Ohio Supercomputer Center

Empower, Partner, and Lead: A Vision for the Ohio Supercomputer Center

November 2009

Executive Summary

The Ohio Supercomputer Center is a statewide resource that provides supercomputing services and computational science expertise to Ohio university researchers as well as Ohio industries. OSC has provided these services for over twenty years, and in fiscal year 2008 we estimate that Ohio researchers that use OSC have won over $85M of research funding for Ohio – a return on investment of 17:1.

Our vision is to be a national center that drives research and development in computational science and the applications of supercomputing, and thus be a strategic transformative force behind Ohio's new economy: by empowering Ohio researchers to new innovations and discoveries that will lead to new products, businesses and services; by partnering with Ohio industries to use supercomputing and computational science as a competitive force; and, in collaboration with Ohio's colleges and universities, in educating Ohio's workforce in the key skills required for future jobs. The plan to realize our vision leverages the significant investments that have already been made by the Third Frontier Program. Specifically, the plan concentrates on the key areas of Advanced Materials, Biosciences and Energy and requires investments for additional technical capabilities, expertise to assist industrial clients, and staff to initiate new workforce training activities. In combination with existing programs across the state in these areas, these investments can be leveraged to position Ohio as the world leader, serving as an attractor for the brightest minds and most innovative firms to move to the state.

Introduction: Today, the economy of Ohio is in significant transition. The state is moving from a historically manufacturing base to a knowledge- and technology-driven economy. The state is investing strategically and aggressively to develop new jobs in emerging sectors, such as energy, advanced materials and biomedicine. Ohio's colleges and universities are being called upon to be the drivers for this new economy by conducting world-class research to augment the state's substantial investments and educating the workforce of the future. At the Ohio Supercomputer Center (OSC), our mission is to empower our clients, partner strategically to develop new research and business opportunities, and lead Ohio's knowledge economy.

Computational science is the application of large-scale, computation-based modeling and simulation that enables researchers to "see" the unobservable – phenomena that are too small (atoms and molecules), too large (galaxies and the universe), too fast (photosynthesis), too slow (geological processes), too complex (jet engines), or too dangerous (toxic materials). For this reason, computational science is recognized as the third leg of scientific discovery (theory and experimentation being the other two). For example, using computational science, researchers are discovering fundamental properties of matter, understanding black holes, and studying living cells at the molecular level. These discoveries are, in turn, used to create new processes, design new products, and develop new drugs. OSC, with its 22-year history of partnering with higher education and industry, is a vital component of Ohio's computational science infrastructure. Going forward, OSC will play a key role in the state's economic future: by working with Ohio researchers for *innovation and discovery* through the power of computational science; by *engaging* with Ohio companies, large and small, in developing products virtually in the computational space of a supercomputer; and by leading the nation in *education and workforce development* in the use of computational science for a wide range of educational, research, and industrial domains. We leveraged our sponsorship from state, federal and private sources to take significant steps in all three areas.

OSC, as its core function, serves a significant portion of Ohio's research faculty across a range of science and engineering fields. In 2008, more than 1,700 researchers executed more than 19-million hours of computational jobs on OSC systems. The major user groups include the chemistry and biochemistry community, materials research, a wide range of engineering disciplines, and significant groups from physics and earth sciences. These researchers depend on the use of OSC resources to study a wide range of topics, from the formation of new molecules, to the binding of drugs to proteins, the long-term changes in the earth's climate, the large-scale circulation of water, and to understanding of the origins of the universe. We will continue to serve these communities in the future. However, our ambition is to become a National Center in research and high performance computing. This will enable OSC and Ohio researchers to compete at the highest national levels for federal center funding while continuing to benefit from the enhanced expertise and hardware capability that will be available.

Our vision is to be a transformative force for Ohio's new economy, providing our universities and industries with world-class computational resources and supercomputing expertise, leading to new goods, industries and services. We describe below how OSC can achieve this vision.

Innovation and Discovery: Many of today's scientific discoveries and inventions would not be possible without the use of modeling and simulation powered by high performance computing (HPC). For example, modeling and simulation are used in creating new composite materials that are lighter and stronger; in designing blades for wind turbines that enable clean, cost-efficient energy; and in developing therapies that are personalized to the genetic makeup of an individual patient. Ohio's academic researchers depend on the availability of the advanced computational resources and expertise at OSC to achieve these breakthroughs. OSC, in turn, must understand the changing computational science landscape, procure and install the HPC systems, storage, and software that enable the breakthroughs, and partner to develop the competitive research proposals that will lead to the next generation of computational science applications. Our vision is to be a vibrant and engaged organization that serves as a magnet to attract the best and brightest minds to Ohio's universities, enabling them to propel Ohio's economy through their discoveries. Biosciences and advanced materials are two key areas of significant strength in Ohio, and we are well positioned to become world leaders in the innovative application of computational science to these areas.

Researchers in the biosciences are striving to understand the workings of human and biological systems at the cellular and molecular level, its relationships to genetics, and the impacts both have on the epidemiology, cause and treatment of disease. Ohio has a strong track record in these areas with its medical schools and related biosciences departments. The three leading academic medical centers (at Ohio State University, Case Western Reserve University and University of Cincinnati) have complementary strengths, and each is closely associated with prestigious Children's Hospitals. All three medical centers are recipients of The National Institute of Health's Clinical and Translational Science Awards (CTSA), which provide for expedited transition of research results from the laboratory to the bedside. Ohio is one of only six states with three or more CTSA sites (CA, IL, MA, NY, and TX). The three CTSAs in Ohio are collaborating on sharing infrastructure and services, particularly in the area of biomedical informatics. Ohio has recently been awarded a $15M federal grant to establish a Health Information Exchange, which further recognizes the position of Ohio in the healthcare information technology arena. OSC has been an important partner in this new endeavor. In addition, Ohio ranks seventh in the number of clinical trials ongoing at the present time. Thus, Ohio is considered a major participant in the health care sector because of our patient numbers, academic medical centers, health information technology expertise and scientific competitiveness/collaboration. Many of the other medical colleges in Ohio (NEOUCOM, Ohio University, University of Toledo, and Wright State University) as well as the community hospitals can benefit from an extension of these biomedical informatics efforts to the entire state thus providing more rapid dissemination of breakthrough treatments, as well as connecting these areas with the world-class medical institutions in Ohio. The statewide Ohio Bioinformatics Consortium (OSC is a member and contributes to the research infrastructure) can serve as a model for developing a statewide Biomedical Informatics Consortium for clinical and translational research, with OSC serving as the provider of computational resources and expertise, and the neutral coordinating site for data and knowledge sharing. This bringing together of the major research academic health centers with additional university and community based researchers and practitioners will position Ohio as the biomedical "discovery engine" attracting investments and engagement by the biotechnology and pharmaceutical industries.

The development of personalized and evidence-based medicine is critically dependent on understanding the genomic, epigenomic, proteomic, phenotypic, and environmental circumstances of the patient, a continuum known as systems biology. This requires a common infrastructure for the sharing of medical information – from the primary-care physician to the research laboratory. High-throughput sequencers for genomics and proteomics produce very large data outputs that must be managed and analyzed. Advanced imaging systems such as late-generation Computerized Tomography (CT) scanners, Magnetic Resonance Imagers (MRI) and Positron Emission Tomography (PET) also result in very large data outputs. Biomedical imaging is a significant research and diagnostic activity across Ohio with major state investments, such as The Wright Center of Innovation in Biomedical Imaging at OSU and Case, with Ohio gaining national recognition in imaging for these advances. Coordinated, evidence-based patient care will require storage and analysis of the resulting data deluge. HPC will be a critical resource for correlating across imaging and other data, not just for individual patients, but also for analyzing data across patients and multiple animal models that will be needed to deliver new insights and new discoveries. OSC is already working in a number of these areas, including exploiting three-dimensional imaging for surgical training simulations, and the analysis of high-resolution, gigabyte-sized histopathological tissue scans. We will play an important role in positioning Ohio as the leader in healthcare delivery and research by providing the computational muscle, storage resources, and intuitive interfaces to powerful computational software that will enable our academic medical centers to translate research data into additional, new discoveries for patient care. In addition, OSC will lead the way in the use of emerging computational methods and their use by the next generation of health care researchers and providers. The ability to bring current research results to community-accessible points-of-care will contribute significantly to the health and well being of all Ohioans.

Advanced materials offer the second area of opportunity. The search for new materials for a variety of industrial and medical applications requires many of the same software advances as those for the systems biology area. For example, high resolution and three-dimensional imaging of materials requires storage and

analysis capabilities similar to that needed for biomedical imaging. Due to their complex structures, these materials must be modeled at the microscopic level of fibers and grains in order to accurately predict the macroscopic behavior. Modeling these materials at the microstructure level to determine strength and life span requires new predictive techniques. Conventional methods for analyzing fatigue – the progressive and localized structural damage that occurs when a material is subjected to cyclic loading – show inconsistencies in their predictions due to lack of underlying physics-based mechanisms and lack of information about the actual material microstructure. Novel techniques are being developed at the research level to provide a higher probability of accurate fatigue failure prediction. Other novel approaches must be adopted in the creation of nanomaterials and nanodevices. Modeling at the sub-microscopic level poses new challenges, as the behavior of physical and biological systems at that scale can be quite different. Here again, Ohio has a community of successful researchers that require HPC to refine and scale-up their simulations necessary for the discovery of important new materials and processes. The universities and Ohio have invested heavily in these areas with several national-level centers in both the materials science and nanotechnology areas – examples are the Institute for Materials Research at OSU and the recent Third Frontier Advanced Materials Program. Ohio universities also have won several significant, multi-year awards from the National Science Foundation in the area of materials research and nanoscale engineering totaling $24M. OSC can offer modeling and simulation expertise, along with the required development of software and the hardware and storage necessary to address these challenging problems.

An important component of these major thrusts is the identification of the USO Centers of Excellence in Ohio, initiating more opportunities for interdisciplinary, inter-institutional research in which OSC will play a significant role. Beyond the two areas discussed above, we expect the centers to increase demand for modeling and simulation capabilities relating to the development of new, cost-effective sources of energy; modeling of transportation; additional, large-scale environmental and agriculture simulations; and the need for systems to handle and analyze large datasets of images from medical, materials, and earth science applications.

Industrial Engagement: Modeling and simulation are competitive tools for many businesses, ranging from consumer-goods manufacturers to insurance and financial-services providers. Today, many of Ohio's largest companies, such as P&G, Goodyear and GE, depend upon HPC to develop their products in a timely and cost-effective manner. For example, Goodyear no longer builds prototypes when they are designing new products, but use modeling and simulation to design long-lasting tires, and P&G has used HPC to design Tide containers that do not break when dropped. For many of these companies, HPC modeling and simulation is an essential and crucial business tool. The Council on Competitiveness, a national think-tank promoting U.S. economic competitiveness, has determined that modeling and simulation also facilitates innovations not previously possible, such as modeling complex systems in energy (e.g., the Smart Grid), transportation, and health care and can help lead the way toward the creation of new jobs, industries, and markets. Many more businesses, typically of small and medium sizes, recognize the value of using modeling and simulation for virtual product development, but face barriers to its timely adoption. These barriers typically revolve around the need for computational infrastructure and lack of expertise. OSC launched the Blue Collar Computing Program in 2004 to address this need, and is acknowledged as a leader in HPC industrial engagement, winning the HPC Wire Readers Choice Award in 2006. Under the Blue Collar Computing program, we have assisted a large automobile manufacturer in Ohio with the design of parts, partnered with the Edison Welding Institute to create a HPC-driven welding simulator, and under a contract from the Defense Advanced Research Projects Agency, assisted two Ohio small businesses to design parts that could only be done using HPC. Our experience with the Blue Collar Computing program can serve as the hub for enabling widespread adoption of HPC for virtual product development by Ohio industry, large, medium and small. We can integrate the infrastructure, software applications, and domain-specific academic computational expertise that can advance the industrial applications of modeling and simulation, and so that industries can use HPC in their everyday work. These efforts are linked to training and education programs discussed below. Our vision is to be a major attractor of businesses to the state because of the value they perceive in the infrastructure, services, and expertise provided by OSC. These efforts also can be linked with the *innovation* investments discussed earlier to bring new jobs to Ohio in important high-technology industries.

Education and Workforce Development: There is widespread national recognition of the need for education and training in computational science and HPC. American computational science education is lagging behind other countries in producing the skilled workforce needed at all levels, from the doctoral student developing algorithms for solving the next great scientific questions to the factory manager designing prototypes for the next successful product. These deficiencies have been cited by many national studies, including the President's Information Technology Advisory Committee, a National Science Foundation blue ribbon panel on the future of engineering, and the Council on Competitiveness. OSC, through the virtual Ralph Regula School of Computational Science (RRSCS), is a national leader in addressing this pressing need. Our vision for education and training is to keep OSC and the RRSCS at the forefront of international computational science education and to expand our efforts into interactive and immersive shared, virtual environments for training. The web portals to complex modeling applications provide a mechanism for both training and on-going use of modeling and simulation in more classrooms and by industry. We are developing, in partnership with Ohio universities and community colleges, companion certificate programs for industry employees, as well as enhancements to the regular curriculum for more traditional students. An introductory computational science certificate program is already in place at Sinclair Community College and will be inaugurated at Columbus State later this academic year. These programs will be extended with stackable certificates in more advanced fields. The first such certificate is underway in Polymer Science and we expect to build other special programs as we work with different industry groups. Such workforce development training will help to build a pipeline of students to fill the research and industry positions in the industries the state is building, will train current faculty, students, and industry employees how to take advantage of new technologies, and build Ohio's reputation as in international leader in computational science education.

Location and Management of OSC: OSC is currently housed at the Ohio State University, which also serves as our fiscal and human resources manager. OSU is the largest user of OSC resources as well as an important partner and collaborator. The location at OSU has helped OSC recruit an interdisciplinary team of highly qualified staff with expertise in both computation and a variety of science and engineering disciplines. Location at OSU also allows us to employ undergraduate, graduate, and post-doctoral students to build the next generation of computational science applications from the widest array of disciplines. OSC's current location in Columbus has the advantage of a central location that is within a 3 hour drive from all areas of the state. At the same time, the growing research programs at OSU Medical Center, the Comprehensive Cancer Center and the Institute for Materials Research as well as related programs in the sciences and engineering will be very valuable in achieving our vision to build a focused, nationally competitive set of research partnerships. Combining these conditions with the long-standing record of OSC's collaborations with all of the higher education institutions in the state, the continued administration of OSC by OSU represents the best positioning of this important resource to achieve status as a national center.

Conclusion: The broad vision we have laid out for the future of OSC is to extend and enhance our impact on research and education at Ohio's colleges and universities, to improve the competitive position of our businesses and industry in the global marketplace, and to provide the training and workforce development in the STEM disciplines necessary for a technically proficient workforce. The ultimate goal is to contribute to improving the lives of Ohio citizens by retaining and creating high-quality jobs around the state.

To achieve this vision, we will accomplish several goals. First, in the area of Discovery and Innovation, our goal is to develop a national center for computational excellence in Biomedical Informatics and Advanced Materials. Second, in Industrial Engagement, our goal is to serve as a statewide resource for businesses to use for virtual product and production process development. Finally, in Education and Workforce Development, our goal is to be a leader in computational science education, preparing the next generation of students at all levels – from the community colleges to the research universities. Additional resources will also be required to achieve this vision:

- Expanded investments in OSC's computational, storage, and technical support capacity to further the Discovery and Innovation focus on Biomedical Informatics and Materials. The investments will produce high returns in terms of increased extramurally funded research, co-investments by vendors, and the long-term prospect of Ohio winning national competitions to advance those fields and to supply those services nationally.
- Industrial Engagement will require expanded funding for industrial modeling and simulation services to provide Ohio firms with a competitive advantage in the development of new products and services and increased profitability in the production of goods and services. This will require staff with specialized modeling and simulation expertise to work with industrial clients and link with faculty research programs that can provide a benefit to industry. Funding also will be needed for commercial licenses for software and to reduce the fees charged by OSC for HPC and staff resources, so that they are affordable to a larger number of firms.
- Expanded funding for workforce training in computational science to encourage students to pursue related careers, to train faculty, students, and industrial users how to take maximum advantage of computational resources, and to attract new computational research faculty and high-technology businesses to the state.

Ohio's historic investment in the human and physical capital embodied in OSC has positioned the Center in a leadership position for the application of modeling and simulation to foster a thriving employment base and develop a skilled workforce. With additional investments, we envision the Ohio Supercomputer Center as a dynamic technology organization that will serve Ohio and lead the nation in the areas of research, industrial engagement and workforce development, all crucial endeavors for the years ahead.