CASE WESTERN RESERVE UNIVERSITY
University Technology

Interested in learning more about research technology support at Case Western Reserve University? Our professionals are available to meet with you to discuss your needs.

University Technology
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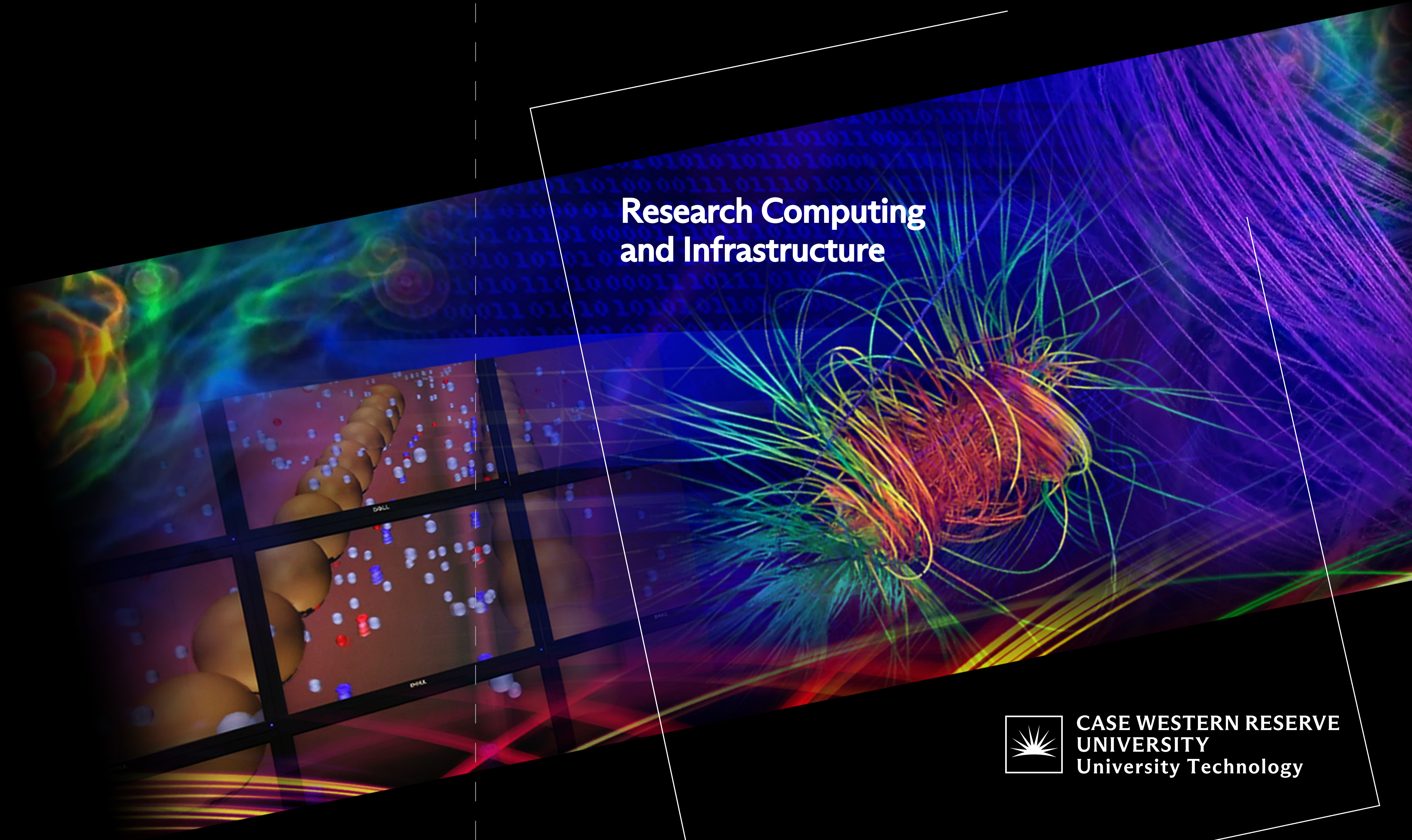

# Research Computing and Infrastructure

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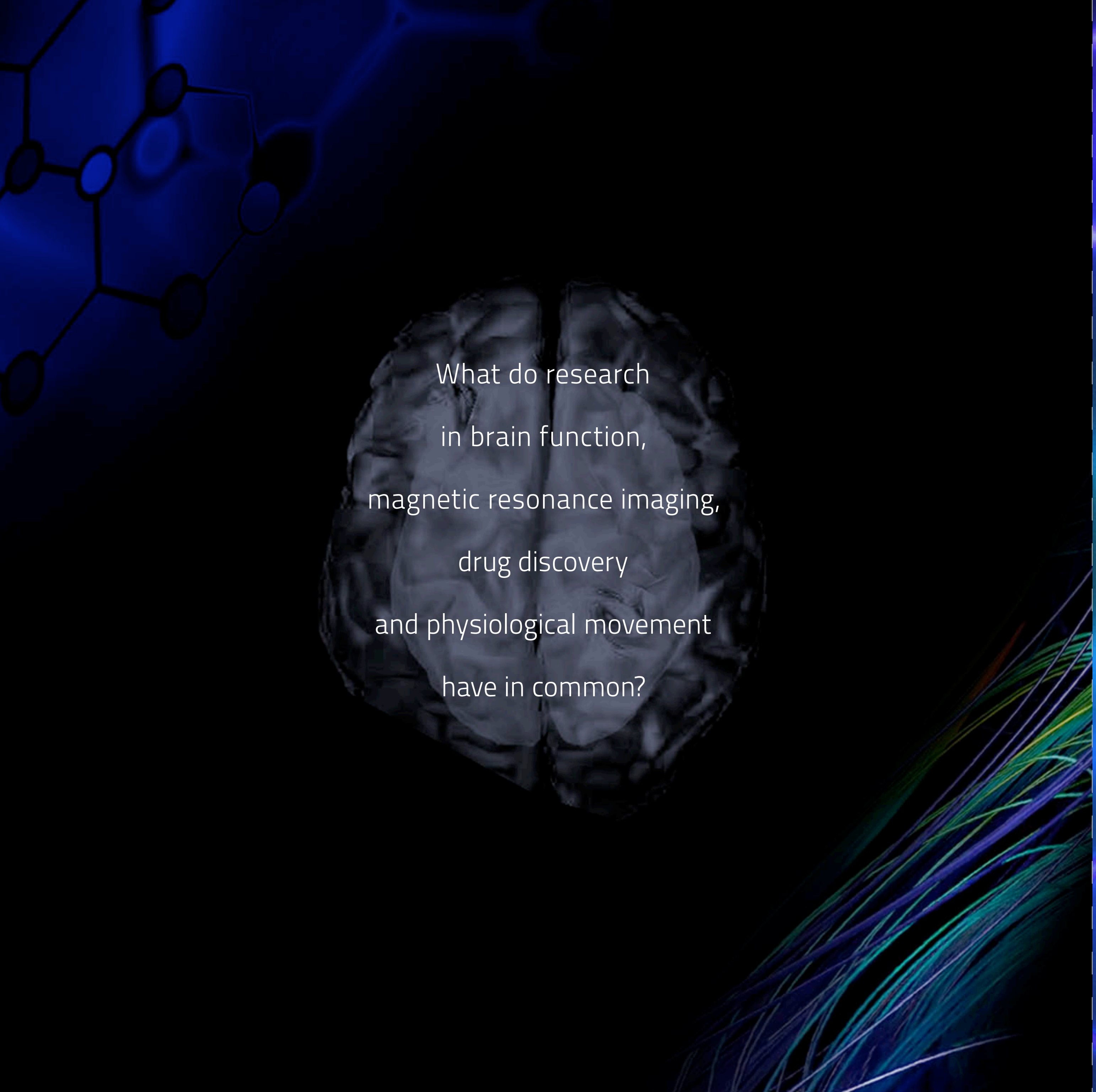



Like other research endeavors in science and engineering, they require significant amounts of computational power. High performance computing (HPC) increasingly is a critical resource for an expanding spectrum of disciplines, since it enables researchers to solve large-scale, data-intensive, advanced computational problems on topics across the disciplinary spectrum faster, more accurately and more efficiently.

A research computing resource comprised of thousands of processors working in parallel; discipline-specific software; visualization tools; multi-tiered, scalable storage; and high-speed networking enables research of this caliber at Case Western Reserve University. The HPC cluster provides immediate, cost-effective access to a supercomputer capable of supporting the work of researchers in all departments, across all disciplines at the university.

In addition to high performance computing, the Research Technologies group provides data visualization and graphics processing; data storage; database creation, management and consultation; a high-speed network; and funding-agency application consultation.

**CWRU's Research Technologies resources have been integral to published studies on:**

- cancer cell growth and mutation
- algorithm development
- chemical bonds
- simulations of protein-protein associations
- topographic studies
- structural calculations
- chemical reactions
- brain rhythms
- fuel cell development
- intracluster light measurement
- organization of protein complexes in 3D
- molecular dynamics simulations

Discover the ways that Information Technology Services supports researchers and frees them to **think beyond the possible.**

# Research Technologies Support

### High Performance Computing

Computationally intensive research is supported through the operation of a scalable high performance computing system based on Dell PowerEdge servers with Intel processors and Red Hat Enterprise Linux. Researchers are encouraged to apply for guest membership in order to explore the cluster's capabilities.

### Research Database Design, Programming and Consultation

Our professional database design and programming services, based upon the Web-based Oracle Application Express (APEX) system, permit researchers to produce sound data management plans and to create secure and effective systems for their research needs. Research Technologies also provides consultation on the creation of data management and sharing plans as required for funding applications to the National Institutes of Health, National Science Foundation and other agencies.

### Data Storage Services

Storage solutions are available to enable researchers to securely store and share data in a collaborative environment. Faculty can purchase multiple terabytes of space, as needed, and can utilize Globus Online, a fast and powerful file transfer service, for moving large files to and from the HPC system.

### Data Visualization and Graphics Processing

Data visualization is transforming how research findings are analyzed and communicated, and provides a powerful new way to gain a better understanding of the complexity of ideas and data through simulations, models, maps and infographics. The Research Technologies team offers consultation on visualization and graphics processing. Additionally, a visualization wall, a large-scale system of multiple liquid crystal displays on a single, expansive wall, can display social science, scientific or engineering data as high-definition computer-generated graphics. Combined with a parallel processor, the visualization wall's 86-million pixels display the complex data patterns and subtleties in information that are necessary for hypothesis formation and scientific research.



### Concierge Services

Value-added services include identifying and helping assemble the full scope of research-computing service requirements, algorithm optimization, grant writing, data-management plan creation and data-management administration. Individualized assistance also is available during office hours.

### High-Speed Network Partnerships

Case Western Reserve has one of the fastest data and voice networks in higher education. The entire campus has access to Internet speeds of up to one gigabit per second. Through a partnership with OARNet, the Ohio Academic Resource Network, researchers can obtain network connectivity access to the Internet2 and National LambdaRail high-speed networks for data exchange rates with other research institutions of up to 100 gigabits per second. CWRU also provides a platform for research of community initiatives through the Case Connection Zone, a one-gigabit network for the University Circle community, which is host to a variety of projects revolving around smart-home technologies; telemedicine; community safety; and science, technology, engineering and mathematics education.

### Award Application Consultation

Many funding agencies require detailed data management and sharing plans during the application review process. Consultation on these services, as well as on research database design, visualization and graphics processing, is available for researchers preparing for the funding application process.

### Advisory Committee

The Research Technologies team offers Information Technology Services on strategic issues in support of the CWRU research community's IT-related needs. For more information, see http://case.edu/its/researchcomputing/advisorycommittee/.

## Additional Technology Support for Researchers

- MediaVision digital technology services to help researchers create a portfolio as a presentation tool to showcase their work and show the value of their research for marketing purposes
  - – Video production to capture interviews and case studies
  - – Digital publishing
  - – Website development and hosting
  - – Animation and motion graphics
  - – Technology training development
  - – Videoconferencing and TelePresence service
  - – Audio-visual event support
  - – Vyvx broadcast fiber services network to transmit live interviews to international media
- Dozens of free software titles through the Software Center, including Qualtrics® online survey software
- Access to collaboration technology, such as Google™ Apps for Education and Adobe® Connect™
- Access to academic technologies, such as Blackboard Learn™ and lecture capture
- Access to advanced learning environments, such as videoconference rooms, the Active Technology Collaboration room and Technology Enhanced Classrooms
- Online storage through Google Drive, offline storage on the Case network, enterprise data protection, server service, and server colocation in one of two datacenters on campus
- Academic technology support from faculty engagement leaders
- Proposal collaboration and pre-award support
- Research administration support
- 24/7/365 technology support through the ITS service desk



## Data Visualization and Processing

The visualization wall is a high-definition display installation for use by Case Western Reserve faculty and their students who are engaged in scholarship and research that require high performance computing and large-scale visual representations of data.

As a science, visualization is the process of representing data in a form that can clearly and effectively communicate its meaning. Most visualizations are computer-generated graphics born from the simulation and modeling of data, which often are 3D. Using visualization, researchers can see both large and small differences across sets of data and discern meaningful relationships. The wall's use is applicable in any discipline where there is a need to identify patterns, singularities and details that otherwise would not be apparent from raw data. Scholars of mathematics, statistics, astronomy, physics, geospatial mapping, art and medical imagery benefit from the ability to visualize data.

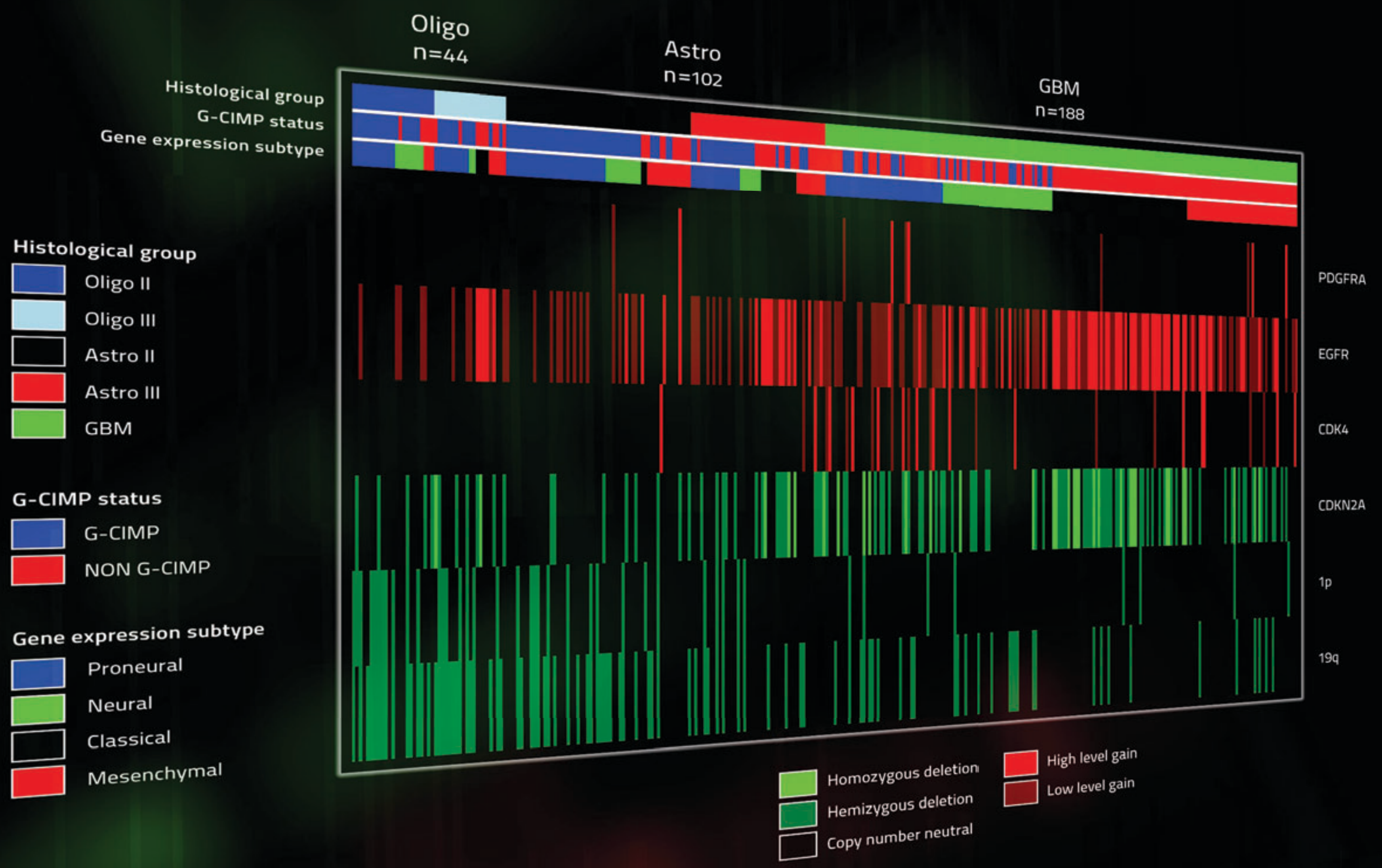
Visualization has been going on at CWRU for many years through the use of the HPC system. The visualization wall adds a new, exciting layer to learning and discovery. With its 630 square inches of display and 86-million pixels, it's bringing complex data patterns and subtleties in information even closer to the eyes of those who will discover them. The wall enables researchers to solve complex problems through the creation, manipulation and envisioning of highly dense and complex images and scientific data.

Visualization goes beyond number crunching. Some examples of research topics that can use visualization include:

- an historian trying to replicate original battlefield conditions to visualize troop configurations, sight lines or lines of attack to be able to consider what the general might have seen on the day of the battle
- a natural scientist who needs to render molecules
- an art historian displaying visual details across multiple works of art or tracing the provenance of different works of art across the centuries
- an archaeologist's reconstruction and analysis of the material remains, including artifacts, inscriptions, monuments, artworks, and human, floral and faunal remains, from an excavation
- an ecologist modeling large-scale climate changes
- a biologist visualizing cell division
- an engineer visualizing the stress point in a beam

"Input from ITS has been critical to us having a federally compliant space within the high performance computing cluster where identifying data on patients can be stored. That is really critical for much of the research that goes on in the Case Comprehensive Cancer Center and, specifically, for my own research in brain tumors."

***Jill Barnholtz-Sloan, Ph.D.***






**Jill Barnholtz-Sloan, Ph.D.**

Associate Professor
Case Comprehensive Cancer Center

The Bioinformatics component for the Case Comprehensive Cancer Center Biostatistics and Bioinformatics Core was envisioned and built by a cross-functional team comprised of individuals from the Case Comprehensive Cancer Center, Case Western Reserve, University Hospitals and the Cleveland Clinic Foundation. As co-director for Bioinformatics for this core, Dr. Barnholtz-Sloan engaged ITS to build the infrastructure, created the work groups that would utilize the data, established a governance framework, implemented institutional reporting, and ensured that security and privacy requirements were followed.

Speaking about her own utilization of the core for her brain tumor projects, Barnholtz-Sloan says, "We'd like to find a biomarker that helps us distinguish between people who live a long time versus people who live a short time after diagnosis with a brain tumor, or a biomarker that helps us distinguish people who will or won't respond to treatment." The ability to store and analyze clinical research data, including patient demographics, survey data, images, pathology data and bio-specimen data, is critical. Continues Barnholtz-Sloan, "The only way we can do that is if we know who these people are. We keep that information so that we can follow them over time."

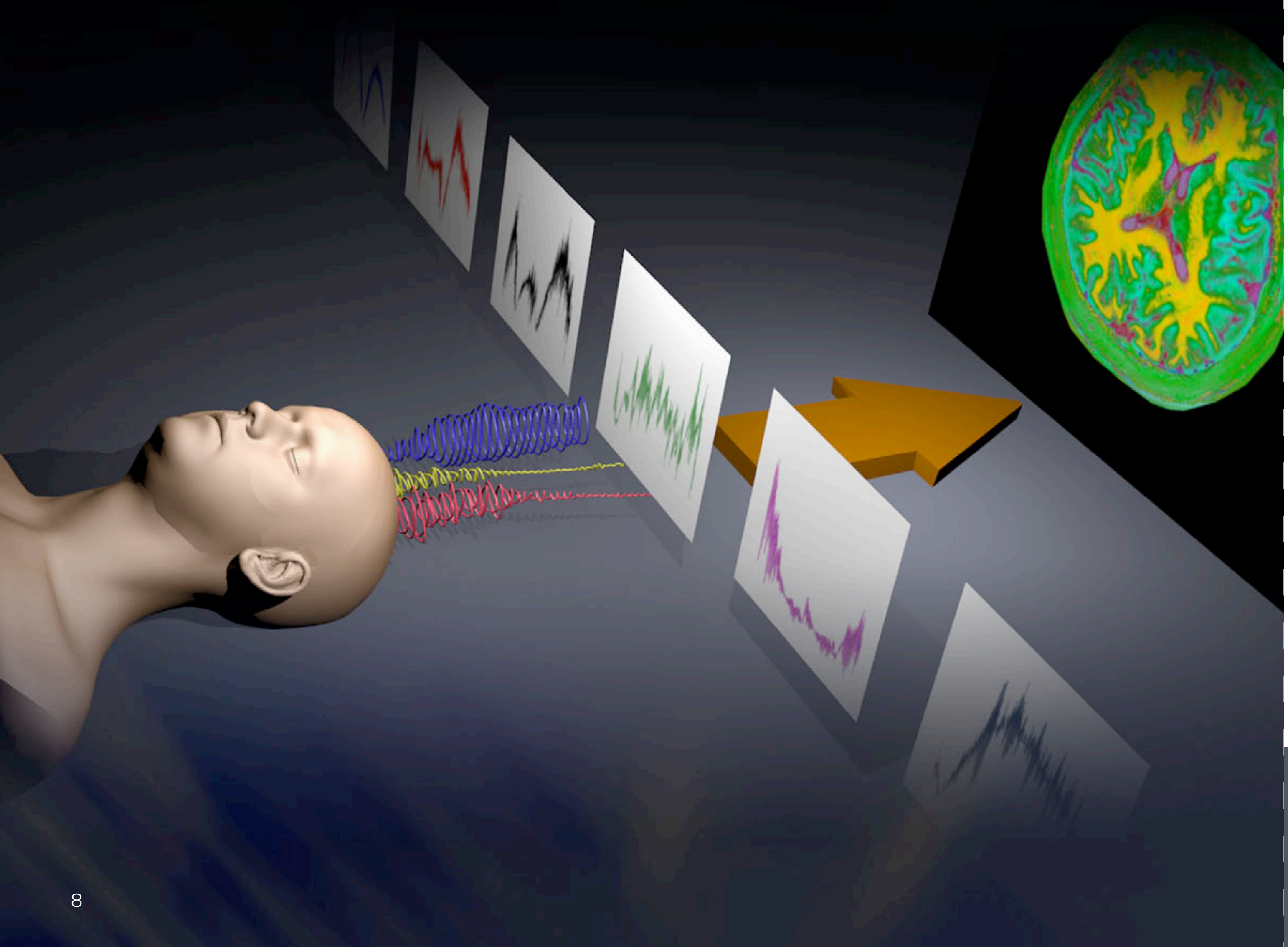
Barnholtz-Sloan's involvement in research advisory and planning committees at Case Western Reserve has made her keenly aware of the need for accessible, secure research storage. She says, "I can't emphasize enough the importance of making high performance computing and storage a priority for the university and having that be an essential piece of its infrastructure that's available to all researchers."

Several research groups utilize the core, including the Barrett's Esophagus Translational Research Network and GI Specialized Program of Research Excellence. "The mission of the Bioinformatics component of this core is to provide expertise in analysis of high throughput data and coordinate and facilitate clinical informatics research support to Cancer Center members," she concludes.

*Jill Barnholtz-Sloan serves as the co-director of the Biostatistics and Bioinfomatics Core Facility at the Case Comprehensive Cancer Center. She received her doctorate from the University of Texas School of Public Health. She is involved in research for the Central Brain Tumor Registry of the United States, the Ohio Brain Tumor Study and the Cancer Genome Atlas Program, among other programs.*

"We are looking to take a current MRI data reconstruction time of five hours and reduce it to 250 milliseconds. This solution fundamentally can change the way we do MRI and fundamentally change the way we do medicine in this country. Thanks to CWRU's high performance computing capabilities, we now can solve computational problems that could, in turn, solve health problems."

***Mark Griswold, Ph.D.***





**Mark Griswold, Ph.D.**

Professor
Radiology

Magnetic Resonance Imaging (MRI) is one of the most powerful clinical tools available today in hospitals. The MRI research team at CWRU, led by Radiology Professor Mark Griswold, is using parallel imaging and a high-speed network to collect MRI data and reconstruct an image in real time – a task that previously could take five hours to accomplish.

To optimize the task of reconstructing MRI data, additional compute and graphical processing unit nodes were installed in the existing HPC system. This gave Griswold's team the ability to perform parallel imaging of MRI data, but they still needed to visualize the data in real time from their lab.

"We are doing experiments where there are needles in a patient's head," describes Griswold. "We can't wait five days for the reconstruction to come back. We need it now, and it needs to be robust; the connection can't break." A dedicated fiber line between the HPC system and the MRI unit created a robust connection that makes data reconstruction time feasible in a clinical setting.

The goal of connecting the MRI to the HPC facility is to collect data and reconstruct it in the same amount of time - an accomplishment that doesn't currently exist. "We have this beast of a machine," says Griswold. "Now we need to show results from it." Griswold and his team are working to reduce MRI data reconstruction time to 250 milliseconds.

*Mark Griswold received his doctorate from the University of Wurzberg in Germany. His research currently addresses the development of software and hardware for fast MRI imaging methods. Griswold has developed many parallel methods since his work in the field first began, including the GRAPPA method. Developing multi-transmitter technology, especially those that utilize on-coil amplifier technology, is an additional focus of his research.*

"The power of the high performance computing system allows us to do analysis we would not have been able to do. With parallel computing, we can do multiple jobs at the same time."

***Robert Kirsch, Ph.D.***




**Robert Kirsch, Ph.D.**
Professor and Interim Chair
Biomedical Engineering

Biomedical Engineering Professor Robert Kirsch and his students use the HPC system to explore the mechanics and control of human movement with the goal of using functional electronic stimulation (FES) to restore motility to people suffering from paralysis and other disabilities. The HPC system is essential to the study of turning thoughts into motion, whereby brain signals from an electrode implanted in a paralyzed person are correlated with the movements of a simulated limb. "Our work requires extensive parameter searches, large-scale optimization problems, artificial neural network training and analysis of massive data sets," explains Kirsch. "We are heavy users of HPC. We wouldn't be able to work without it."

One part of Kirsch's study takes a mathematical approach to identifying the locus of bodily movement. Because current technology cannot extract all of the independent commands produced by the brain to create movement, the HPC system is being used to optimize the data so the minimum number of commands required to create movement can be identified and then replicated. "To find commands is very complicated with many variables," adds Kirsch. "The HPC system optimizes the massive data."

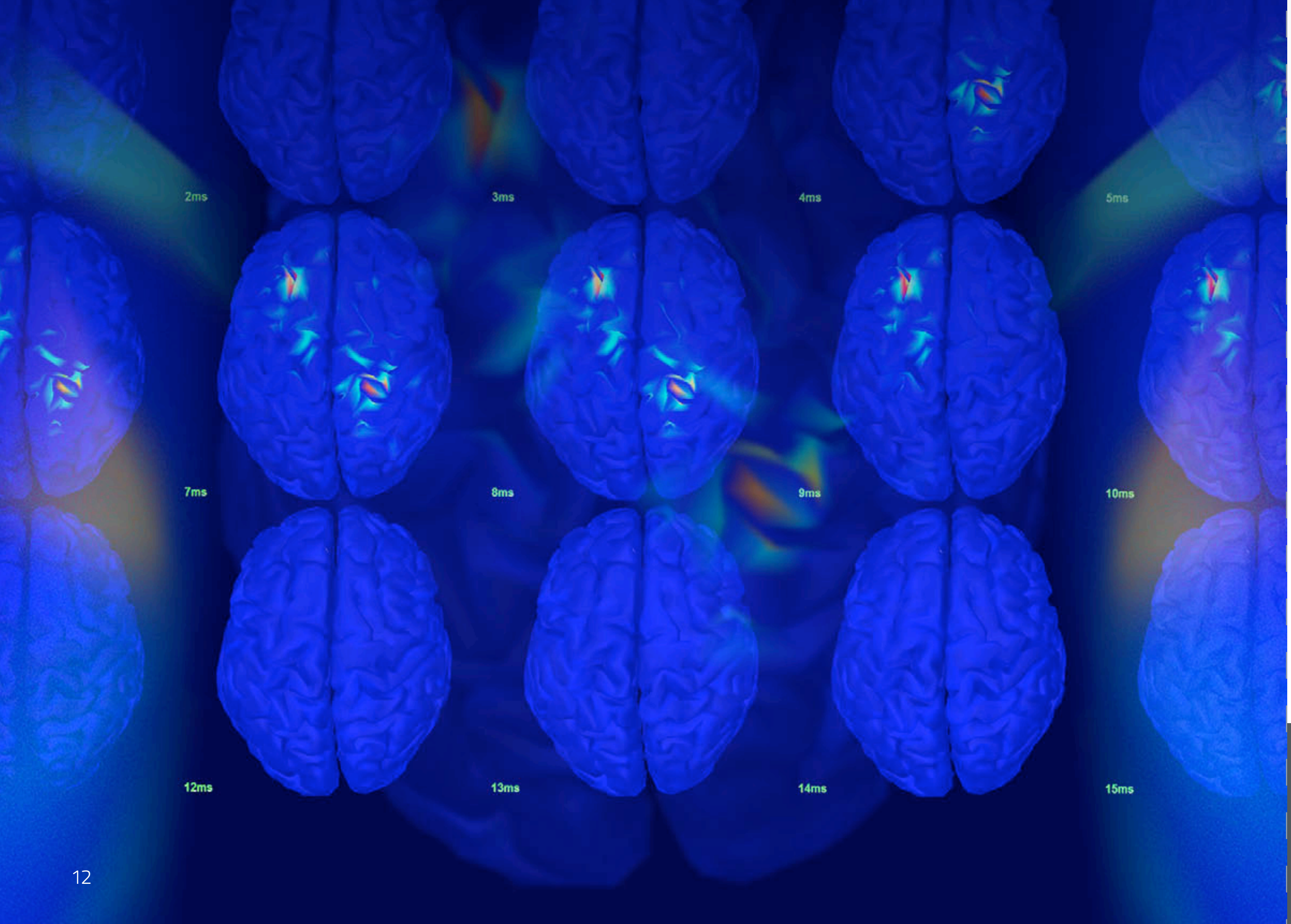
Developing advanced feedback control algorithms for FES arm reanimation requires developing and testing as many as 500 different arm morphologies that involve intense computations. The HPC system revolutionized this project, which allowed the group to test candidate algorithms in an hour – a process that previously took 20 days on a personal computer.

Studies of proprioception, a feedback mechanism for adapting and altering bodily movement, and of artificial neural network controllers for upper limb prostheses also use the HPC system to perform large optimizations and parameter searches.

*Robert Kirsch currently serves as the executive director of the Cleveland FES Center. He received his master's of science and doctorate in biomedical engineering from Northwestern University.*

"High performance computing continues to gain importance in many areas of research, and its role at our institution is becoming more and more pivotal as the university positions itself as one of the leaders in promoting the new vision of energy and health sciences. The Department of Mathematics, Applied Mathematics and Statistics, where high performance computing is well represented, has embraced the vision that HPC will continue to gain popularity and has added new courses addressing the mathematical and algorithmic changes needed to take advantage of computing resources. At present, all graduate and undergraduate students in applied mathematics are expected to be educated in the foundations of HPC when they graduate, and an increasing number of students majoring in technical disciplines populates the courses where such notions are taught."

***Daniela Calvetti, Ph.D.***






**Daniela Calvetti, Ph.D.**
Professor and Chair
Department of Mathematics,
Applied Mathematics and Statistics

Expertise in scientific computing is a significant characteristic of the university's applied mathematics students. Both undergraduate and graduate students are achieving success and recognition in their research and finding continued success in education and employment. A contributing factor was the Mathematics, Applied Mathematics and Statistics Department reshaping its curriculum around HPC. Courses, including parallel scientific computing, linear algebra and applications, computational inverse problems and numerical optimizations, have been expanded with the goal of transforming students into high performance computing experts.

Dr. Calvetti sees HPC as a permanent part of academic life. "I am working on a lot of large problems, which, even with smart algorithm, require a great deal of computing time," she says. "In addition, I am doing a lot of computational statistics, which is, by its own nature, computationally demanding; so, the only way to think about my future research is in terms of HPC."

Currently, researchers are using the HPC system to examine the use of electrical impedance tomography to improve breast tumor classification and to examine focal source localization of nerves and the brain for the control of prostheses and to determine sources of epilepsy.

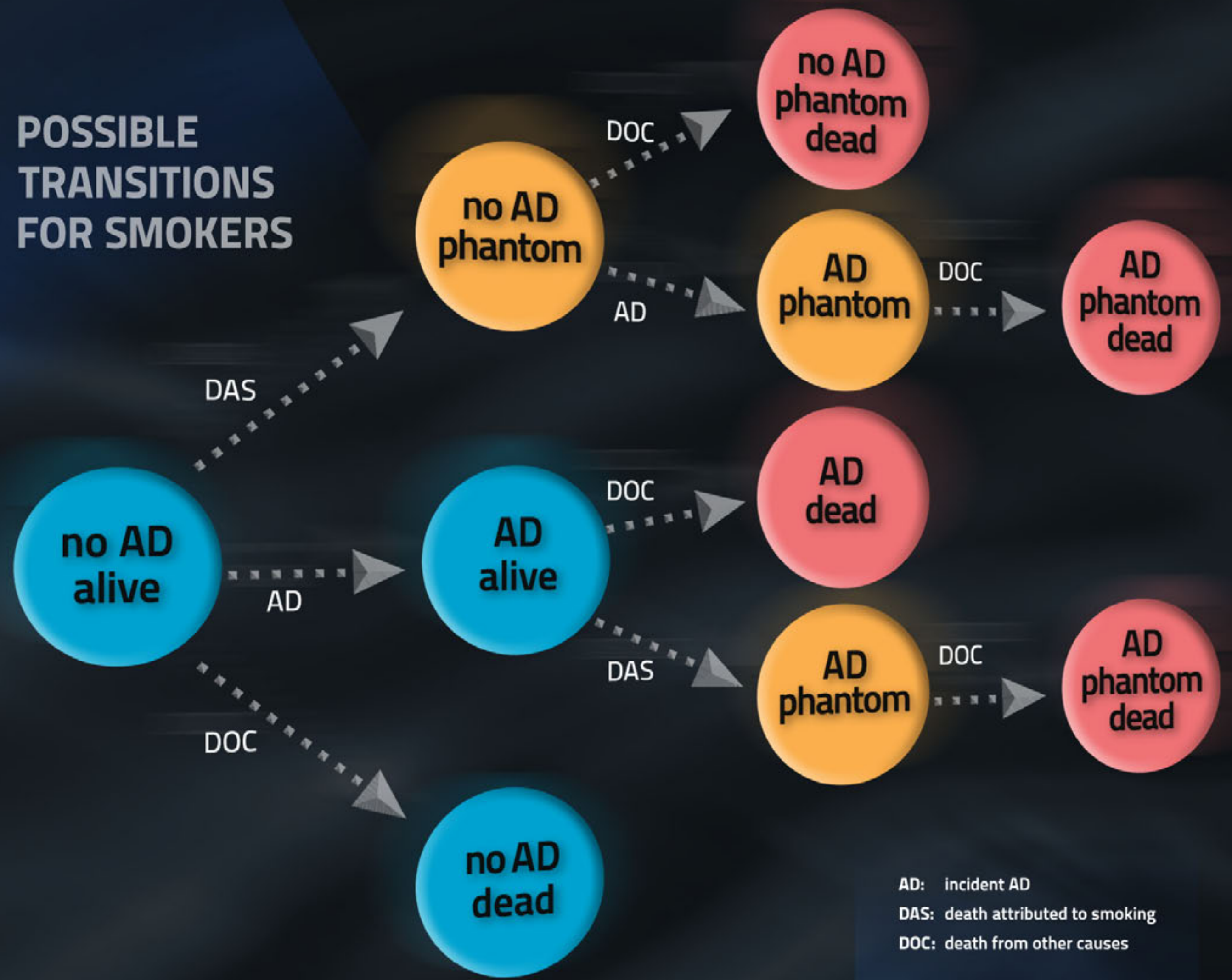
"High performance computing gives us the possibility of testing algorithms on real problems, which would be prohibitive to run on desktop computers, not only from the power element, but the time element, as well," says Calvetti. "Three days of testing with normal resources can be reduced to a few hours with the cluster. And, the support provided by ITS takes away the fear of working with parallel computing and really gives you confidence that it is a powerful, yet approachable, machine."

*Daniela Calvetti earned her doctorate and master's in mathematics from the University of North Carolina at Chapel Hill. Her articles have appeared in numerous journals and publications. She has served on the International Advisory Board on Inverse Problems and has been an associate editor for the SIAM Journal on Matrix Analysis and Applications, the Electronic Transaction on Numerical Analysis, Inverse Problems and Imaging, and Mathematics of Computation.*

"The efforts of the Research Technologies staff in assisting faculty in writing research proposals and contributing to the research itself provide tremendous value to faculty in carrying out the research mission of the university."

*Sara M. Debanne, Ph.D.*

## POSSIBLE TRANSITIONS FOR SMOKERS






**Sara M. Debanne, Ph.D.**
Professor
Epidemiology and Biostatistics

Dr. Sara Debanne, professor of Epidemiology and Biostatistics at the School of Medicine, also holds a secondary appointment as professor of community dentistry at the School of Dental Medicine and is professor plenario (adjunct) in the Departamento de Investigacioǹ, Universidad Belgrano, Buenos Aires, Argentina. She has extensive experience in collaborative research, particularly in the design, conduct and analysis of clinical trials. She is a co-principal investigator on several research projects in the School of Medicine.

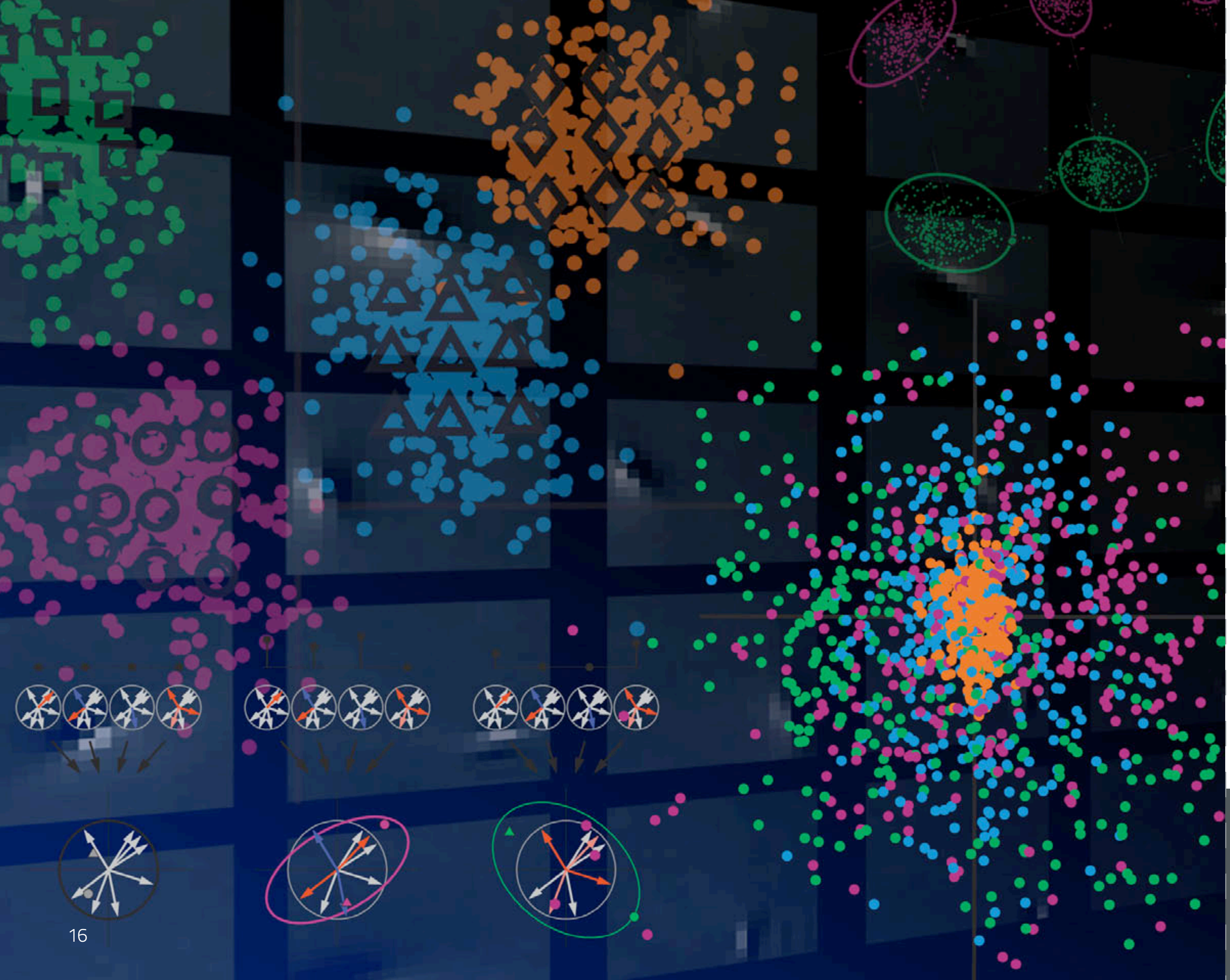
In a recent research effort, Dr. Debanne and her co-investigators used simulation modeling to assess the extent of bias present in cohort studies of the association of Alzheimer disease and smoking due to the competing risk of smoking-related diseases. One co-investigator on the study, who is also a member of the Research Technologies team, designed and programmed the simulation software that was a critical part of the research. More recently, another member of the ITS team, ported that software to the HPC system for improved performance.

She says, "The availability of APEX database subscription services and database design and programming has been critical to the success of several clinical trials on which I have collaborated. The APEX service provided by ITS has been solid with an excellent record of reliability, security and flexibility. The contributions of the Research Technologies team, in both research proposal preparation and in designing data management plans, has been valuable to our success, as have its contributions in working with the research teams throughout the projects. The participation of such experienced professionals has permitted us to focus on research rather than on technology."

*Sara Debanne received her doctorate in mathematics from Case Western Reserve. Her research focuses on the mathematical modeling of disease progression, and she has received grants from the Center for Disease Control and Prevention and the World Health Organization to model epidemiological aspects of tuberculosis and poliomyelitis. She is a sought-after reviewer for the National Institute of Health and has served as an expert witness for the Occupational Safety and Health Administration.*

"Using the cluster saves us tremendous amounts of time. With the faster cycles we can get results in a day. That makes a huge difference. It allows us to run larger simulations, change models, try something different and not wait weeks to see if the simulation works. We can store and collect huge amounts of data and tackle much larger problems."

***Mike Lewicki, Ph.D.***





**Mike Lewicki, Ph.D.**

Associate Professor
Electrical Engineering and Computer Science

How does the human visual system process natural scenes? What computations does the brain perform, and what occurs as we perceive the world around us? Associate Professor Mike Lewicki's team in the Department of Electrical Engineering and Computer Science uses an interdisciplinary approach to attempt to answer these questions by understanding the universal principles of representation, processing, and learning of pattern structure in natural visual and acoustic environments in both biological and machine vision systems.

Using the resources available in the HPC system, the project utilizes computational principles of information processing in the nervous system to form a theory describing what functions the brain solves and if they are being solved in an optimal way. "If we understand what the principles are, we can predict how the brain processes information, and we can build similar devices," says Lewicki.

By developing new classes of models that robustly infer representations of the natural environment, the project has the potential to bring about significant benefits to speech- and hearing-related technologies and fundamental advances in neuroscience, computation and perception. Lewicki also is studying optimal ways to process the natural sound environment. Theoretical models from this research predict the organization and the processing of the peripheral auditory system. The HPC system is being used to search possible biological filters from a database of natural sounds and recreate the adaptive process. Applying the idea of efficient coding, algorithms are created to develop optimal codes for creating theoretically optimal models. The result is that theoretical characteristics and physiological characteristics are almost exact.

*Michael Lewicki holds a doctorate in computation and neural systems from the California Institute of Technology. He was a postdoctoral fellow in the Computational Neurobiology Laboratory at the Salk Institute. In 1999, he joined the faculty of the Computer Science Department at Carnegie Mellon University and the CMU-University of Pittsburgh Center for the Neural Basis of Cognition. He was a fellow at the Institute for Advanced Study in Berlin, Germany, during the 2008-2009 academic year.*

"After years of hardware building for the LUX dark matter search, we are entering a data-rich decade; so, we are excited about partnering with the Research Technologies team for this next chapter in our project."

***Dan Akerib, Ph.D.***

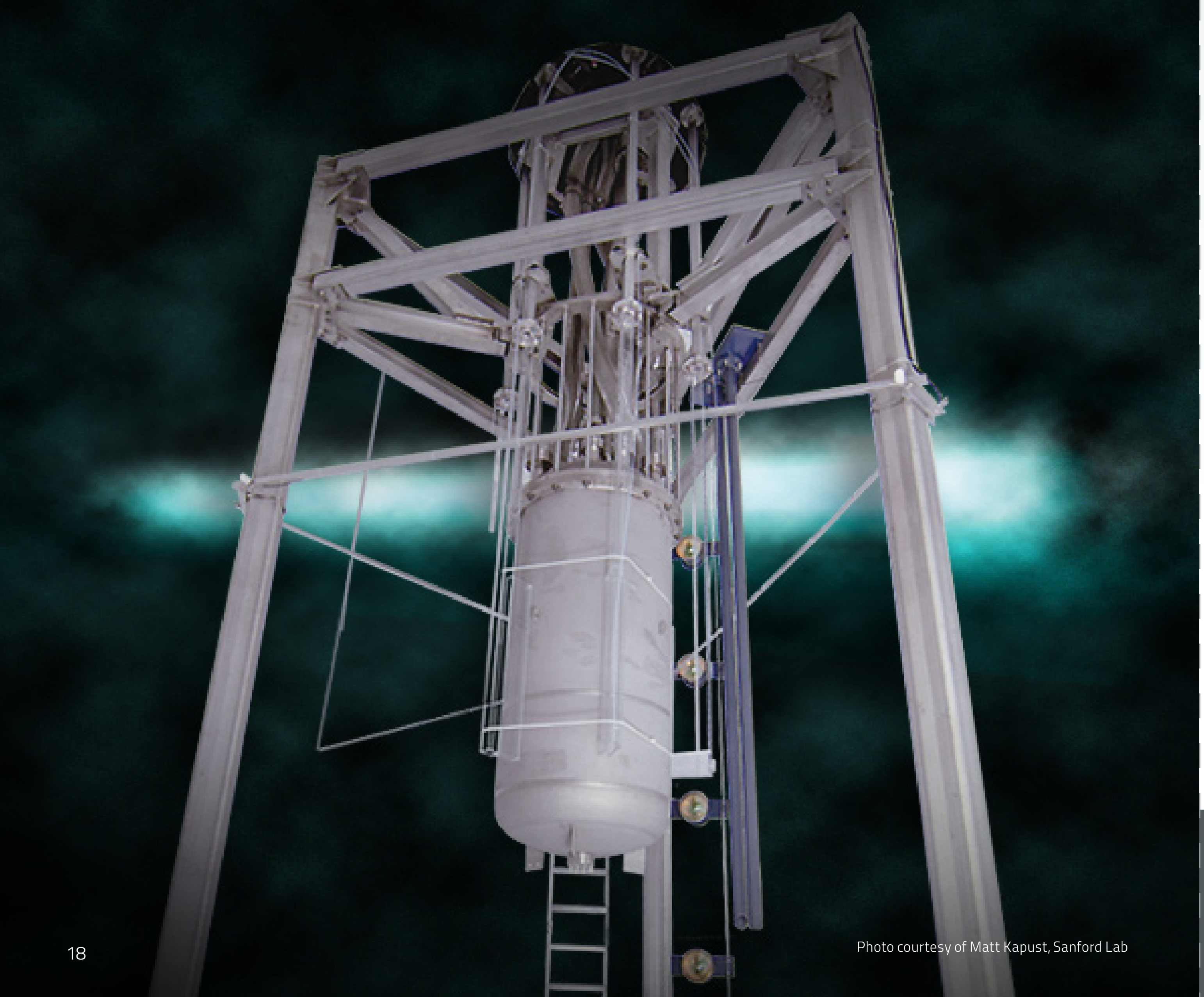


Photo courtesy of Matt Kapust, Sanford Lab



**Dan Akerib, Ph.D.**

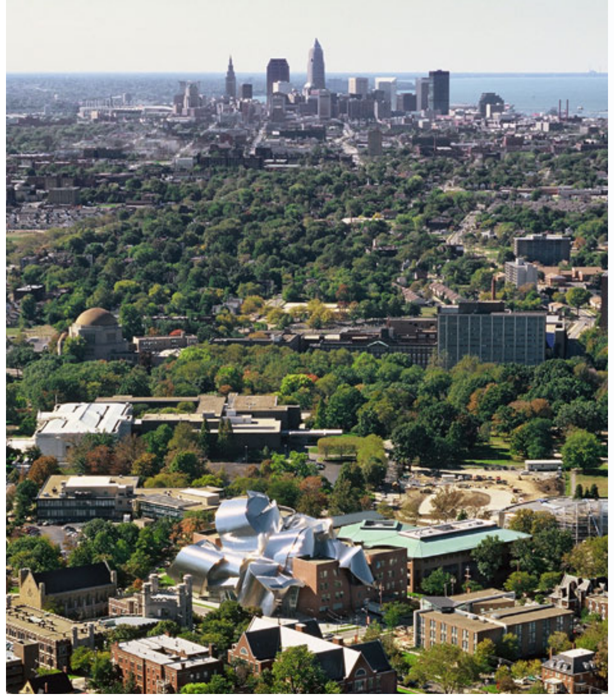
Professor
Physics

Our understanding of gravity hinges on the detection of a substance known as dark matter that we think could make up some 80 percent of the matter in the universe not yet observed in the laboratory. Dark matter is so named because it doesn't emit or absorb light or other electromagnetic waves and goes unseen by telescopes. One hypothesis is that dark matter is made up of weakly interacting massive particles (WIMPs) that were produced moments after the Big Bang. If WIMPs exist, they may be detectable with very sensitive particle detectors.

Dan Akerib has been chasing these particles for 20 years. In 2008, he joined forces with CWRU faculty member Tom Shutt and his group to complete construction of the Large Underground Xenon (LUX) experiment. Their project consists of a 300-kilogram liquid xenon detector that will scintillate or emit brief flashes of UV light should a WIMP collide with a xenon nucleus. To shield the detector from ordinary radiation, it is surrounded by four meters of ultra-pure water in a cavern one mile underground at the former Homestake Mine's Sanford Lab in western South Dakota. In 2012, they moved it into the newly refurbished Davis Cavern, the site of the pioneering solar neutrino detector.

The group carries out a broad range of activities, from detector construction and testing to numerical simulations and long-range R&D. In 2012, it began using the HPC system to process data from its experimental detector. One hundred and twenty two sensitive light detectors, or photomultiplier tubes, continuously view the xenon in the detector and record the brief flashes of light for offline analysis. During the next couple of years, the group will search this rich stream of data–gigabytes per day – for the particular patterns that are characteristic of WIMP interactions and are distinguishable from residual background events. To help with these interpretations and to design follow-up observations, the group also is preparing to use HPC to run simulations of the detector using the GEANT4 open-source physics software developed at The European Organization for Nuclear Research (CERN).

*Dan Akerib received his doctorate in physics from Princeton University. He joined CWRU in 1996 and served as department chair from 2007 to 2010. He was awarded a National Science Foundation CAREER award in 1997. He is a fellow of the American Physical Society and serves as chair for the APS's Primakoff Award. He also serves on the SLAC Particle Physics and Astrophysics Advisory Committee and was a member of the STFC (UK) Dark Matter Oversight Committee, the NRC's Neutrino Facilities Assessment Committee and co-chair of the Dusel Dark Matter Working Group.*



Case Western Reserve University is located in the University Circle neighborhood of Cleveland, Ohio, where it maintains close relationships with world-renowned cultural and medical institutions including the Cleveland Orchestra, Cleveland Museum of Art, the Cleveland Clinic Foundation and University Hospitals Case Medical Center.

Case Western Reserve has eight schools operating within the university: the College of Arts and Sciences, School of Engineering, School of Medicine, Mandel Center for Applied Social Sciences, Frances Payne Bolton School of Nursing, School of Dental Medicine, School of Law and Weatherhead School of Management. Faculty often collaborate and share resources with colleagues across schools, local businesses and partner institutions, including the Case Comprehensive Cancer Center, Seidman Cancer Center and Cleveland Clinic Lerner College of Medicine.

Case Western Reserve receives more than $400 million in external awards each year from the National Institutes of Health, National Science Foundation, NASA, the Department of Defense, and other industries, institutions and agencies. More information on the Case Western Reserve research enterprise can be found at case.edu/stage/research.



"Having local HPC resources has helped our competitiveness for research grants. Being able to say that we have preferential access to computing resources is an advantage over the general access at national facilities. The CWRU HPC resources have helped us significantly in our simulations of the evolution of galaxies and galaxy clusters, a major piece of our research effort. These resources also have given our students hands-on experience in high performance computing and have made them more competitive in today's computationally intensive academic job market."

***Chris Mihos, Ph.D.***

Professor and Chair
Astronomy

"The efforts of ITS to support the research mission of the university are critical to the success of the School of Medicine. The ability to stay in front of this ever-changing environment and to quickly ramp up computational needs has been instrumental as we further expand informatics-based research."

***Pamela B. Davis, M.D, Ph.D.***

Arline and Curtis Garvin Research Professor
Dean and Vice President for Medical Affairs