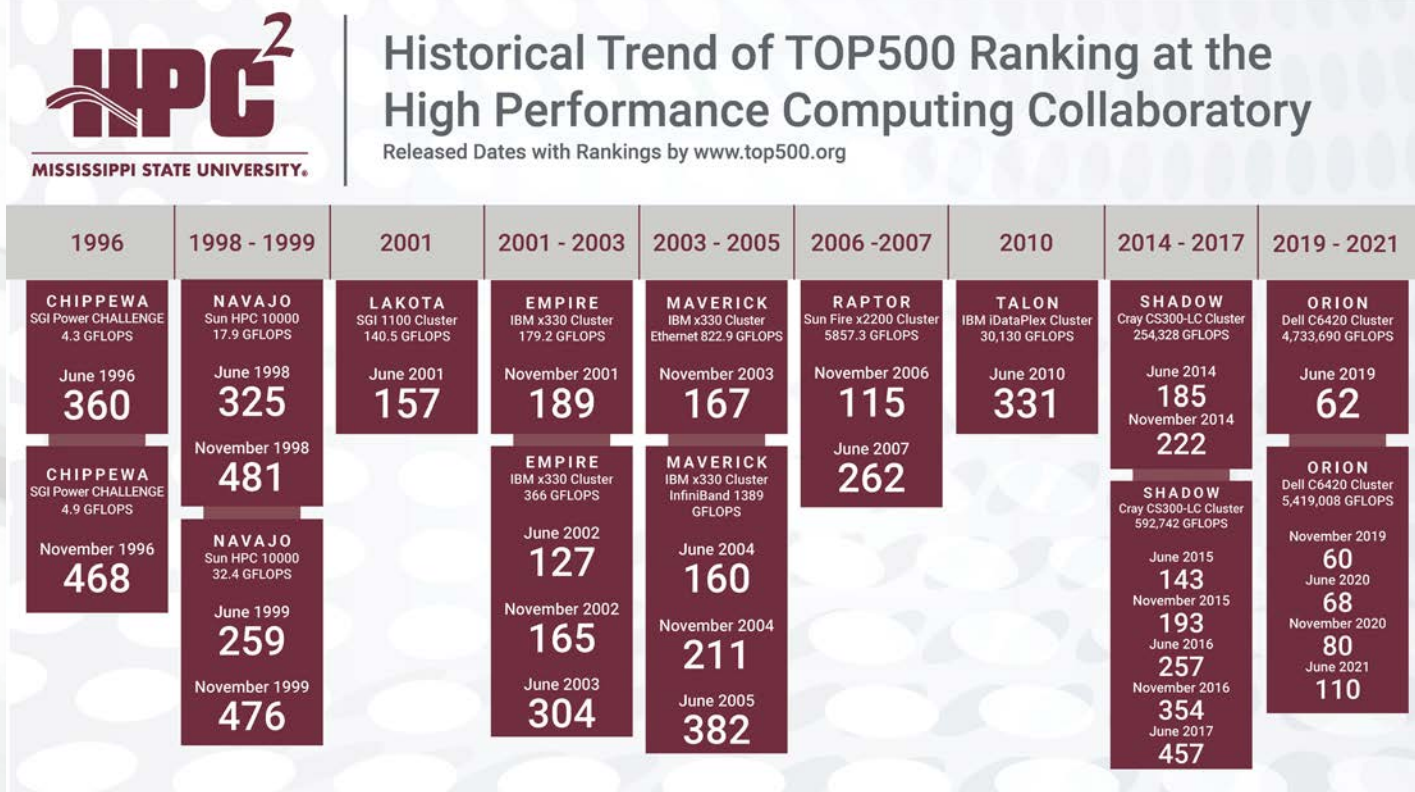HPC²

MISSISSIPPI STATE UNIVERSITY™
HIGH PERFORMANCE
COMPUTING COLLABORATORY

Capabilities Overview

HPC² Overview

The High Performance Computing Collaboratory (HPC²) at Mississippi State University is a coalition of member centers and institutes that share a common core objective of advancing the state-of-the-art in computational science and engineering using high performance computing; a common approach to research that embraces a multi-disciplinary, team-oriented concept; and a commitment to a full partnership between education, research, and service. The mission of the HPC² is to serve the university, state, and nation through excellence in computational science and engineering.

HPC² History

Historical Trend of TOP500 Ranking at the High Performance Computing Collaboratory
Released Dates with Rankings by www.top500.org

MISSISSIPPI STATE UNIVERSITY.

1996	1998 - 1999	2001	2001 - 2003	2003 - 2005	2006 -2007	2010	2014 - 2017	2019 - 2021
CHIPPEWA SGI Power CHALLENGE 4.3 GFLOPS	**NAVAJO** Sun HPC 10000 17.9 GFLOPS	**LAKOTA** SGI 1100 Cluster 140.5 GFLOPS	**EMPIRE** IBM x330 Cluster 179.2 GFLOPS	**MAVERICK** IBM x330 Cluster Ethernet 822.9 GFLOPS	**RAPTOR** Sun Fire x2200 Cluster 5857.3 GFLOPS	**TALON** IBM iDataPlex Cluster 30,130 GFLOPS	**SHADOW** Cray CS300-LC Cluster 254,328 GFLOPS	**ORION** Dell C6420 Cluster 4,733,690 GFLOPS
June 1996 **360**	June 1998 **325**	June 2001 **157**	November 2001 **189**	November 2003 **167**	November 2006 **115**	June 2010 **331**	June 2014 **185** November 2014 **222**	June 2019 **62**
CHIPPEWA SGI Power CHALLENGE 4.9 GFLOPS	November 1998 **481**		EMPIRE IBM x330 Cluster 366 GFLOPS	MAVERICK IBM x330 Cluster InfiniBand 1389 GFLOPS	June 2007 **262**		SHADOW Cray CS300-LC Cluster 592,742 GFLOPS	ORION Dell C6420 Cluster 5,419,008 GFLOPS
November 1996 **468**	NAVAJO Sun HPC 10000 32.4 GFLOPS		June 2002 **127**	June 2004 **160**			June 2015 **143** November 2015 **193** June 2016 **257** November 2016 **354** June 2017 **457**	November 2019 **60** June 2020 **68** November 2020 **80** June 2021 **110**
	June 1999 **259**		November 2002 **165**	November 2004 **211**				
	November 1999 **476**		June 2003 **304**	June 2005 **382**				

The High Performance Computing Collaboratory at Mississippi State University originated as the National Science Foundation Engineering Research Center for Computational Field Simulation, which focused directly on the application of high performance computing for computational field simulation of fluid flow, heat and mass transfer, and structural mechanics for applications to aircraft, spacecraft, ships, automobiles, environmental, ocean, and biological flow problems. Initially funded by the NSF Engineering Research Center Program in 1990 -- one of three funded that year out of 48 proposals - it was the only one with a focus directly on high performance computing. Over the 11-year life cycle as an Engineering Research Center, the MSU center increased its annual funding by an order of magnitude, graduating from the NSF program in 2001, and now continuing as a self-sufficient research unit with funding from a range of federal agencies and industry. As cited by the NSF Director in the January 1999 issue of *ASEE Prism*, the MSU Center was a prime example of a successful NSF Engineering Research Center, noting that it "...effectively demonstrates that you can institute change in a very positive way."

Computing Overview of the HPC²

The HPC² provides an advanced computing infrastructure in support of research and education activities of the collaboratory's member centers and institutes. This infrastructure includes high performance computing systems, high performance storage systems, a large capacity archival system, high-bandwidth networking systems, and an extensive number of traditional desktop workstations. The HPC² operates four primary computational systems: (1) a 5.5 PetaFLOPS cluster with 72,000 Intel Xeon Gold 6148 (Skylake) processor cores, 350 terabytes of RAM, and a Mellanox HDR InfiniBand interconnect; (2) a 914 TeraFLOPS cluster with 11,520 Intel Xeon Platinum 8260 (Cascade Lake)
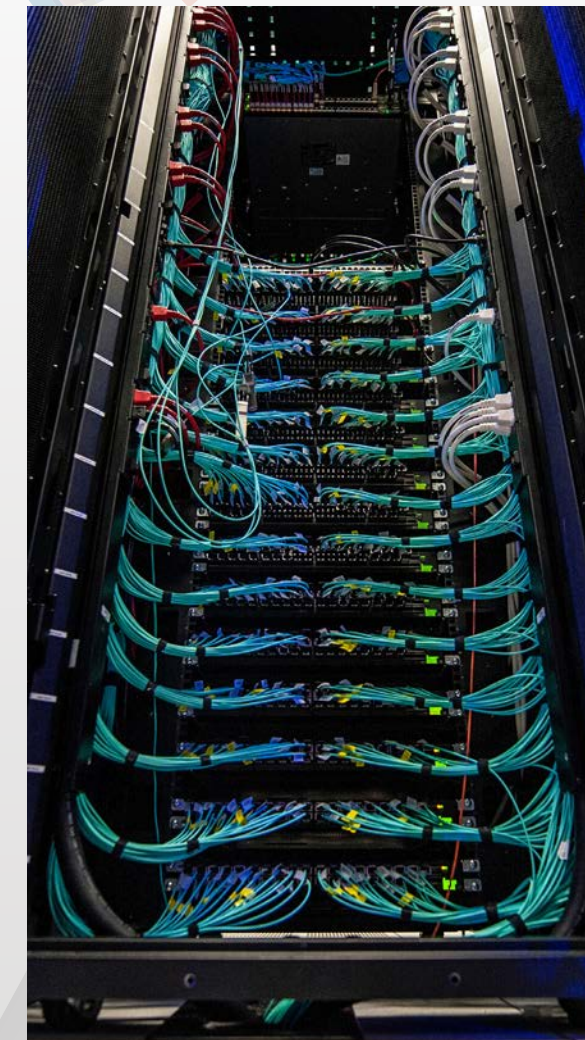

processor cores, 101 terabytes of RAM, and a Mellanox HDR InfiniBand interconnect; (3) a 593 TeraFLOPS cluster with 4800 Intel Xeon E5-2680v2 (Ivy Bridge) processor cores and 28,800 Intel Xeon Phi cores, 72 terabytes of main memory, 4 terabytes of Xeon Phi memory, and a Mellanox FDR InfiniBand interconnect; and (4) a 138 TeraFLOPS cluster with 12,800 Intel Xeon E5-2680 (Sandy Bridge) processor cores, 26 terabytes of RAM, and a Mellanox FDR InfiniBand interconnect. Data storage capabilities include 45 petabytes of high performance RAID-enabled disk systems, including a large parallel file system, and a 31 petabyte near-line storage/archival system.

Networking at the HPC²

The HPC² networking infrastructure backbone consists primarily of 100-Gigabit and 40-Gigabit Ethernet networks interconnecting the organization's primary computing and storage systems, as well as an extensive number of high performance edge switches providing connectivity to the organization's more-than 500 high-end desktops and laptops. This network infrastructure supports full redundancy at the core and allows for aggregated connections to support high-bandwidth activities. Each of the three HPC² facilities obtains wide area (external) network connectivity to the commodity Internet and Internet2 through geographically diverse paths to the Mississippi Optical Network (MissiON), a regional optical network supporting research activities within the state. The two MissiON network connections provide for high-availability and fault tolerant communication channels to the Internet2 connector site in Jackson, Mississippi which supports a potential capacity of more than 8 terabits per second. The HPCC and CAVS buildings are connected via dual 100 Gigabit/sec circuits; the STC facility is connected via dual 10 Gigabit/sec circuits. Additionally, the MissiON network peers with the Defense Research and Engineering Network (DREN) via a dedicated connection at the USACE Engineer Research and Development Center in Vicksburg, MS. These robust wide area network connections give the HPC² researchers the ability to share large sets of data with collaborators across the country and around the globe.
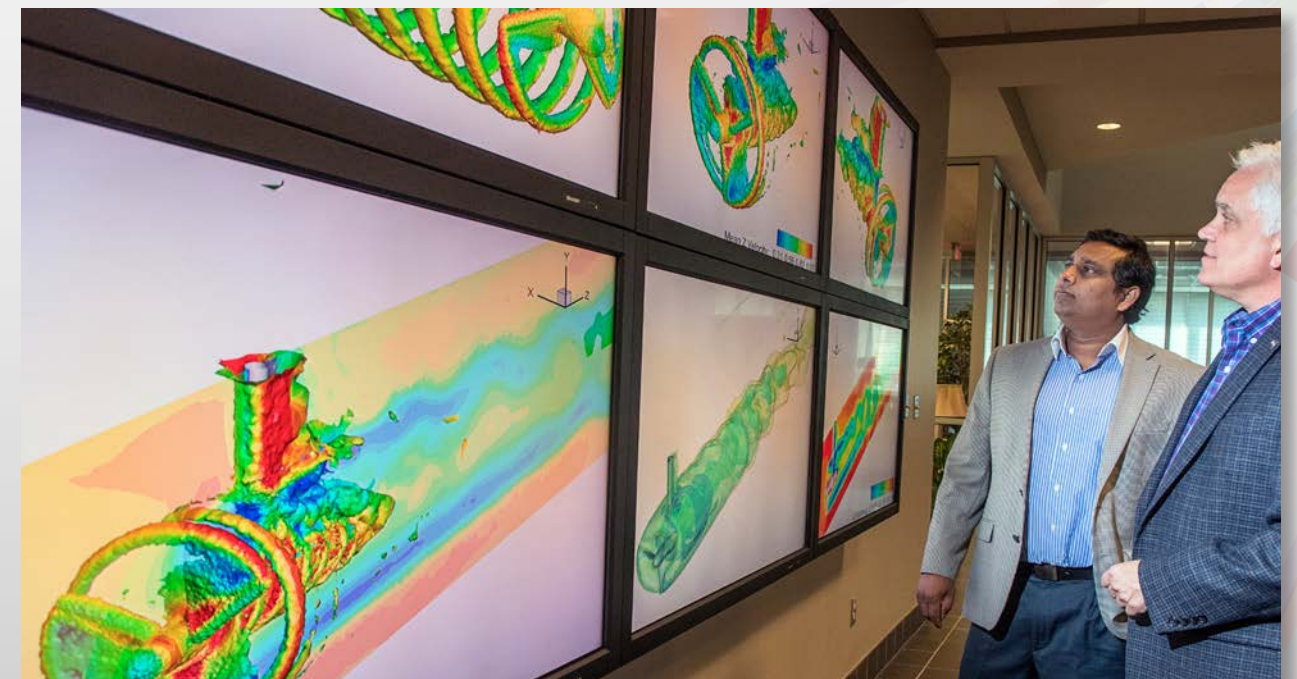
Facilities of the HPC²

The High Performance Computing Collaboratory, an evolution of the MSU NSF Engineering Research Center for Computational Field Simulation at Mississippi State University, is a coalition of member centers and institutes that share a common core objective of advancing the state-of-the-art in computational science and engineering through the utilization of high performance computing; a common approach to research that embraces a multi-disciplinary, team-oriented concept; and a commitment to a full partnership between education, research, and service. The HPC² member units are the Alliance for System Safety of Unmanned Aerial Systems through Research Excellence; the Institute for Computational Research in Engineering Science that oversees the Center for Advanced Vehicular Systems, the Institute for Imaging and Analytical Technologies located at Mississippi State, the Center for Advanced Vehicular Systems Extension located in Canton, Mississippi, and the Institute for Systems Engineering in Research located in Vicksburg, Mississippi; the Center for Cyber Innovation; the Center for Computational Sciences; the Geosystems Research Institute; the Institute for Genomics, Biocomputing & Biotechnology; and the Northern Gulf Institute.

The HPC² facilities include two buildings, the Portera High Performance Computing Center and CAVS buildings, within the Thad Cochran Research, Technology, and Economic Development Park, adjacent to the Mississippi State University campus in Starkville, Mississippi, the CAVS-E building in Canton, Mississippi, and the Science and Technology Center building at the NASA John C. Stennis Space Center (SSC) near Bay St. Louis, Mississippi. The Portera HPCC is a 71,000 square foot facility designed in an open manner to facilitate multi-disciplinary interactions and houses the organization's primary data center. The CAVS building is a 57,000 square foot facility consisting of numerous office suites, experimental laboratories housing an extensive array of equipment in support of materials, advanced power systems, and human factors research activities, as well as a small data center. The Science and Technology Center building at the NASA SSC is a 38,000 square foot facility consisting of office space, classroom space, and a data center.

The CAVS-E building located in Canton, Mississippi was built to serve as a facility where business leaders, government officials, educators, and other professionals can gather to plan or train. CAVS-E has state-of-the-art telecommunication capabilities, video conference meeting rooms, manufacturing and quality laboratories, as well as computer class rooms. The Science and Technology Center building at the NASA SSC is a 38,000 square foot facility consisting of office space, classroom space, and a data center.

To honor Mississippi State University's 16th president and his emphasis on computer research, institution leaders named the HPC building the Malcolm A. Portera High Performance Computing Center.

During the West Point native's tenure from 1998 through 2001, Portera continually advocated for the National Science Foundation's Engineering Research Center for Computational Field Simulation on campus. Eventually, the research unit evolved to become the High Performance Computing Collaboratory; a coalition of independent, multi-disciplinary research units focused on the application of high performance computing. The core operations of the Collaboratory are based in the facility, the Malcolm A. Portera High Performance Computing Center, named for the veteran administrator at the dedication in the Thad Cochran Research, Technology and Economic Development Park.

As a result of Portera's work, enrollment increased as MSU's research and development capabilities expanded, and key aerospace and automotive development activities have contributed to billions of dollars in capital investment in Mississippi and Alabama.

The center has become central to MSU's research enterprises.

Exploration Command Center

Thanks to a long-standing partnership between Mississippi State University and the National Oceanic and Atmospheric Administration, the new Science and Technology Center at the NASA Stennis Space Center is home to the world's seventh NOAA Exploration Command Center (ECC). A state-of-the-art communication hub, it enables research scientists at sea and colleagues on shore to simultaneously view live video streams of the undersea life, sunken treasures, and changing geology. MSU's High Performance Computing Collaboratory provides the computing infrastructure and technical support for the effort.

The ECC enables scientists aboard vessels to be in constant contact with others on shore through a combination of high-definition cameras and remotely operated underwater vehicles. The network includes an Internet-enabled intercom system for voice communication as the ship's remotely operated vehicles send a continuous stream of live video and data.
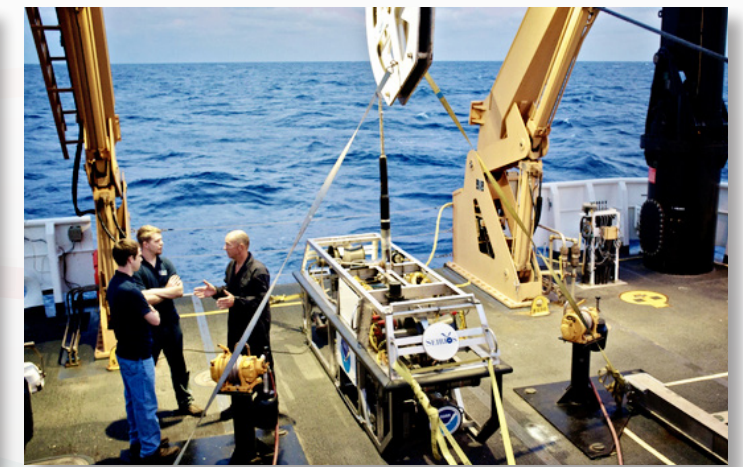
Current Centers and Institutes

The High Performance Computing Collaboratory's member centers and institutes are focused on multidisciplinary, team-oriented research activities for the application and advancement of computational science and engineering. This effort spans a wide range of application disciplines, including fluid dynamics, structural mechanics, materials modeling, astrophysics, molecular modeling, transportation modeling and planning, cyber security, weather and ocean modeling, geographic information systems, genomics, and bioinformatics. Additionally, several of these member units have extensive physical and experimental modeling and analysis capabilities to complement their computational efforts.

Mississippi State University's ASSURE is the Federal Aviation Administration's Center of Excellence for UAS research. The COE's vision is to help UAS grow into its multibillion dollar market potential by conducting research that quickly, safely and effectively gets UAS flying alongside manned aircraft around the world. Twenty-five of the world's leading research universities and over a hundred leading industry, government partners comprise the Alliance for System Safety of UAS through Research Excellence, or ASSURE.

ASSURE possesses the expertise, infrastructure and outstanding track record of success that the FAA Center of Excellence for Unmanned Aircraft Systems demands.
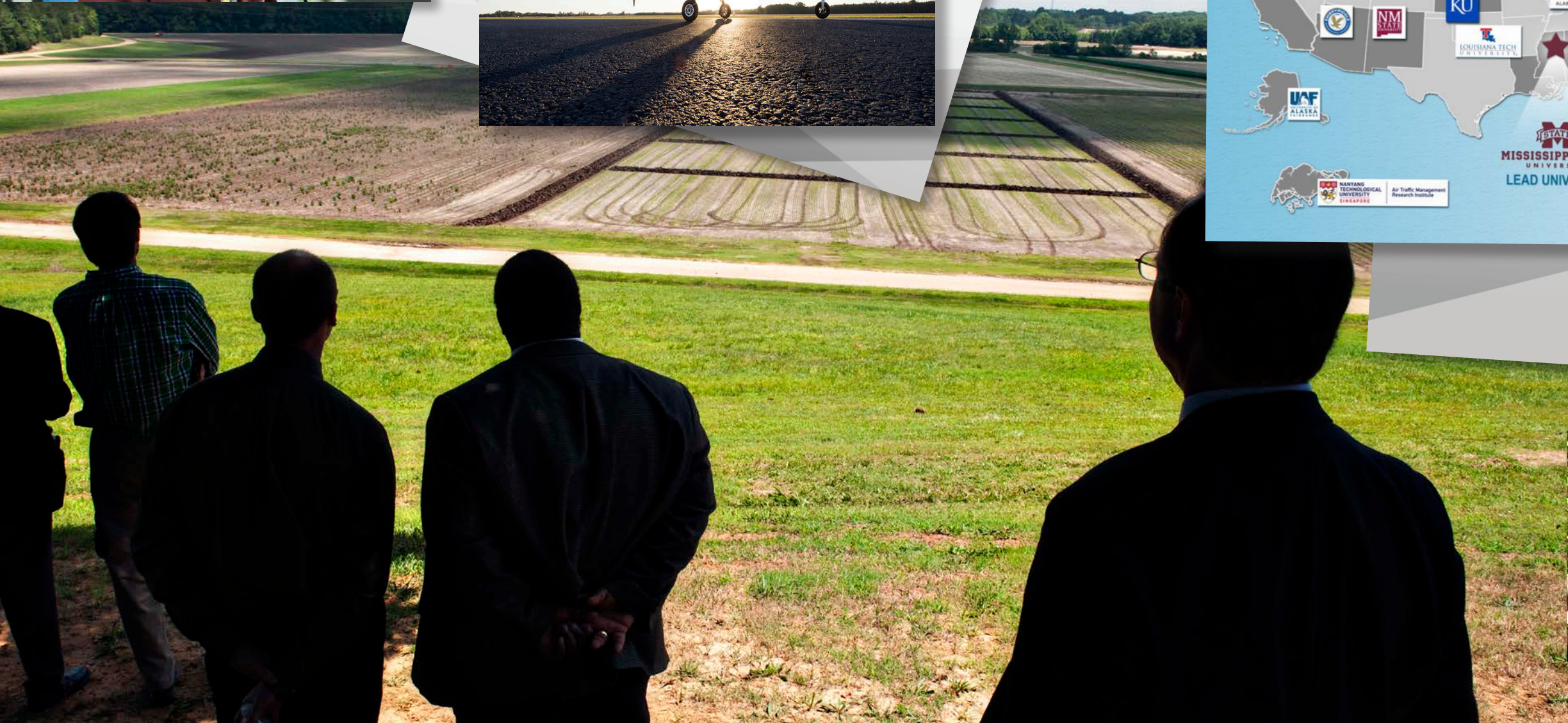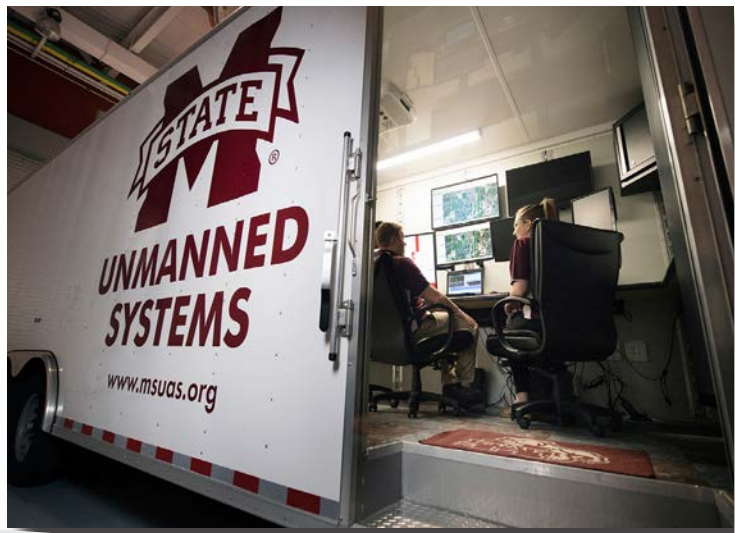
The Institute for Computational Research in Engineering and Science
www.icres.msstate.edu

ICRES

CAVS · CAVS-E · ISER · I2AT

The Institute for Computational Research in Engineering and Science (ICRES) strives to be a world-class center of excellence for research, technology and education equipped to address engineering challenges facing the nation's industrial base. Utilizing high performance computational resources and state-of-the-art analytical tools for modeling, simulation, and experimentation, ICRES will provide a distinctive, interdisciplinary environment that will support economic development and outreach activities throughout the State of Mississippi and beyond.

The institute is composed of four MSU research/economic development centers - Center for Advanced Vehicular Systems (CAVS) in Starkville; Center for Advanced Vehicular Systems Extension (CAVS-E) in Canton, the Institute for Systems Engineering Research (ISER) in Vicksburg, and the Institute for Imaging and Analytical Technologies (I2AT) in Starkville, Mississippi.

CAVS -The Center for Advanced Vehicular Systems mission is to research and develop manufacturing and design means and methods for producing vehicles of superior quality with advanced features and functions at preferable costs, focusing on computational tools and exploiting the underlying technologies for broader industrial use. CAVS research and development activities are based on: industrial needs and priorities; opportunities for providing added value; and building on the state's investment by securing external funding related to broadening the reach of technologies.

CAVS has developed a global reputation for interdisciplinary education and research to expand and enhance the design, technology, production and infrastructure necessary for sustainable mobility. At HPC^2, CAVS researchers have access to one of the world's most advanced supercomputers.
www.cavs.msstate.edu
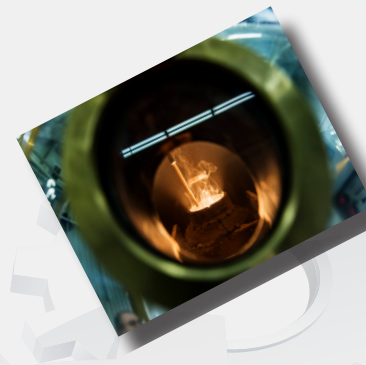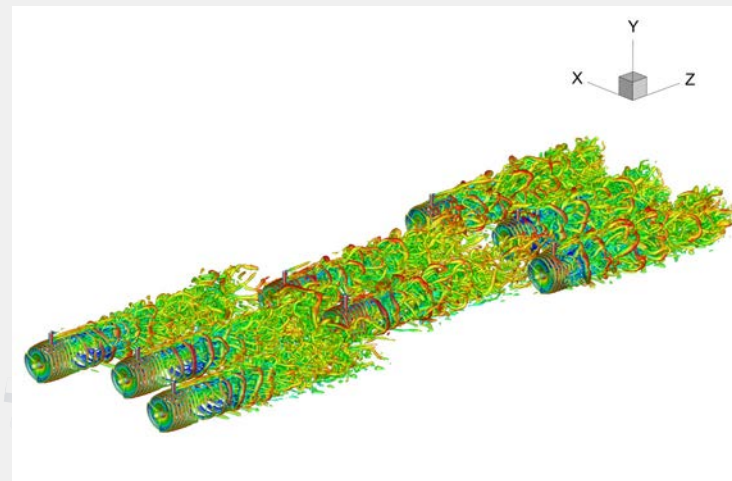
CAVS-E - The CAVS Extension Center in Canton, Mississippi provides direct engineering support for Nissan and its major suppliers; engineering extension work for Mississippi's manufacturers; workforce development, education, and training; and business systems and information technologies.

www.cavse.msstate.edu

ISER - The Institute for Systems Engineering Research is a collaborative effort between the U.S. Army Engineer Research and Development Center and Mississippi State University. The goal of ISER's efforts and products is to mitigate risk, reduce cost and improve efficiency in Department of Defense (DoD) acquisition programs, serve as an additional asset for the state's industrial base for systems engineering related tasks, and create an environment that draws DoD and civilian industry development to the state of Mississippi. www.iser.msstate.edu

I2AT - The institute for Imagingand Analytical Technologies supports research and outreach activities to develop partnerships with local, regional and national industries. Through collaborative interaction with other institutions and industry affiliates, I2AT leverages state of the art technologies and expertise in a way that is mutually benefical for all parties. The technological resources and expertise serves R&D, quality assurance and quality control needs facing many life-science, engineering and industrial operations.

www.i2at.msstate.edu

CCI develops cutting-edge solutions for Defense, Homeland Security and the Intelligence Community. The primary focus of CCI is to research, prototype and deliver cutting-edge cyber solutions that support global national security, homeland security and peacekeeping operations. CCI capitalizes on Mississippi State's world class strengths in unmanned aerial systems, advanced composites, vehicular engineering, motion imagery analysis and hyperspectral imaging processing to provide top notch solutions to our warfighters and their industry partners.

Located at one of the few universities in the country with every academic accreditation awarded by the National Security Agency, CCI can deliver secure cyber solutions for both offensive and defensive cyber operations.

CCI is supported by one of the fastest high performance computers in the country, and is committed to providing world-class cyber analysis and engineering services and solutions. The ability to test concepts and validate through demonstrations leveraging Test and Evaluation capabilities is critical to CCI's success.

The T&E capabilities support Title 10 Acquisition, Service Operational Test Agencies (OTA), Combatant Commands (COCOM), Non-Title 10 Acquisition, DOD Staff Agencies, Intelligence Community, FAA, NASA, DHS and etc. MSU's Secure Compartmented Intelligence Facility will soon be operational, allowing the CCI to work collateral and special compartmented intelligence solutions for government and industry.

CCI develops cutting-edge solutions for Defense, Homeland Security and the Intelligence Community.
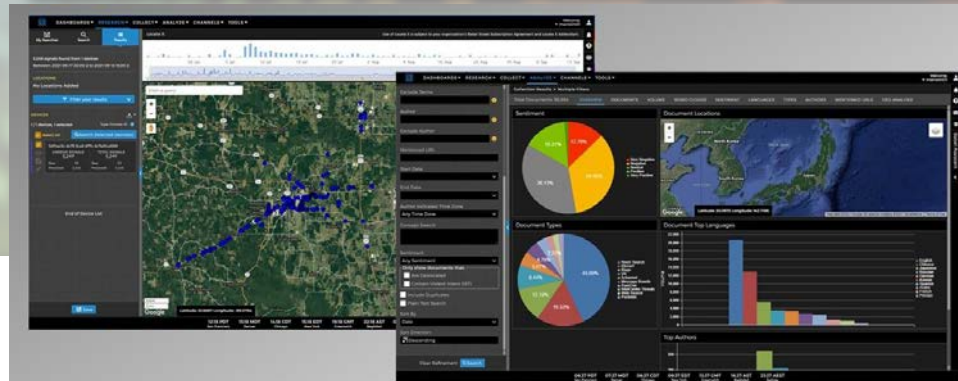
MSU's MOSES is developing collection and analysis methods to use publicly available information to improve safety, security and prosperity. Simultaneously MSU is studying the legal, policy and ethical issues associated with the use of publicly available information.
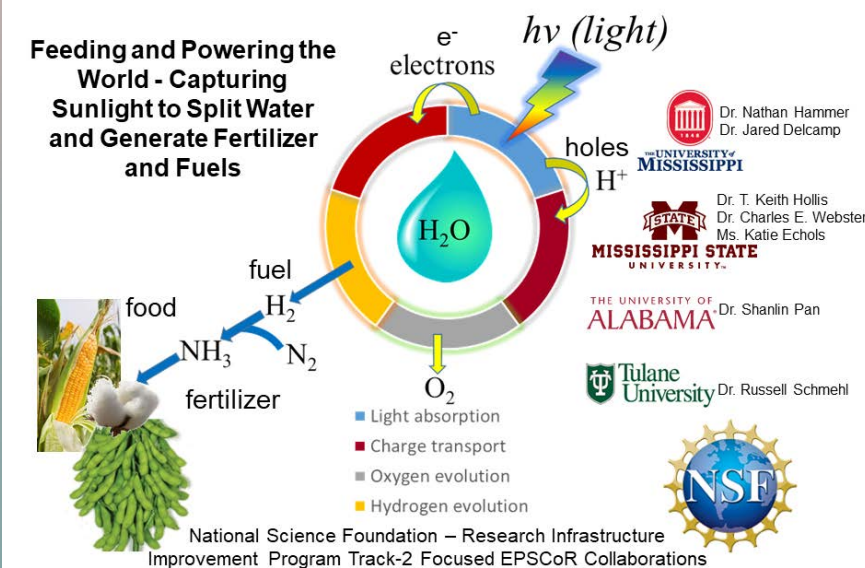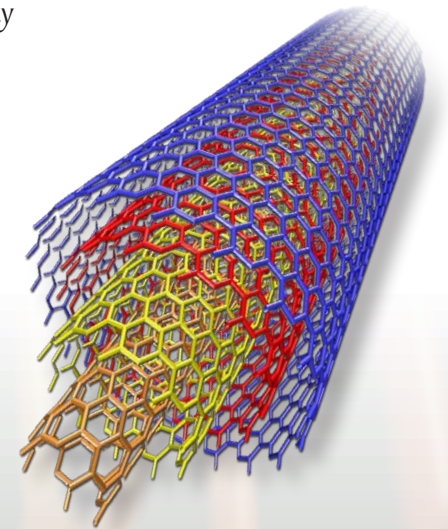

A university alliance with cyber readiness company Circadence Corporation is customizing an existing MSU-designed Netmapper computer program to develop next-generation cyber learning and training software that can scan and map the military's complex computer network infrastructures. This innovative replication of network infrastructures on virtual cyber ranges creates events for training information technology personnel, giving them the skills and defense mechanisms they need in warding off complex attack vectors.

The Center for Computational Sciences (CCS) at Mississippi State University (MSU) is a College of Arts and Sciences center with a mission to foster interdisciplinary research in both the fundamental understanding of and application of all the natural sciences by modeling and developing integrated computational environments and crosscutting tools that allow a comprehensive, cross-disciplinary approach to problem-solving.

The major research activities/initiatives of CCS include: (1) an NSF funded project "Feeding and Powering the World - Capturing Sunlight to Split Water and Generate Fertilizer and Fuels" (2) a DOD funded project "QuAnCo applied to Boltzmann Machines"; (3) a DOE funded project "Nuclei in a relativistic framework: at and beyond density functional theory"; (4) An NSF funded project "Theory and simulations of unconventional superconductors"; (5) NRF funded project "First-principles design of functional electrides using a highly efficient computational platform."

The CCS contributes to the state of Mississippi in numerous ways. Its programs generate a better educated populace and a better-trained workforce by educating students at both the undergraduate and graduate levels in interdisciplinary research, providing them with strong skills in computers, modeling, and the application of the scientific method. These skills are required in a multitude of varied industries and businesses. The CCS introduces MSU scientists from diverse fields to different research and new methodologies. This uniquely positions our scientists to fashion multidisciplinary proposals. Such multidisciplinary approaches to problem-solving are often requirements in requests for proposals from federal agencies and industries. CCS thus creates new opportunities for leveraging resources within MSU as well as drawing resources to MSU.

Feeding and Powering the World - Capturing Sunlight to Split Water and Generate Fertilizer and Fuels

hv (light)

e^- electrons

holes
H^+

H_2O

fuel H_2

food

NH_3 N_2

fertilizer

O_2

- Light absorption
- Charge transport
- Oxygen evolution
- Hydrogen evolution

Dr. Nathan Hammer
Dr. Jared Delcamp
THE UNIVERSITY OF MISSISSIPPI

Dr. T. Keith Hollis
Dr. Charles E. Webster
Ms. Katie Echols
MISSISSIPPI STATE UNIVERSITY

THE UNIVERSITY OF ALABAMA — Dr. Shanlin Pan

Tulane University — Dr. Russell Schmehl

NSF

National Science Foundation – Research Infrastructure Improvement Program Track-2 Focused EPSCoR Collaborations

Geosystems Research Institute
www.gri.msstate.edu

The Geosystems Research Institute (GRI) and the Northern Gulf Institute (NGI) are sister organizations. The NGI was established as a NOAA cooperative institute by GRI. Both entities function independently, but work closely together to capitalize as appropriate

on the unique strengths of each. GRI supports MSU's land-grant mission of Research, Learning, and Service by acquiring and disseminating knowledge about earth and its systems, integrating geosciences and engineering, translating geospatial technologies and skills into useful tools, and transitioning science and technology into practice to support our stakeholders and improve policy and public awareness.

GRI has distinctive competencies in agricultural and natural resource systems, coastal and ocean processes, sensor design, systems engineering, remotely sensed data verification and validation, large scale data and information handling, modeling, and visualization.

GRI has developed nationally recognized research strengths with strong relationships and inherent respect from state, regional and national agencies and business entities. Application disciplines encompass typical departmental subject areas – plant pathology, biology, engineering, geosciences, wildlife conservation, etc. GIS and remote sensing include phenomenology, platforms, sensors, and remotely sensed data verification and validation, which are essential to providing unique capabilities and improve competitiveness.

GRI has developed unique geosystem data streams and modeling capabilities that have responded to sponsor needs, inter-disciplinary perspectives, and systems engineering principles, using advanced geospatial knowledge, observational data, information technology, and modeling utilizing high-end visualization and high performance computing.

The Northern Gulf Institute
www.ngi.msstate.edu
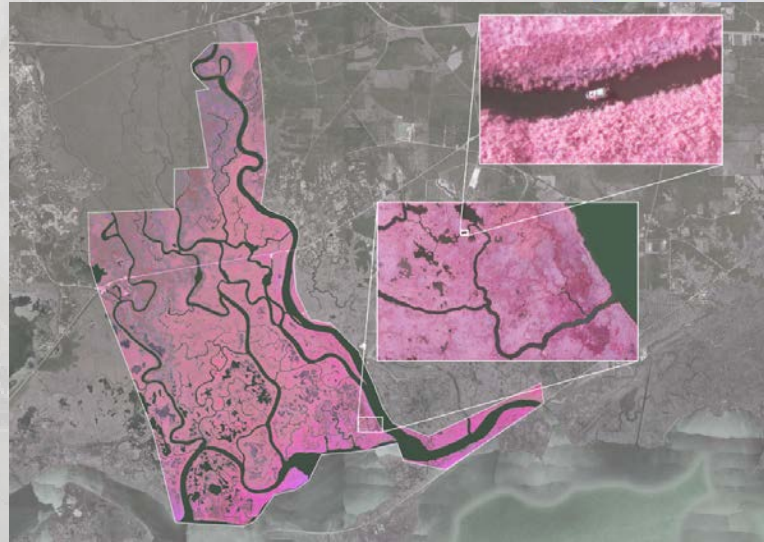
Recognizing the need to integrate research and technology to more effectively address the needs of the Gulf of Mexico, NOAA's Office of Oceanic and Atmospheric Research (OAR) evaluated and awarded the Northern Gulf Institute Cooperative Institute to the team led by Mississippi State University.

The NGI operates between MSU and NOAA, the NOAA notice of award to MSU, NOAA's review of MSU administrative and grants processes, and the NOAA Cooperative Institute Interim Handbook. NGI's approach to the Gulf of Mexico regional issues, problems and opportunities is closely aligned with NOAA's strategic and research priorities.

The NGI is also guided in its mission by a number of sources, the White House's Ocean Action Plan and related orders and comprehensive report of the congressional U.S. Commission on Ocean Policy, the Gulf of Mexico Alliance, and others. The result is an approach that is science driven, regionally focused, and coordinated with other Gulf of Mexico Basin activities.

NGI is a consortium of six academic entities led by Mississippi State University. The NGI partnership includes Mississippi State University, the University of Southern Mississippi, Florida State University, Louisiana State University, the Alabama Dauphin Island Sea Laboratory, the University of Alabama in Huntsville, and the National Oceanic and Atmospheric Administration. NGI conducts research that builds an integrated, comprehensive understanding of natural and human impacts on Gulf of Mexico ecosystems and associated economies to improve its management. Research is conducted under four themes: ecosystem management, coastal hazards, effective and efficient data management systems supporting a data-driven economy, and climate change and climate variability effects on regional ecosystems. Research-driven transformations in regional ecosystem-based management enable managers and communities to improve the resilience and health of ecosystems and people and the sustainability of resources in the Gulf of Mexico.

The Northern Gulf Institute engages nationally and internationally recognized academic experts who provide intellectual and technological capacity to address comprehensive regional ecosystem approaches to science and management in the Gulf of Mexico.
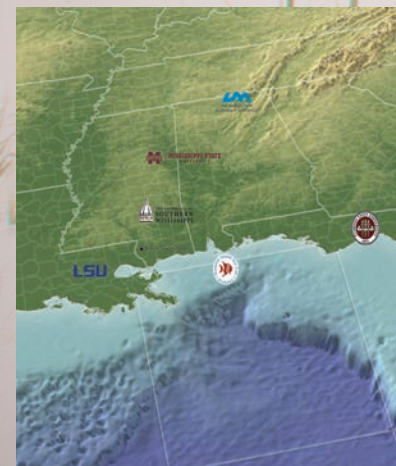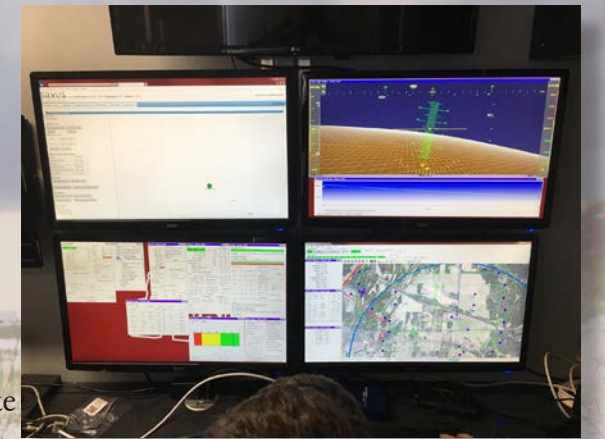
The Institute for Genomics, Biocomputing & Biotechnology (IGBB) functions as both a Mississippi State University research institute and a service center.

With regard to its function as a research institute, the IGBB has recently played leadership roles in (a) the exploration of genomic diversity and molecular evolution in cotton and cotton relatives; (b) improvement of cotton, maize and other crop species; (c) de novo genome sequencing and marker-assisted improvement of fish; (d) study of plant viruses and their control; and (e) computational analysis of gene pathways controlling important biological functions. Funding for IGBB projects comes from a variety of federal agencies including the U.S. Department of Agriculture, the National Science Foundation, the Department of Energy, the U.S. Agency for International Development, and the U.S. Army Corps of Engineers.

The IGBB Service Center provides MSU researchers and their local, national, and international collaborators access to a team of highly-skilled professionals trained in…

- Biological Sample Preparation
- Isolation & Quantification of Biomolecules
- Genomics & Transcriptomics
- All DNA/RNA Sequencing Methods
- Proteomics & Metabolomics
- Computational Biology & Bioinformatics
- Analysis of Complex Molecular Datasets
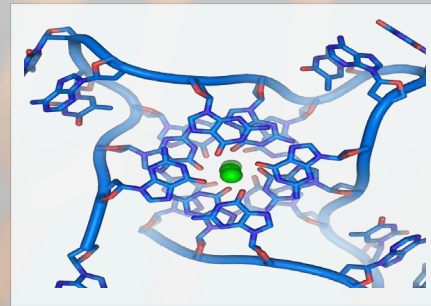
Moreover, the IGBB is home to state-of-the-art molecular analysis instrumentation that the IGBB staff can help you utilize in meeting your scientific goals. As a member institute of the HPC[2,] the IGBB leverages HPC[2] super-computing power to efficiently derive biological knowledge from large, diverse, datasets.

HOW CAN WE HELP YOU?

CONSULTATION WITH RESEARCH EXPERTS - The IGBB's lead genomics, proteomics, and computational biology research associates are happy to meet with you to discuss your research and ways you can reach your scientific goals. Whether you are a pro or a complete novice in high-throughput molecular research, the IGBB research associates will help you chart a course toward success.

PROPOSAL PARTNERSHIPS - Partnering with the IGBB has allowed numerous faculty members to overcome the scientific, technical, personnel, and organizational issues that may have prevented them from successfully obtaining extramural grant funding in the past. We can help you plan, write, and submit your grant proposals in a way that fully leverages the strengths of the IGBB and the HPC2 while building on your research expertise.

EXPERTS FOR HIRE - Most research includes customization of techniques and considerable problem-solving. Trying to figure out how to do new genomics, proteomics, and/or computational biology experiments can be overwhelming, and training a student or postdoc to conduct this work for you may be very expensive and frustrating. Considerable time and resources can be saved by hiring a highly skilled IGBB expert to help you achieve your genomics, proteomics, and/or computational biology research goals.

SERVICE CENTER - Have the IGBB do standard low-risk proteomics, genomics, and computational tasks for you on a fee-per-service, cost-recovery basis. Use our convenient Services Catalog to learn about the standard services we perform and obtain pricing information.

The FAA's Center of Excellence for UAS Research
✕ ASSURE
Alliance for System Safety of UAS through Research Excellence

ASSURE is a 24 university coalition and over 100 industry and government partners from around the world that transform UAS problems into FAA—approved solutions.

CENTER FOR CYBER INNOVATION

CCI develops cutting-edge solutions for Defense, Homeland Security and the Intelligence Community.

CCS
Center for Computational Sciences

CCS models and develops integrated computational crosscutting tools that allow multidisciplinary approaches to problem-solving.

ICRES
CAVS • CAVS-E • ISER • I2AT

ICRES is composed of four research affiliates, and strives to be a world-class center of excellence for research, technology and education. Under ICRES, CAVS is equipped to address engineering challenges facing the nation's industrial base.

GRI
Geosystems Research Institute

GRI competencies are in Ag and natural resource systems, coastal and ocean processes, sensor design, systems engineering, remotely sensed data, large scale data and information handling, modeling and visualization.

IGBB
Institute for Genomics, Biocomputing & Biotechnology

IGBB is a leader in cutting-edge genomics, proteomics and computational biology research.

NGI
NORTHERN GULF INSTITUTE
a NOAA cooperative institute

NGI, a NOAA cooperative Institute, conducts research that builds an integrated, comprehensive understanding of natural and human impacts on the Gulf of Mexico ecosystems and associated economies to improve its management.

MISSISSIPPI STATE
U N I V E R S I T Y™

HPC²
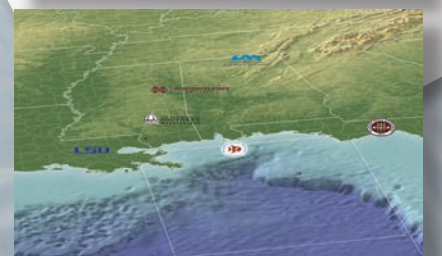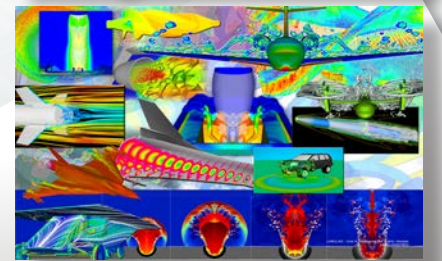
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