Elevating Research Computing Cyberinfrastructure at UW-Madison

I. MISSION STATEMENT

The University of Wisconsin-Madison Advanced Computing Infrastructure will support our emergent research capabilities by making effective computing resources accessible and more readily adopted by campus investigators. The successful outcome will provide expertise, hardware, and software in the right ratio to empower the research mission of UW-Madison through computation.

An infrastructure will be established that facilitates the use of computation for scholarly endeavors, and enables to the greatest extent possible research on our campus. We begin from a position of strength. Our Center for High Throughput Computing (CHTC), the Grid Lab of Wisconsin (GLOW), and Open Science Grid (OSG) are shared resources funded by national agencies and the UW to provide millions of CPU hours per year. We have enviably successful but stand-alone physical science experiments that break barriers in computational research (e.g. Ice Cube, CIMSS, LHC). And yet, these established components of an advanced computing infrastructure exist alongside nascent ones across UW-Madison; they lack interconnectedness, unified leadership, and visibility and support for newcomers to computational science. High performance computing at UW-Madison currently operates on a piecemeal cluster-in-the-closet basis that is not sustainable. We propose a UW-Madison-tailored approach to augment cyberinfrastructure on this campus so that it best serves our mission. Under the umbrella of the Madison Advanced Computing Infrastructure (MACI), local expertise will be coupled with global experience through a modestly hierarchical structure that will encourage exchange of ideas and training of students, faculty and staff in best practices.

This effort began a year ago, when a Research Computing symposium and many cross-campus conversations led to the recommendations contained in our Research Computing White Paper\(^1\). Here we suggest coordinated action and central campus support for the most impactful items in that report. In particular, MACI will (1) hire a Research Computing Officer\(^2\) who will (2) accelerate the pace at which an easily navigable portal is created to disseminate information and encourage participation in our computing infrastructure, (3) establish a pool of highly skilled Facilitators with expertise in domain-specific research computing who will provide an on-ramp to the advanced computational infrastructure and match research and scholarship goals with the appropriate computational tools or resources and (4) provide additional HPC (CPU and GPU) computing hardware because this is seen by many as the current computational limitation.

A function of MACI is to ensure that the vibrant research programs on the UW-Madison campus are not limited by computational infrastructure. Research cyberinfrastructure is a staple of world-class scholarship in the 21\(^{st}\) century and our needs will become only more acute. Our peer institutions have recognized and invested wisely, each according to its needs, on this front. The Minnesota Supercomputing Institute (www.msi.umn.edu) supports research across the state, sponsors workshops, provides summer REU opportunities, and recently opened a new GPU computing center. Purdue’s Rosen Center for Advanced Computing (www.rcac.purdue.edu) will unveil the newest of its ten community clusters, with 10,000 computing nodes, in the spring. Princeton’s Institute for Computational Science and Engineering (www.princeton.edu/researchcomputing) has completed construction of a 47,000 ft\(^2\) green building to house its endowed $2-3 Million/year campus-wide research computing infrastructure. Without a cyberinfrastructure that matches research and scholarship goals with appropriate computational...
tools and resources, the opportunity costs to UW-Madison in missed grant dollars, lost research creativity, and inability to attract and retain the best faculty and students are great. Future competitiveness will be coupled to augmenting our computational infrastructure and the way it interfaces with the scholars and researchers it serves.

ALL researchers – in physical and biological sciences, engineering, social sciences, arts, education and humanities – are potential beneficiaries of MACI. Examples of the very catholic problems to be addressed include dynamics of granular materials with applications in the pharmaceutical industry, simulation of combustion processes for designing greener engines with improved fuel efficiency, modeling millions of simultaneous protein:protein interactions within a human cell, refining protein structures against low resolution data, analysis of unprecedented amounts of satellite image data for modeling the impact of ancient humans on the landscape, mining ancient texts for new linguistic insights, or creating original works of graphic art. We have not yet imagined most of what we will discover.

In keeping with the central mission of UW-Madison in education and training of the scientific leaders of today and tomorrow, resources devoted to MACI will lead synergistically to the development of new courses (both workshops and semester-long) and open up novel possibilities for undergraduate and graduate research. By supporting six-eight senior research assistants as part of its Community of Practice, the MACI mission will explicitly encompass training of graduate students in modern computational methods and experimental design, and give them experience in teaching and mentoring. These students will also serve as ambassadors to broaden awareness and the user base across campus for these shared resources.

Acknowledging the central role that computation plays in 21st century scientific research, we seek a sustained commitment from the University of Wisconsin-Madison to support research computing at a high level as an integral part of our infrastructure.
II. LEADERSHIP AND GOVERNANCE: Where does this proposal fit into the current ecosystem and how will the Infrastructure be run?

A team approach to leadership is recommended. There are three planes of management:

(1) UW-Administration including the Provost, Vice Chancellor for Research and CIO will provide fiscal support, institutional oversight, and coordination between the sponsors and the Steering Committee.

The current proposal to create a UW-Madison Research Computing Officer (RCO), who will link the CIO’s office and the office of the Vice Chancellor for Research, forms an important cornerstone for the smooth operation and complete success of the MACI (see detailed job description in Appendix II). In particular, the RCO will connect the MACI to other aspects of Cyberinfrastructure at UW-Madison by sponsoring a vibrant, information-rich and integrated Web-based portal for research computing at UW-Madison. The MACI will become a forum for the research computing community to meet and interact, and the regular updates, highlights, calls for proposals, seminar announcements and calendars available at the on-line portal will be a critical tool for the network of users.

(2) The Faculty Director and Faculty Steering Committee

This visionary faculty director will have a highly respected research program that relies heavily on or develops methodologies in HPC and/or GPU and/or cloud computing. We propose this could be a new faculty position. This individual will provide an outward face for the MACI. S/he will develop grant proposals that may support it, will provide high-level connections between other faculty members who might benefit from collaborative use of the Infrastructure, and will speak nationally and internationally to promote our work.

The Faculty Director will chair a Steering Committee broadly representative of campus researchers. This permanent Steering Committee, composed of faculty members and scientists and advised by technical staff, will play an active role in guiding the MACI and setting policies and priorities for use of its resources. Using its own discretion, this committee may consult with other researchers and faculty members from UW-Madison or, when appropriate, from other institutions.

The Faculty Director and the Faculty Steering Committee will review the implementation and
the success of the MACI and will develop milestones that can be celebrated and used as evidence of
the impact this framework has on campus research. We expect, for example, new federal or private
grants to be won, new research areas to be opened up, new cross-disciplinary and cross-campus
collaborations to ensue, recruitment of world-class faculty, an increasing number of UW researchers
who use high level computing resources each year, a jump in the number and quality of PhD theses
earned for work using these resources, new undergraduate courses that will be developed, and news
articles to appear in local or national press about work happening here.

One role of the Steering Committee will be to monitor the ecosystem of the MACI and to
periodically review the roles and responsibilities of the staff members. Because the nature of the
staff positions is that they will change over time in unpredictable ways, the steering committee will
make recommendations for how the positions should evolve.

The Faculty Director of MACI will work closely with the Technical Director.

(3) The Technical Steering Committee.

The MACI Staff, led by the Technical Director, will facilitate the adoption of appropriate
computational infrastructure and methodologies by campus researchers to advance their research
and position them to take advantage of 21st century funding opportunities. We refer to this group as
the “Community of Practice”. The Staff is key to success of the MACI. The Staff will work directly with
campus researchers on the necessary technical issues, advise them on best practices, help them form
connections and collaborations with other researchers, and transmit information to and from the
researchers. These staff members are the bridges from the central MACI into individual domain
science and scholarly research groups.

The Technical Director of the MACI will be responsible for acquiring, instantiating, and
sustaining the core computing hardware and software deemed to limit campus research. He/she will
have responsibility for successful daily operations. This Community of Practice level of management
will also be guided by a steering committee, whose members will be peers with technical expertise.
Current research and technical staff on campus including experts within CHTC, Ice Cube, SSEC, and
individual PI-sponsored computational programs are likely members of this Technical Steering
Committee. An predicted outcome is increased communication, problem solving, expertise sharing,
and professional training for this group of research computing technical staff.

The anticipated close connection between the newly envisioned MACI and the extant and very
successful Center for High Throughput Computing (CHTC) will be a great benefit to the MACI and its
users. The Faculty Director and the Technical Director will work closely with staff of CHTC and with its
director, Miron Livny. Professor Livny is a world leader in distributed computing and a key developer
of CONDOR and of the Open Science Grid. As the boundaries between specific computational
modalities blur further, the CHTC director will continue to collaborate with and/or serve as a member
of the MACI Steering Committee to ensure a straightforward evolution that strengthens the
capabilities of the CHTC within the broader framework of the MACI.
III. INITIATION: How do we get started?

The initial investment in staff and hardware are presented in the Budget (item V). We project a ramp-up over three years to an annual investment of approximately $3 Million. We stress that the organization, funding, governance and user interface aspects of this project are tantamount to its success. With this structure firmly in place, future growth will not require major restructuring. The most important investment will be in the staff. An immediate investment in 3-4 full time research computing experts who can serve as Facilitators to be deployed as needed for getting new research computing projects up and running is recommended. Initially, these employees could be accommodated within the current framework of the CHTC or other campus computing facilities offering shared resources and as additional computational resources are acquired and brought on line their positions would evolve.

In terms of the physical facility and hardware purchases, we recommend a cluster that is large enough to create opportunities on campus that do not exist but small enough to build organically in response to increased demand. MACI should facilitate access to GPU or CPU clusters already on campus by working closely with PIs or directors of those clusters (Manos Mavrikakis, Dan Negrut, Qiang Cui, Martin Merck, and others) and providing manpower as needed so that available cycles can be shared. We anticipate rapid growth over the next five years and the business plan should allow for this. One possibility for the physical facility is the WID/MIR building. Future expansion would be to a separate, larger physical space (or, for the sake of continuity of service, to one central MACI space with additional remote sites). At this point, design and planning for such future space is left to the MACI Steering Committee, but a vision for a green-design MACI home, where the community of researchers can gather and where they can be seen, is an exciting possibility. We stress, given the current Administrative Excellence planning, that physical space, power, and cooling for a growing computational infrastructure must be included in any long-range planning.

IV. BASIC OPERATING STRUCTURE: How will the Advanced Computing Infrastructure operate and how will resources be allocated if demand exceeds supply?

This will be a research hub, rather than an administrative unit. It will be a place to get work done!

1. The university pays for the MACI staff, the physical facility, and matching nodes (for example 20% of the total nodes up to a capped maximum), thereby augmenting researchers’ contributions and providing CPU cycles for new users who are not (yet) committed to or able to purchase their own nodes.

2. New users will be paired with the most appropriate Facilitator for getting new projects started. The research computing team will have a diverse set of skills appropriate to matching with researchers in all of the scholarly divisions on campus. All of us will benefit when this is done correctly. An important aspect of the responsibilities of the MACI staff is to help researchers identify the best research computing tool for their particular application, whether this tool be Cloud Computing, HTC within the CHTC, HPC, GPU computing or another resource outside UW-Madison.

3. New users will have access to MACI resources at no cost, in order to determine if a certain approach is feasible or to carry out pilot projects that lead to future larger engagements. To meet this need, a designated fraction of computing cycles (for example, 10%) remain available for new users.
4. Experienced users will have straightforward direct access to computing cycles and submit jobs themselves.

5. As demand grows, a more formal process will be put in place by which <1 page proposals will be solicited from potential users and these will be reviewed with a very quick turn around time for priority setting and resource allocation.

6. A researcher buys in to the MACI co-op model with a given number of CPU nodes. The type and price of nodes is generally specified by the computer management team - they purchase nodes periodically, and get discounts by buying large volumes from regular vendors.

7. The researcher never needs to see the nodes. They are ordered, installed and maintained by the MACI staff.

8. The researcher has access to at least all of her/his dedicated nodes, which s/he owns for five years. After that point s/he needs to contribute a portion of the purchase price for replacement nodes (see also #9).

9. The university provides a substantial fraction of replacement costs for equipment purchased with non-federal funds, since such equipment generates indirect return over its depreciation period (typically five years) equal to its purchase value.

10. When researchers’ nodes are not in use, they can be allocated to other users. Allocation of unutilized nodes is carried out on the basis of brief semiannual proposals (see also #5).

11. At any given time the nodes that a researcher owns can be replaced with more recent nodes. The MACI staff is continually upgrading its computing equipment and providing the same CPU power to all its clients. The number of CPU nodes that a researcher owns can increase or decrease, but the actual number of computing units that s/he owns never goes down, and it can actually increase as better and cheaper products reach the market.

12. The MACI staff is responsible for all maintenance. All a researcher does is pay at the beginning.
### V. BUDGET PROPOSAL

#### Salaries and Fringes

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Budget Proposal Footnotes:

1. A Steering Committee will be formed and will take immediate responsibility for the budget, and the budget will be reevaluated in 18 months.

2. Although Cluster Administrators and Facilitators are listed as full FTEs for the purposes of this budget, we anticipate at least some of these MACI members could be appointed partly through MACI and partly through independent research groups, colleges, or schools.

3. Graduate Research Assistants will have a different role than Facilitators, with a greater focus on training, mentoring, ambassadorship. These students are ones who will be carrying out their own research using MACI resources.

4. The acquisition of new centrally-funded hardware will not be automatic even if it is budgeted. Rather MACI Steering Committees will assess current usage and demand, co-op model CPU availability and demand, and expected near term growth in demand based on established users' needs and expected new users. Based on these factors, new hardware will be added organically.

Appendix I. RCO position description
Appendix II. UW-Madison Research Computing White Paper 2011