Improving Access to the National Computational Infrastructure

The Role of Regional Organizations

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Gregory E. Monaco, Kansas State University and the Great Plains Network
Donald F. McMullen, Texas A&M University

This bulletin is drawn from “The Role of Regional Organizations in Improving Access to the National Computational Infrastructure,” a conference report funded by and submitted to the National Science Foundation (NSF) in response to a request for guidance on computational infrastructure needs and solutions in the 2017–20 time frame. The authors of this bulletin participated in producing the report to NSF and have here distilled the key points of that report. The quotes included below are taken from the white papers that were submitted by interested parties in advance of the conference.

Introduction

Providing the U.S. scientific and research communities with access to the cyberinfrastructure (CI) tools that meet their computational and data needs is accomplished through the coordination of resources across multiple levels of what has come to be known as the cyberinfrastructure ecosystem.

Cyberinfrastructure is understood to be the “enabling hardware, algorithms, software, communications, institutions, and personnel” for conducting research. The complex coordination process that ultimately provides leading-edge infrastructure and expertise to researchers on campuses involves the joint activity of a large number of people across many organizations, ranging from campus research computing centers to state and regional networks and national and international CI. Regional organizations include state and regional networks that provide the communications infrastructure, as well as academic high-performance computing centers and other specialized organizations that serve multiple institutions.

Although CI resources are critical for enabling scientific discoveries, there are some inherent limitations to the current configuration of advanced CI resources and the manner in which they can be discovered and accessed:

- **Centers of expertise may become islands of expertise.** As organizations become more mature, they also become more adept at their core business and, as a result, more specialized.

- **Communication across islands may be limited.** Specialization often leads to a situation in which personnel communicate most frequently with personnel at other organizations that provide similar or closely related services.

- **Lines of communication between users and providers that were once necessary for establishing advanced services go unused, become less efficient, and disappear.** State and regional networks and their operating organizations were initially created to ensure that researchers...
on campuses are connected to nationally funded, shared research computing infrastructure. During these early stages, the end-user community of researchers was closely involved in the development and delivery of network services. However, with the efficient and reliable delivery of network services, close communication is no longer perceived as necessary.

- **Although essential, the regional layer is often neglected in national CI discussions.** State and regional networks represent a major success in the development of U.S. national cyberinfrastructure for science and education. They are self-sustaining, provide excellent service, and represent a significant return on research investment. They are also overlooked in discussions of the U.S. CI ecosystem.

- **There is no way of knowing whether users are being adequately served.** There are thousands of scientists at smaller academic institutions who are trained to do computational- and data-intensive science who would like to and are qualified to train their students in these skills but do not have access to the technology appropriate for meeting their needs.

Over time, new projects have emerged not only to deliver new services but also as workarounds to limitations to the status quo of existing systems. Efforts such as XSEDE Campus Bridging, the Advanced Cyberinfrastructure Research and Education Facilitators (ACI-REF) program, and Open Science Grid (OSG) are aimed at creating a more consistent campus-to-national environment. These projects have been successful at expanding access to specific services but are not necessarily sustainable in the long term, nor are they well integrated with the broader CI community.

In October 2015, an NSF-funded meeting brought together representatives from campuses, regional research and education networking organizations, and national computational facilities to discuss current limitations to expanding access to advanced CI resources and to identify ways to better coordinate their efforts. The meeting focused on the role of regional organizations in providing broader support to computational researchers and how these organizations might expand engagement beyond faculty and students at research-intensive universities. The ultimate goal was to initiate a process for charting a more coherent course of action that will contribute to a stronger computational and CI landscape by:

- Clarifying the roles of campus, regional, and national resources and services in the overall computational ecosystem
- Identifying scalable operating models for effective and dynamic delivery of computational resources and services to geographically distributed researchers
- Identifying collaboration models that reduce barriers across different environments while preserving efficiency and innovation
- Creating effective learning and workforce development programs to ensure next-generation capability in the most advanced computational science for all disciplines

**Establishing State/Regional CI Centers of Excellence, Champions Leadership Team**

The national high performance computing (HPC) centers […] conduct excellent community engagement, but […] can’t visit every campus, attend every conference and workshop, or reach out to the many people that would most benefit from knowledge about and access to advanced digital resources.
To prepare for this meeting, white papers were solicited from universities (both small and large), scientific research collaborations, state and multistate regional organizations, and national organizations. In all, 36 white papers were received, representing at least 98 authors and 80 organizations. These papers were meant to identify ways that regional organizations could provide timely and relevant education and outreach efforts to computational researchers over the long term, as well as promote and coordinate the sharing of hardware, software, and expertise across campus, state, and regional boundaries. White paper authors were invited to a conference in Kansas City. This bulletin highlights what was learned from the white papers and the subsequent meeting, and it outlines recommendations for the higher education community.

The Role of Regional Organizations

Regional organizations such as regional optical networks and regional high-performance computing centers can serve as the connector between users and CI resources. Proximity to their campus members and familiarity with regional priorities and interests allow these organizations to focus on challenges and opportunities characteristic of the region, as well as to promote new capabilities and resources beyond individual campuses.

One or more regional organizations can potentially serve as a CI hub and occupy a key strategic position between campuses and national computational resources. With respect to computational- and data-intensive science and research, regional organizations have shared values and are poised to move the national science agenda forward through more effective education, outreach, coordination, and sharing of resources, including developing personal relationships to support and sustain initiatives.

In order to do this most effectively, coordination across regional organizations is necessary to develop tactics to maximize adoption of successful activities, minimize duplication of effort, and gain a better understanding of what works. Some key areas where this work can occur include broadening access to the computational infrastructure, promoting CI awareness and literacy, developing a culture of bridging the gap, and sharing resources.

Barriers to Accessing the Computational Infrastructure

There is a growing expectation that the undergraduate experience will include exposure to computational research methods and solutions. Further, industry demand for these skills is growing, increasing the need to expand CI engagement beyond a small set of highly advanced and specialized sciences. To meet these needs, higher education resources must be readily available to train new computational scientists. There are populations of students and faculty at smaller colleges and universities—institutions that typically have less funding to offer tools and services—who want to be intellectually engaged by becoming a part of larger projects. Engaging these individuals in the larger computational fabric is critical for training future generations of scientists.

At research-intensive universities, faculty and students—particularly in STEM disciplines—have access to a human support network that guides them to needed resources and supports them in using those
resources. They also benefit from administrators who understand the importance of CI and are committed to providing what they need to be successful in research and scholarship as well as teaching. This guidance may be lacking in some disciplines and at smaller campuses.

Even in cases where some advanced CI resources exist, additional barriers may limit broader adoption of these resources, including:

- Existing resources that are insufficient or inappropriate for one's particular problem
- Minimal awareness among potential consumers of the CI resources available
- Lack of adequate training and understanding of how to use them
- Concerns around intellectual property protections when working with the “sharing culture” of CI facilities

Other barriers exist, as well. Because of geographic remoteness and sparse populations, faculty, staff, and students located in rural regions find it difficult to access CI resources, expertise, and training. There is no readily available central repository of resources and expertise for states and regions, and geographic isolation leaves many rural researchers unaware of rapidly evolving research-computing capabilities. The development of robust CI is critical to ensuring that these institutions remain competitive. However, the costs of deploying enhanced CI can be high. Regional organizations can aggregate the voices of rural institutions to ensure collaborations serve the entire region.

Regional organizations are in a strong position to assist underrepresented institutions in expanding the adoption of advanced CI, including both networking and computing infrastructure. Institutions with a wide range of missions may be effectively aggregated at a regional level to promote the use of computational resources by an ever-expanding user base.

**Promoting CI Awareness and Literacy**

Promoting awareness of and literacy about advanced CI among researchers, students, and IT staff is an important objective in the overall effort to build national cyberinfrastructure. Outreach and training to the research community is difficult at the campus level and even more so at the regional level. Although outreach efforts from “CI aware” campuses to other campuses—particularly smaller campuses and those in more remote and rural environments—are highly desirable, models for successful regional coordination of outreach activities are few.

National CI organizations provide their communities of users with information and resources related to their range of services and interests. A key role for a regional CI organization is to organize and provide access to the following resources across its membership, building on existing resources and services but tuning them to specific regional requirements:

- Training (online and in person) and educational materials and services
- Shared CI infrastructure, tools, and services
- Community information sharing and professional development events

There is a substantial reservoir of potential future computational scientists who are currently enrolled in small colleges throughout the United States with professors who wish to introduce them to high-performance computing but lack the resources to do so.

*A Personal Perspective on High-Performance Computing at a Small Liberal Arts College*,
Gail S. Blaustein
Developing a Culture of Bridging the Gap

The development of a core community of successful CI consumers within underrepresented communities is critical for expanding the use of computational cyberinfrastructure into a diverse set of users that includes both rural and smaller organizations. Developing a set of professionals who can speak the language of their peers and bridge between CI providers and CI consumers is essential for successful outreach on a regional level and to build collaborations with researchers and students at smaller institutions.

Resource Sharing

XSEDE and OSG represent two points along the sharing spectrum. There are increasing efforts to merge the sharing efforts of these respective communities. The OSG provides a viable opportunity for a campus to share computing resources with the broader scientific community. For example, the high-energy physics community proved that when the incentive for broad sharing is sufficient, the difficulties in sharing physical resources and data can be overcome. As communities become interested in advanced CI, there is an opportunity for regional organizations to provide an introduction to the field and to encourage member involvement in CI-related activities. The challenge is to identify these communities, welcome their members, and provide outreach and education. The twin issue of expanding and improving access is a “people problem” and is amenable to the study of those factors that influence behavior at the individual and organizational levels. Engaging social scientists (psychologists, economists, sociologists) to focus on increasing uptake of advanced CI is one key approach.

White paper contributions have demonstrated that there are meaningful things to learn. Social science methodology and rigor can help us form meaningful hypotheses about variables that influence adoption of advanced CI and help to institute valid, meaningful metrics.

In addition, technology may help improve access to and use of computational infrastructure. Just as new smartphone applications such as Uber and Airbnb have led to more seamless sharing of rides and rooms, the use of technology can lead to increased sharing of computational cycles and storage. Although cloud computing is one new model for resource sharing, to date it is still weak in enabling the distributed sharing of local, autonomous resources between organizations. Sharing mechanisms and services must be seamless and work much as the Globus high-performance data mover application does, where anyone can put a Globus end point on his system.

Recommendations

In order to make computational and data resources pervasive, connected, shared, distributed, and dynamic, it is important to find approaches that cut across communities, agencies, and projects. The guiding principles behind these recommendations are that 1) robust, regionally based CI efforts will support a stronger national infrastructure; and 2) for the CI ecosystem to be more than a collection of parts (e.g., networking, computing, and storage), higher education must foster a culture in which all of the components of the system are complementary and communicate with one another. Improving the overall...
CI ecosystem, however, calls for some specific recommendations for each of the key players: regional organizations, CI projects, and funding agencies.

**Regional Organization Recommendations**

Regional networks are well positioned to help expand access to all components of the CI ecosystem, including computation, data storage, and expertise. They are self-sustaining and have connections to smaller colleges and universities. Although regional organizations were originally created to improve access to the national computational infrastructure and improve science, their missions have become more focused on the provision of reliable Internet services. Regional organizations can continue to improve access to the national computational infrastructure by more broadly adopting the following practices:

- **Add personnel dedicated to computational education and outreach efforts.** These are professionals who can communicate about both the science and the cyberinfrastructure. Their role is to enable researchers to more effectively and efficiently reach their research goals.

- **Actively seek out and communicate with researchers at smaller institutions who have unmet data-storage and/or computational needs.** Regional network personnel are in a unique position to help these researchers—who often have limited time and limited local resources—navigate the CI terrain.

- **Identify and catalogue computational and data resources across their region.** Even within campuses, computational and other network-reachable resources are often unknown to researchers and campus IT departments. An inventory of resources would be invaluable, not only for researchers but also for regional network organizations in order to provide more resources while keeping costs down.

- **Facilitate the sharing of computational and data resources across their region.** Not all computational resources are appropriate for all research problems, and not all researchers have ready access to computational resources. Sharing of resources across campus boundaries will expand the availability of the most appropriate resources to researchers who need them.

- **Expand educational and meeting activities to include topics of interest to researchers with computational and data storage needs.** Regional networks are geographic centers for CI and can convene researchers from larger and smaller campuses to learn from one another, to problem solve, and to obtain campus, state, regional, and national updates.

- **Coordinate efforts with one another (e.g., via The Quilt).** State and regional networks have a long history of working together and assisting one another. The Quilt, the member organization of regional networks, currently has an initiative to strengthen researcher engagement and increase coordination efforts within the research and education networking community.

- **More closely coordinate with national activities like XSEDE Campus Champions, OSG, and ACI-REF.** Regional networks can serve as a communication conduit regarding campus and regional infrastructure and requirements while sharing information about national computation resources with their campus communities.
• Coordinate efforts with national research and education networks such as Internet2 and ESnet. These networks have similar goals to support academic research for the benefit of furthering scientific exploration.

• Coordinate end-to-end performance troubleshooting. When problems occur, it is important to rapidly discover where things went awry and get them back on track. This can be done by actively implementing and promoting performance measurement tools such as perfSONAR.

**CI Project Recommendations**

Emerging and established projects have been developed to fill gaps and work around many of the inherent difficulties with engagement and education. These projects include ACI-REF, XSEDE Campus Champions, XSEDE Campus Bridging, and virtual research communities, among others. These kinds of projects should be encouraged, particularly through the following recommendations:

• Recruit participation of other, established communities in meaningful roles to assist in advisory, development, promotion, and cross-fertilization of communities. These projects can benefit from the capabilities, infrastructure, and expertise of regional organizations.

• Extend the reach and broaden the impact of project activities by coordinating with other regional organizations when working with a campus also supported by them. Through partnerships with regional organizations, these projects can promote their services more broadly (e.g., to smaller campuses, community and tribal colleges, etc.).

• Increase the audience for training opportunities. Regional CI organizations can help provide training for multiple institutions in place of a one-time event at a single campus.

• Improve the sustainability of support and training activities by involving regional organizations. Regional organizations can help in the provisioning and delivery of these activities, bringing these services to campuses within their reach. Many regional organizations are self-sustaining and can help sustain valuable services when the project’s lifetime has ended or when key personnel depart the project.

**Funding Agency Recommendations**

Funding agencies play a vital role in providing direction to the national CI community by identifying priorities and changing dynamics. This role has a direct bearing on research capabilities available for researchers on campuses, but it is focused more on provisioning resources and less on making those resources available to a broad range of users. Regional organizations are well positioned to assist funding agencies in making CI infrastructure and services accessible to researchers and students at a broad range of institutions.

• Support acquisition of regional CI resources to serve a geographic region. This should be done where the performing regional organization shows commitment to some or all of the following:
  - Operation of the CI resource (including funding the system administration staff, operations cost of the resource, and network connectivity)
  - User support, outreach, training, and education
Integration of the system with national CI (e.g., level-two XSEDE provider and OSG partner, and other regional CI)

Low barrier of entry for regional researchers to increase and broaden participation

Integration of research instruments with high-performance networking and advanced data-transfer and data-sharing capabilities

- **Fund regional centers of CI excellence that are committed to the principles of sharing, education, and outreach.** Regional centers of CI excellence would assist with sharing resources at multiple levels, with engaging underserved groups, and with increasing educational opportunities in the region. These centers would also provide a liaison function between campuses and national infrastructure. Successful models are starting to emerge. However, rather than cloning existing models, it is essential that regional CI centers are unique to and meet the needs of a geographic area.

- **Develop a policy to require a resource-sharing plan akin to a data-management plan.** If reasonable for the funding program, a document should be included describing how the resources that will be funded by a proposal will be shared outside the immediate user community.

- **Create a forum for sharing technical expertise developed within university systems on behalf of their campuses and the national community.** In parallel with groups like the XSEDE Campus Champions, which bring technical expertise from NSF supercomputer centers to researchers on campuses, it would be useful to develop mechanisms by which expertise at academic HPC centers can be shared with peers across the United States.

- **Invest in workforce development.** For example, NSF awards to fund the creation of and initial support for Campus Cyberinfrastructure Engineers has led to increased awareness for this area of specialization across the United States. Since crossover between domain knowledge and technical expertise is to be encouraged, new career paths would be open to domain scientists who have acquired sufficient expertise in a given technology to become a critical component of the current CI workforce.

### Recommendations to the Broader CI Community

The cyberinfrastructure community has other needs that may not be neatly addressed by regional organizations, funding agencies, or specific projects. Members of this community must work together to bring about changes that will cultivate computational scientists and CI professionals and encourage a climate of sharing.

- **Incentivize training of the next generation of computational scientists.** The availability of advanced CI to faculty and students at smaller colleges should no longer be a barrier to participation and use. The primary barriers that remain are related to outreach, training, and support. Approaches to lowering this barrier to the use of national and regional CI include:
  - Incentivize training at smaller colleges and universities to include computational science in undergraduate discipline-specific curricula (e.g., chemistry, physics, biology, agriculture), using CI resources available at the national and regional levels.

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**Given the fast-paced changes of available tools and technologies, the connection between teaching and research is crucial.**

*White Paper for the Workshop on the Role of Regional Organizations in Improving Access to the National Computational Infrastructure*, Don Engel and Jack Suess
Partner with existing, proven computational and CI training groups, particularly those that cross boundaries (e.g., HPC University, Software Carpentry, and Data Carpentry) to engage in an organized way with smaller colleges and universities.

Support the active inclusion of smaller schools in support networks like XSEDE Campus Champions and the ACI-REF programs.

**Incentivize training the next generation of CI professionals.** The opportunity exists to create new career paths for CI professionals who will help improve existing systems, broaden their reach, and help discover new uses. The creation of careers such as cyberinfrastructure engineer and data science research specialist are examples. In addition to well-defined job descriptions and expectations, there needs to be:

- Encouragement and credit for interdepartmental and multidisciplinary work
- Incentives for domain scientists to gain expertise in relevant technologies that help advance their field
- Certification programs on proficiency in emerging technologies

**Promote a culture of sharing and coordination of existing resources.**

- Encourage discussion, arbitration, and development of voluntary standards within a region or a discipline that promote the sharing and use of resources beyond campus boundaries
- Recognize effective and/or novel efforts in resource sharing
- Measure sharing at campus and regional levels—how much utilization is shared beyond campus members

**Conclusion**

There are many regional organizations in the space between campuses and nationally shared CI facilities, and these organizations enable the use of advanced cyberinfrastructure in research. The higher education community plays a significant role in the funding, leadership, and management of these state and regional organizations. Investments in shared networking infrastructure and expertise, for example, have resulted in benefits to individual campuses and researchers. Now is the time to harness the collective energies of these organizations and focus them more broadly on innovating CI infrastructure and expertise and sharing those solutions on an intra- and interregional basis.

By carefully considering the information presented here and choosing to implement the recommendations from this report, it may be possible to accomplish broadscale change across the CI landscape in support of future computational and data-intensive science in the United States and beyond. To accomplish these goals, regional organizations need support from the entire higher education community.

**About the Authors**

Gregory E. Monaco is Research Associate Professor, Department of Psychological Sciences, Kansas State University, and Director for Research & Cyberinfrastructure Initiatives at the Great Plains Network. Donald F. McMullen is Associate Director of HPRC Enablement, Texas A&M University.
Citation for This Work


Notes


3. The white papers are publicly available for download.

4. In some cases, the authors were listed as a community. In many cases an author represented more than one organization.

5. For an example of such an effort, see Internet2’s Broadening the Reach of Cyberinfrastructure Breakthroughs project.

6. Many university consortia that might compete to acquire and operate regional CI resources on behalf of multiple members are dissuaded from doing so when the consortium is administered by a member university. The consortium must first compete on a member campus to acquire a limited submission slot in response to infrastructure solicitations (e.g., NSF’s Major Research Instrumentation competition). At one time, consortia were exempt from limitations and did not compete for slots on their own campus. This made it easier for funding agencies to award funds for resources to regional consortia (with bylaws and clearly executed membership agreements) on behalf of their entire membership.