Computational Science

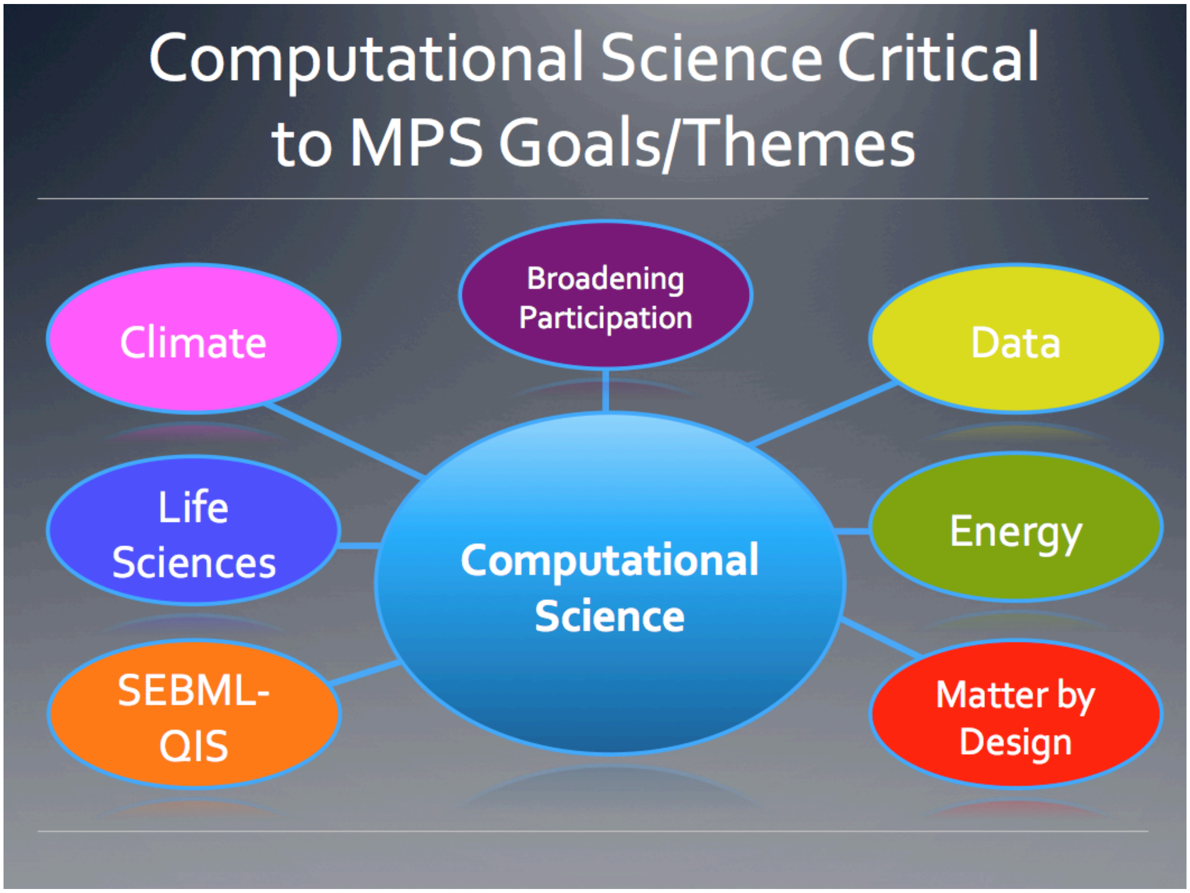
White Paper submitted by the MPSAC Working Group
May 14, 2010

Background and Introduction

Computational Science is now well recognized by the scientific community as a critical enabling discipline underpinning modern research and development in all fields of science, engineering, and medicine. Many fields of science, such as climate and atmospheric sciences, elementary particle physics, and chemistry, have been transformed by computational modeling and simulation. The prediction of material properties and self assembly, emergent behavior in complex systems, and the formation and interaction of stars and galaxies have likewise benefitted in critical ways from the development and application of mathematical models and algorithms, software, and ever-increasing computer speeds. Indeed, numerous recent studies, reports and articles [1-14] identify the enormous opportunities and challenges that await the application of computational modeling and simulation to the many disciplines within the Mathematical and Physical Sciences (MPS) Directorate at NSF, along with their partner directorates across the foundation.

> *"The computational landscape is changing rapidly with the US invention of many-core computer processors integrated to provide a thousand-to-million-fold increase of computational power over that of today's computer. Remarkable advances in numerical algorithms and solvers for handling complex equations are providing additional many-fold increases in compute power. At the same time, the ability to store unprecedented amounts of digital data continues to grow rapidly. The increases in computational capability will allow simulations that will drive solutions to problems from Alzheimer's and alternative energy, creating unlimited opportunities for tackling the most important issues facing our nation and creating new venues for renewed national and individual prosperity, wealth and security."*
>
> – NSF-commissioned report on *Inventing a New America through Discovery and Innovation in Science, Engineering and Medicine: A Vision for Research and Development in Simulation-Based Engineering and Science in the Next Decade*, 2010 [1]

Despite this growing awareness of the importance of Computational Science to the scientific enterprise, NSF has not taken a leadership role in its stewardship and support, and Computational Science has no well-defined, visible "home" at NSF. This long-term lack of a visible, permanent commitment to Computational Science has important and far-reaching consequences: (i) The critical infrastructure supporting U.S. Computational Science is eroding or missing. (ii) Universities are wary of creating permanent programs and faculty lines in an area where there is no clear line of funding. (iii) Too few students are being trained in computational science. As a result, Computational Science cannot realize its full abilities as an equal partner to experiment/observation and theory/modeling, and science suffers. As a recent report states, "America's historic leadership role in this field is diminishing as other nations aggressively scale up investments in computational science."[2]



Computational Science is critical to MPS Goals/Themes.

This white paper presents a set of recommendations by the MPSAC Working Group on Computational Science, working in partnership with the MPS Internal Cyber Working Group. The recommendations were developed through a series of group and individual discussions and heavily informed by community input gathered from recent reports. Questions addressed by the working groups included:

- What should MPS be doing in Computational Science?
- What critical activities in Computational Science are important to the community but not adequately (or at all) addressed or supported by MPS or elsewhere at NSF?

Our recommendations comprise a new and holistic vision for computational science within the directorate that we believe is necessary for the directorate to provide leadership and stewardship to the MPS computational science community and its beneficiaries in theoretical, experimental and observational science.

Needs, Opportunities and Recommendations

To realize the full promise and impact of Computational Science, MPS should consider six clearly identifiable and high priority opportunities and or issues.

First and foremost concerns the very ***identity of Computational Science and its recognition by MPS***. While MPS has various important programs within its divisions supporting theory, modeling and simulation activities, these are not synonymous with supporting computational science. *NSF does not currently support computational science holistically as an enabling discipline – as a critical infrastructure for theory, modeling and simulation.* Activities in computational science are instead often funded indirectly, as secondary to the science, a practice that appears to stem, at least in part, from the reviewing process in which science always trumps infrastructure. At NSF, no one "owns" computational science, and no one yet takes responsibility for it, despite the recognition by the scientific community of its importance. As a result, core elements of scientific computation critical to MPS (and other NSF) activities currently fall between the cracks, and opportunities are lost. Examples of "orphaned" core elements include, but are not limited to, (i) the development and long-term stewardship of software, including new and "staple" community codes, open source codes, and codes for new or nonconventional architectures; (ii) the development of models, algorithms, and tools and techniques for verification, validation and uncertainty quantification; (iii) the development of tools, techniques, and best practices for ultra large data sets; (iv) the development and adoption of cyber tools for collaboration, sharing, re-use and re-purposing of software and data by MPS communities; and (v) education, training and workforce development of the next generation of computational scientists.

Recommendation 1: MPS (as well as all of NSF) should embrace Computational Science as a "discipline" in its own right - it has its own identity that should be recognized and nurtured as such.

A second issue concerns the present ***lack of long-term support of computational science*** activities. Model, algorithm and software development are long-term activities that often span multiple generations of students, and for which scientific impact and recognition may take years. After all, no cover of Science or Nature has even gone to the development of a new piece of software, just to the science done with the code.

Recommendation 2: MPS must commit to long term support of the computational science community, and put in place permanent programs that provide substantive, long term, pan-generational funding and support for endeavors for which scientific impact may be many years off, with appropriate reward metrics.

A third critical issue involves the ***development, dissemination, maintenance and stewardship of computational codes (software) central to MPS activities***. Software is the single most important tool in computational science. Without software to implement algorithms and solve models, computational science is not possible. Thus software must be supported for the critical infrastructure that it is, and thought of in the same way as we think about large facilities for experimental science. Computational science is key to scientific discovery in all MPS divisions, yet there is presently little commitment to software development within MPS and the existing divisional and program structure may make it difficult to do so. Examples of successful programs include PetaApps and CyberChemistry, but these were not established as long-term programs. Computational codes for new and emerging architectures (e.g. multicore, graphics processors, and FPGAs and other accelerators) are demonstrating enormous promise for MPS programs, yet no clear, permanent home for such code development that would benefit entire fields or application domains exists. Examples of needed MPS programs include the funding of MPS Software Centers, as well as large and small teams and single investigators. These programs should be designed to leverage new Software Institutes being established under OCI. Key to the success of these activities will be a fundamental shift in attitude toward viewing and supporting – as “facilities” – community codes important to the MPS mission.

Recommendation 3: Software development and stewardship must be supported by MPS for the critical infrastructure that it is.

A fourth critical activity not being supported holistically within MPS is the collaborative development by domain scientists and mathematicians of ***approaches and tools in validation, verification and uncertainty quantification that underlie predictive computation***. Without VV&UQ, it is impossible to quantitatively bridge from atoms to enterprise in a way that allows risk assessment and, ultimately, policy decisions based on the underlying science.

Recommendation 4: MPS should encourage interdisciplinary interactions between domain scientists and mathematicians on the topic of uncertainty quantification, verification and validation, risk assessment, and decision making.

Also critical to the future of MPS is the education, training and development of a future workforce in Computational Science. Many studies have demonstrated the weaknesses in our nation’s current approach to workforce development in this area. Relegating workforce development in Computational Science to others means that future mathematical and physical scientists lack the education and training they need to fully leverage the present and coming computational capabilities in solving the scientific problems central to MPS. The need for education and training spans undergraduate, graduate and postdoctoral levels, as well as K-12 and continuing learning and retraining. Examples of needed programs include support for the development of new curricula in the core competencies of Computational Science and new ways of sharing and disseminating curricula; virtual centers, institutes, and schools in computational science; undergraduate scholarships & REUs focused on computational science; IGERT-like graduate fellowship block grants in Computational Science; internships, practica and partnerships with industry, national, government labs and supercomputing centers, where MPS can serve as a matchmaker; continued learning opportunities for those already in the workplace; and transitional grants such as portable postdoctoral fellowships in MPS computational science disciplines that take one through the equivalent of tenure.

Recommendation 5: MPS should support workforce development at all levels to expand literacy and broaden participation in computational science.

Finally, it should be recognized that supporting computational science may differ in many respects from supporting traditional domain math and science disciplines. As an enabling yet unconventional discipline with its own set of core competencies but which also spans all of mathematical and physical science, it will important to leverage and integrate activities where possible in order to have the maximum impact.

Recommendation 6: MPS should support unconventional and high risk activities in computational science, and be nimble to evolve while maintaining a long-term, pan-generational commitment, to achieve transformative change.

Next steps

Strategies and tactics for implementing the above recommendations should be developed by MPS with guidance from the MPSAC Working Group on Computational Science. Questions to be addressed include:

- How should MPS undertake these new programs in Computational Science? What form should they take, and how should they be implemented?
- How should/can MPS activities leverage CF21?
- What aspects of Computational Science should MPS take the lead on, vs. partner on, with OCI as well as other directorates?

As noted by the MPS Cyber group, "how to create this new opportunity for the MPS community in the most efficacious fashion should be discussed among all the stakeholders, the community, the divisions and the MPS front office. The focus should be the value added of this activity, and be a grass-roots, program officer managed effort, as opposed to a top-down activity." At the same time, the MPSAC Working Group urges a holistic, integrative, and long-term view.

Contributors

The MPSAC Working Group on Computational Science contributing to this White Paper includes Sharon Glotzer, David Keyes, Joel Tohline and Jerzy Leszczynski.

Member of the internal MPS Cyber Group participating in discussions leading to this document includes Morris Aizenman, Estella Blaisten, Evi Goldfield, Daryl Hess, Leland Jameson, Andy Pollington, Tom Russell, and Barry Schneider.

References

1. P.T. Cummings and S.C. Glotzer, “Inventing a New America through Discovery and Innovation in Science, Engineering and Medicine: A Vision for Research and Development in Simulation-Based Engineering and Science in the Next Decade,” WTEC Workshop Report, 2010, in press.
2. Glotzer, S. C., Kim, S., Cummings, P. T., Deshmukh, A., Head-Gordon, M., Karniadakis, G., Petzold, L., Sagui, C. and Masanobu Shinozuka, “WTEC Panel Report on International Assessment of Research and Development in Simulation –Based Engineering and Science,” World Technology Evaluation Center, Inc., 2009. http://www.wtec.org/sbes/SBES-GlobalFinalReport.pdf
3. Keyes, D., Colella, P., Dunning Jr., T. and Gropp, W. “A Science-Based Case for Large-Scale Simulation - Volume 1, Department of Energy – Office of Science Workshop Report,” 2003. http://www.pnl.gov/scales/
4. Keyes, D., Colella, P., Dunning Jr., T. and Gropp, W. “A Science-Based Case for Large-Scale Simulation - Volume 2, Department of Energy – Office of Science Workshop Report,” 2004. http://www.pnl.gov/scales/
5. Benioff, M. and Lazowska, E. “Computational Science: Ensuring America’s Competitiveness; President’s Information Technology Advisory Committee (PITAC) Report,” 2005. http://www.nitrd.gov
6. Pollock, T. M., Allison, J. E., Backman, D., Boyce, M., Gersh, M., Holm, E. A., Lesar, R., Long, M., Powell, A. C., Schirra, J. J., Whitis, D. D. and Woodward, C. Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security; The National Academies Press: Washington, DC, 2008.
7. “White Paper: U.S. Manufacturing— Global Leadership Through Modeling and Simulation,” Council on Competitiveness, 2009. http://www.compete.org/publications/detail/652/us-manufacturingglobal-leadership-through-modeling-and-simulation/
8. R. Stevens, T. Zacharia, and H. Simon, "Modeling and Simulation at the Exascale for Energy and the Environment " Department of Energy Office of Advance Scientific Computing Reserach, Washington, DC, Report on the Advanced Scientific Computing Research Town Hall Meetings on Simulation and Modeling at the Exascale for Energy, Ecological Sustainability and Global Security (E3), pp. 174, 2008.
9. Jagadish Shukla ed., Workshop Report World Modeling Summit for Climate Prediction, Reading, UK, January 2009.
10. SIAM Working Group on CSE in Undergraduate Education, “Undergraduate Computational Science and Engineering Education,” SIAM Review, submitted.
11. SIAM Working Group on CSE in Education, “Graduate Education in Computational Science and Engineering,” SIAM Review, vol. 43, no. 1, 2001, pp. 163–177.
12. S.C. Glotzer, R. Panoff, and S. Lathrop, “Challenges and opportunities in preparing students for petascale computational science and engineering,” Computers in Science and Engineering, **11**(5) 22-27 (2009).
13. *Challenges in Climate Change Science and the Role of Computing at the Extreme Scale*, Workshop Report, November 6-7, 2008, Washington D.C. (http://extremecomputing.labworks.org/climate/report.stm)
14. Large Hadron Collider (LHC) (http://public.web.cern.ch/Public/en/LHC/Computing-en.html).
15. NSF-OCI Task Force on Cyberscience: Enabling Transformative Research and Education Through Advanced Computing, Data and Collaboration, Interim Report, May 2010.