty with full membership. The Institute will bring together faculty with expertise in their own discipline to work in areas with common methodologies, fostering synergy and interdisciplinary interactions.

Figure 1. **Research Thrusts supported by ICER.** Faculty in the Institute will have access to enabling technologies and resource personnel noted in the middle layer with core facilities and infrastructure defined in the center of the diagram.

Also, research activities in the computational chemistry and physics and in the inverse and multiscaled modeling thrust areas will be greatly advantaged by the development of petascale systems. The proposed Institute will help develop linkages for these faculty to such systems.
Allocation of Resources

Resources available through the Institute and the HPCC will be provided on a competitive basis. There will be continual analysis to consider the addition, continuation, or discontinuation of resources available through the Institute based on faculty needs and impact on research productivity. Developing policies and procedures for the allocation of resources within the Institute will be carried out by the Faculty Steering Committee and the Director with input from the Executive Committee and the HPCC Advisory Committee. The Executive Committee is comprised of the Deans of the Colleges of Social Science, Natural Science and Engineering, the Director of the NSCL, the Vice Provost for Libraries, Computing and Technology, the Institute Director, and a representative from the Office of the Vice President for Research and Graduate Studies. The Faculty Steering Committee will be comprised of faculty of the institute, at least one from each of the five thrust areas and four at large.

- **Time allocation on HPCC.** The suggested policy for access to HPCC CPU cycles will be to provide 50% of cycles to high priority, externally funded researchers, 15% to work in support of proposal preparation, 15% to open testing and new users (new faculty), and 20% to the Director’s discretion. This policy will be reviewed annually by the Faculty Steering Committee with input from the HPCC users advisory group. Changes will be initiated by the Director in consultation with the Faculty Steering Committee. Budget for hardware and maintenance - $800K. Budget for HPCC personnel - $350K.

- **Resource personnel in the Institute.** Policies for access to the personnel resources will be developed by the Faculty Steering Committee together with the Director and with input from the Executive Committee. This process will give preferential access to the “high performance” faculty of the Institute. Personnel within the HPCC will be specifically responsible for support and use of that infrastructure, while personnel in the Institute support general programmatic activities of the Institute. Budget for Institute personnel - $320K.

- **Faculty Scholars Program.** An application process and policies will be developed by a subcommittee of the Faculty Steering Committee and will be approved, first by the full committee, and then the Director, with input from the Executive Advisory Committee. A subcommittee of the Faculty of the Institute will serve as the review committee to recommend to the Director which applications will be approved for funding. Faculty Scholars are appointed and funded for one year. Budget for Faculty Scholars - $150K.

- **Postdoctoral/Visiting Scholars Program.** The process for developing policies and procedures for the Postdoctoral/Visiting Scholars Program for selecting the funded applications and level of support will be similar to that for selecting Faculty Scholars. It should be noted that a category of Adjunct Postdoctoral Associates of the Institute will be considered. These Postdoctoral Associates would not be funded by the Institute but would serve as resources for the faculty of the Institute and may have some priority access to the Institute’s resources. A process for selecting Adjunct Postdoctoral Associates would then be developed. Budget for program - $180K.

- **Graduate Student Fellowships.** The policies and processes for selecting Graduate student Fellows of the Institute will be similar to that for the Faculty Scholars and Institute Postdoctoral Associates. Preference will be given to those students in programs that are the main thrusts of the institute or associated with the enabling technologies. Budget for Fellowships - $120K.

- **Graduate curriculum.** Developing new courses requires resources, in particular, faculty time. New courses associated with the Institute would be offered by departments and often joint across several departments. This approach provides the faculty teaching new courses with credit in their own department. The development of a specialization or even a joint Ph.D. program would be developed similar to that of the QBl and EEBB – as a joint Ph.D. While developed and offered by departments, proposed courses that use resources of the Institute
should have the endorsement of the Faculty Steering Committee and the Director. The Institute will have the responsibility of connecting with the Virtual School of the Great Lakes Petascale Computational Center and coordinating course offerings from that school to MSU students.

- **Seminar series** will be developed in collaboration with a number of other programs such as “Science at the Edge”, the Quantitative Biology Initiative, and departments to minimize costs. These seminars will be posted on the Institute’s web site. Budget for seminar series - $10K.

- **Workshops and retreats.** The Institute will offer workshops on specific topics on advanced computing for the MSU research community. The Institute will schedule an annual retreat for the Institute Faculty to review the activities of the Institute. The retreats will include presentations of research by the faculty and students in the Institute. Budget - $20K.

- **Web Site.** The Institutes website will provide information about the center and its resources, activities and programs. Funds will also be needed to support the Institute Office. Budget for SS&E and Web site - $50K.

The resources of the Institute are presented in layers in Figure 2, below, with the core resources having the highest priorities. These layers will be built over the next several years as funding for the Institute becomes available. It is anticipated that by the third year the $2M will be needed to support all of these layers, but that investment is expected to provide a 2 – 4 fold return in external grants (depending on thrust areas) for projects that would not otherwise have been funded. The establishment of this institute is critical for MSU faculty to be successful in the competition for many funding opportunities, such as the NSF CDI funding, and for participation in the GLPCC.

The Director and Faculty Steering Committee will consider opportunities for generating resources and revenue streams including hardware buy-in policies and fees for service.

**Figure 2. Resource layers of the Institute.** The core resources of the Institute are at the center and the additional resources needed are indicated in the outer layers, presented in priority order.
Evaluation of the Institute and Revision of Programmatic Activities and Research Thrust Areas

It will be essential to develop metrics that evaluate programs and resources that are productive and implement processes to modify, expand or discontinue programs and resources that do not meet expectations, as noted below.

- An Annual report will be prepared by the Institute with input from the HPCC personnel. Faculty identified as members of the Institute must submit information regarding ICER associated publications, grants, and national meeting presentations. ICER faculty will list the postdoctoral associates, graduate students and undergraduates working on CER related research. Awards to students, postdoctoral associates, visiting scholars and faculty associated with the CER Institute will also be submitted each year. Submission of an annual report to the Director will be a requirement for retaining membership in the Institute. Metrics that will be monitored annually for each thrust area include: total grant funds awarded, number of peer reviewed publications, number of invited talks at national and international meetings, number of major awards.

- The Director, with assistance from the Assistant Director, will assemble the productivity reports of the faculty, outline the activities of the Institute to include the seminar series, any workshops offered, and outline future plans for the Institute. The Director, in consultation with the Faculty Steering Committee, will be expected to evaluate the impact of each of the programmatic activities of the Institute and justify continued funding. The Director will evaluate the external funding of each of the thrust areas. It is expected that if the external funding is not increasing in a thrust area at a rate that would project a 2-4 fold increase (depending on thrust area) in five years from the initial base year (2008-09), that area will be under consideration for discontinuation. Similarly, the enabling technologies will be scrutinized to determine their impact. The Annual Report will be reviewed by the Faculty Steering Committee.

- The Annual report will be submitted to the Executive Committee for input and then to the Provost and the Vice President for Research and Graduate Studies.

- The Institute’s funding each year is dependent on acceptance of the report and recommendations from the Director and Faculty Steering Committee.

- The Faculty Steering Committee will annually review the reports of the faculty and consider discontinuation of full membership.

- The Director, in consultation with the Faculty Advisory Committee and the External Advisory Committee, will annually review the progress made in each of the initial thrust areas. This group will also review recommendations for adding thrust areas to respond to unforeseen opportunities or discontinuing thrust areas that are not performing to minimum expectations.

As shown in the table below, faculty linked to the research thrusts and enabling technologies of the proposed Institute are some of the most productive, as indicated by their grant funding, and have a high potential for growth in the use of advanced computing technologies. Institute resources will be critical in advancing the research programs of these faculty. Note that this table may not include all faculty linked to these thrusts and the analysis used an initial estimate of the faculty’s primary research area.
Table 1. Research productivity of faculty linked to research thrusts and their potential for growth in use of advanced computing.*

<table>
<thead>
<tr>
<th>Thrust Areas</th>
<th>Total Grants (over last 3 yrs)</th>
<th># Grants Submitted</th>
<th># Grants Awarded</th>
<th>Faculty #</th>
<th>Grant $/faculty</th>
<th>% Faculty with High potential for growth in Advanced Computing</th>
</tr>
</thead>
<tbody>
<tr>
<td>Computational Biology</td>
<td>$36,437,381</td>
<td>262</td>
<td>105</td>
<td>15</td>
<td>$2,429,159</td>
<td>73%</td>
</tr>
<tr>
<td>Climate and Environmental Modeling</td>
<td>$14,007,723</td>
<td>109</td>
<td>52</td>
<td>10</td>
<td>$1,400,772</td>
<td>50%</td>
</tr>
<tr>
<td>Computational Chemistry &amp; Physics</td>
<td>$11,104,249</td>
<td>149</td>
<td>79</td>
<td>12</td>
<td>$925,354</td>
<td>42%</td>
</tr>
<tr>
<td>Materials, Nanoscience &amp; Energy</td>
<td>$8,521,461</td>
<td>178</td>
<td>91</td>
<td>10</td>
<td>$852,146</td>
<td>20%</td>
</tr>
<tr>
<td>Inverse and Multiscaled Modeling</td>
<td>$10,198,155</td>
<td>149</td>
<td>78</td>
<td>11</td>
<td>$927,105</td>
<td>55%</td>
</tr>
<tr>
<td>Enabling Technologies</td>
<td>$17,511,605</td>
<td>313</td>
<td>144</td>
<td>21</td>
<td>$833,886</td>
<td>33%</td>
</tr>
</tbody>
</table>

*Based on an analysis of the research programs of 79 faculty identified by Chairs, Directors and Deans as using advanced computing or having the potential for applying advanced computing to their research.

Impact of Programmatic Initiatives

The Institute will provide resources for major projects that are computationally intensive. The Institute resources could be presented as institutional support for external grants. For instance, two of the Science and Technology Center proposals to be submitted this fall are in the research thrusts of the Institute and are computationally intensive. The Principle Investigators for one of these projects has indicated that they would like to include the development of the Institute as institutional support of their proposal.

- **Time allocation on the HPCC.** Use of the HPCC will be prioritized providing preferential support of the highest performing faculty and will promote research in specific thrust areas. Time will also be available for development and testing of new projects, including research of new faculty, establishing their research.
- **Access to resource personnel in the HPCC.** These personnel will improve the efficiency and effectiveness in the use of the cyber infrastructure associated with HPCC. These personnel will help to maintain the hardware and provide advice for upgrades of hardware and software.
- **Access to resource personnel in the Institute** will provide faculty with important technical support.
- **Faculty Scholars Program** will provide buy-out for the submission of large center and multidisciplinary proposals, especially in the thrust areas. In addition proposals for the GLPCC will be promoted by these scholars – help develop a connection to that Center.
- The postdoctoral fellows program – impact on the faculty mentor and to the rest of the ICER faculty.
- **The Graduate Student Fellowships.** These recruitment fellowships assist in attracting the very best students into the research programs of Institute faculty.
- **Graduate curriculum** —will help connect the institute to the virtual school and to recruit students to CER faculty programs. Provides more efficient and effective education of students in CER faculty labs
- **Website** helps to provide connections and collaborations within and across the thrust areas
- **Seminars and workshops/retreats** will provide connections and collaborations within and across the thrust areas.
Composition and Roles of the Committees and Personnel Associated with the Institute

- **Faculty Steering Committee.** The steering committee will be composed of one representative from each of the thrust areas and four additional institute faculty. Each member will serve serves a three year term. Initially members of the Steering committee will be selected by the Director and Executive Committee, with three of the initial members serving a one-year term, three serving a two-year term, and three serving a three-year term. New Faculty Steering Committee members will be selected by the Director in consultation with the Current Faculty Steering Committee and the Executive Committee. The Steering committee will provide advice and guidance regarding investments in enabling technologies that meet the needs of the Institute.

- **HPCC advisory committee** will consist of five MSU faculty members with a vested interest in the success of the HPCC. The HPCC advisory committee will be selected by the HPCC Director with input from the Institute’s Steering Committee and Director. This Committee would provide recommendations and approaches for the architecture and tools in the HPCC. The committee would have budget responsibility for the resources in the Center and would develop queuing mechanisms, and for implementing a hardware buy-in policy for access.

- **External Advisory Committee** will consist of internationally prominent scientists, some of whom are MSU alumni and friends of MSU in the fields of computing and science, and possibly with significant “advancement capabilities,” as well as distinguished members not only of the academic community but also from key industries. This board will provide visibility for the Institute and help set scientific directions, as well as provide help with fundraising efforts.

- **The Executive Committee** is comprised of the Deans of the Colleges of Social Science, Natural Science and Engineering, the Director of the NSCL, the Vice Provost for Libraries, Computing and Technology, a representative from the Office of the Vice President for Research and Graduate Studies and the Institute Director (ex officio).

- **Director of the Institute** will be selected for a five year term. Director is a Tenured Faculty selected through a search process developed by the Executive Committee in consultation with the Faculty Steering committee. The Executive Committee will provide input to the Director’s Chair and Dean regarding annual performance in this administrative role. A five year review of the Director will be conducted as a component of consideration for reappointment. The Director will set policies and procedures for the Institute as described above, have responsibility for evaluating the activities of the Institute to include the development and presentation of the Annual Report

- **Assistant Director of the Institute** will assist with the detailed operations of the Institute, including organizing seminars and workshops. The Assistant Director will also help maintain the Institute’s web site which will contain information about courses, programs, and events, a listing of the faculty and institute resources.

- **Director of the HPCC (50% appointment)** will have the responsibility for maintaining and upgrading the hardware and software of the HPCC and for hiring HPCC staff, with input from the Institute Director. The Director will have input on developing policies for the use of the HPCC and will be responsibility for implementing policies and procedures in the Center.