PARTNERSHIP FOR AN ADVANCED COMPUTING ENVIRONMENT (PACE) FALL 2019 NEWSLETTER
From the director’s desk

PACE was formed in 2004 with a mission to provide Georgia Tech’s faculty and researchers with sustainable leading-edge research cyberinfrastructure and support. Since this time, resources managed by PACE have accelerated research for over 4,000 users, including nearly 1,500 who have been active in the last year.

2019 is a pivotal year for PACE. We’ve moved to a new home in CODA. We’ve deployed a state-of-the-art NSF funded cluster called Hive, the first resource to become operational in the cutting-edge CODA data center, increased instructional resources available to courses that use HPC resources, and expanded our team to 25 funded positions.

All of this would not have been possible without the collaboration, partnership, and support we have enjoyed and appreciated from across the Institute. For this opportunity to serve our community, we thank you all.

In this inaugural edition of the quarterly PACE newsletter, we showcase a portion of the great work accomplished by the Georgia Tech research community that has been enabled by PACE resources, as well as selected highlights of our own activities.

I’d like to communicate that PACE is committed to advancing the research goals of all disciplines within Georgia Tech’s research community through advanced computational and data science cyberinfrastructure and expert consultation. We welcome opportunities for collaboration; please reach out if we can provide any assistance.

Neil Bright
Associate Director for Research CyberInfrastructure

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Astronomers detect light that originated around supermassive black holes during the universe’s infancy, when it was only 700 million years old. How these behemoths grew so rapidly is still a mystery. Research led by Dr. John Wise and his collaborators provides a promising scenario for their birth. They found that massive black holes between 1,000 and 10,000 solar masses can form in dense starless regions that are growing rapidly. This discovery overturns the long-accepted scenario where they only form in regions bombarded by intense ultraviolet radiation. Black holes formed in this manner, though rare, may be common enough to explain the origin of most supermassive black holes located in galaxy centers.

Their findings were based on the Renaissance Simulations, some of the most physics-rich simulations of early galaxy formation. They ran this simulation suite on NSF’s Blue Waters supercomputer, but they needed to re-simulate two candidate pre-galactic objects at 200x higher resolution. Wise used PACE to rapidly prototype new routines in the open-source simulation code Enzo, specifically for this study. The team increased the resolution by splitting particles in an intermediate restart output and made the adaptive mesh refinement (AMR) more aggressive. However, they restricted AMR to occur only around the candidate objects to increase efficiency. These targeted and efficient simulations only took five days to run on a computer cluster, compared with three months in the original simulation.

Above: A 30,000 light-year region from the Renaissance Simulation centered on a cluster of young galaxies that generate radiation (white) and metals (green) while heating the surrounding gas. A dark matter halo just outside this heated region forms three supermassive stars (inset) each over 1,000 times the mass of our sun that will quickly collapse into massive black holes and eventually supermassive black holes over billions of years. Credit: John Wise (inset) and Advanced Visualization Lab, National Center for Supercomputing Applications.

Performance is the name of the game in High-Performance Computing! Understanding how to identify potential issues in the code which may be impacting how fast and efficient your code is running is a powerful tool to have in a scientific programmer’s toolbox. In this short workshop introduced in Fall 2019, users will benchmark, profile, and improve a serial code using matrix multiplication, which is one of the most common numerical operations in scientific programming.

Prerequisite: Familiarity with a programming language such that the attendee will be able to read and follow code with guidance. Greater familiarity is encouraged but not required. The times and locations for upcoming Optimization 101 sessions are available at pace.gatech.edu.
NSF AWARDS PACE, PARTNERED WITH CENTER FOR RELATIVISTIC ASTROPHYSICS, $400K TO EXTEND OPEN SCIENCE GRID AT GEORGIA TECH

Research scientists Dr. Mehmet Belgin and Semir Sarajlic from the Partnership for an Advanced Computing Environment (PACE), in collaboration with Center for Relativistic Astrophysics (CRA) faculty Drs. Laura Cadonati, Nepomuk Otte, and Ignacio Taboada, received a $400k National Science Foundation (NSF) grant (award OAC-1925541) to extend the Open Science Grid (OSG) service to the Georgia Tech campus. OSG is an NSF-funded national computational grid that provides shared resources to run massive numbers of short/small computations, commonly referred to as High Throughput Computing (HTC). Since 2004, PACE has been successfully providing federated services for long-running, large-scale computations, known as High Performance Computing (HPC). In recent years, the number of HTC-type users utilizing PACE has grown rapidly relative to the number of conventional HPC-type users. As a first step towards supporting HTC-type workloads, PACE deployed a custom OSG cluster for the Laser Interferometer Gravitational-Wave Observatory (LIGO) project led by Cadonati. Peter Couvares (Caltech), chair of Computing for LIGO, said, “Georgia Tech’s collaboration with the Open Science Grid has been of tremendous benefit to LIGO, and I’m looking forward to PACE’s growing capabilities.” With this grant, PACE will be able to extend OSG support to the rest of the researchers on campus, which will improve the overall efficiency and utilization of campus resources. The three main features of the proposal include:

- Providing a centralized OSG support structure to Georgia Tech researchers, who can benefit from HTC, with an option to invest their research funding directly into OSG;
- Providing new GPU resources that are currently in high demand in OSG for large-scale, highly-parallelized computing; and
- Growing OSG’s data federation with the addition of the first “Stash-Cache” service in the southeastern United States to enable fast, convenient access to large data sets.

“We are excited about the significant contributions this grant will add to GT’s existing capabilities,” said PI Belgin. “Perhaps more importantly, it marks the beginnings of a centralized PACE service to support very large numbers of relatively small and short computations -- a common type of computation that has been on the rise at GT.”

The immediate benefit of this grant will be to the multi-messenger physics programs supported through CRA faculty research. The augmentation of the existing LIGO cluster with additional resources brings new capabilities for Cadonati, who will be able to extend her analysis work and test the new GPU-based LIGO software stack. Cadonati explained, “This cluster is placing Georgia Tech at the forefront of the quest for understanding the mysteries of the universe, analyzing data from gravitational waves, photons and neutrinos; we are now pushing the frontiers of science!” Also benefiting from these GPU nodes will be Taboada of the IceCube collaboration, which currently consumes more than 99% of OSG’s GPU resources. Otte, whose work with the Cherenkov Telescope Array (CTA) and the Very Energetic Radiation Imaging Telescope Array System (VERITAS) entails hundreds of terabytes of data, will benefit from a StashCache instance local to Georgia Tech. CTA computations have been run in Europe, mostly due to the lack of a high-capacity StashCache server to store large sets of CTA simulation productions. Those computations will now be able to run in the US.

This NSF award will profoundly impact scientific research. The addition of computational resources locally provides more than just an increase in hardware; it complements the existing HPC infrastructure at PACE with a new HTC-focused model and provides increased opportunity for all researchers on campus and nationwide that participate in the OSG.

Left: Not only are there more HTC-type users than HPC-type users on PACE clusters, the growth rate for HTC-type users is double that of HPC-type users. The graph, from XDMoD, shows PACE usage since May 2015.
CESM2 EARTH-SYSTEM MODEL IMPLEMENTATION PREDICTS EFFECTS OF CLIMATE CHANGE

Future generations may well view climate change as the defining issue of our time. A central goal of the climate research directed by Dr. Jie He is to understand, as well as to predict, the potential impacts of climate change, including sea level rise, prolonged heat stress, increasing probability of storms and melting of the Arctic Ice. To study the issues associated with climate change, scientists use earth system models, which are numerical tools developed for providing the most reliable and comprehensive simulations of the Earth’s climate. Such simulations are computationally expensive and require a combination of cutting-edge computer architecture and state-of-the-art software and workflows.

A newly developed earth system model - the Community Earth System Model, version 2 (CESM2) - was recently implemented on Georgia Tech's high-performance computing system via a collaboration between the Partnership for an Advanced Computing Environment and the Climate Dynamic and Modeling Group at the School of Earth and Atmospheric Sciences. CESM2 is the latest version of CESM developed at the National Center for Atmospheric Research. It includes suitably accurate representations of the atmosphere, ocean, land, sea ice and biogeochemistry, and in each case including elements of human activities that affect these systems. The implementation of CESM2 provides the Georgia Tech research community with an exciting opportunity to study the various components of climate and climate change.

Currently, the Climate Dynamic and Modeling Group is utilizing CESM2 to understand future changes in global rainfall. The challenge lies in the fact that rainfall changes are highly connected with various aspects of climate change, such as the evolving chemical composition of the atmosphere, the warming of the Earth’s surface and changes in land use and plant physiology. These effects are difficult to dissect during transient climate change, which makes rainfall one of the most complex subjects of climate science. To address this issue, the Climate Dynamic and Modeling Group applies the technique of temporal decomposition, where the various factors of rainfall changes are separated based on their differing responding times to climatic forcing (as exemplified in He and Soden, Nature Climate Change, 2017). Central to this technique is CESM2, which has the flexibility to set up climatic forcing at various timescales, as well as the capability to represent the various components of climate change.

Our question:

Our approach: climate modeling (CESM1 and CESM2)

UPCOMING PSI4 WORKSHOP BY AUTHOR, DR. DAVID SHERRILL

Quantum-chemical computations are an increasingly important component of modern chemical research. Psi4 is a freely-available, open-source program providing many popular electronic structure methods, including those based upon density functional theory, many-body perturbation theory, coupled-cluster theory, and configuration interaction. It has been designed to be as user-friendly as possible, both for beginning computational chemists and for advanced users. For users who want to automate complex workflows, Psi4 can now be called from a Python script as a regular Python module. This workshop will introduce the Psi4 program and how it can be used in research or education. A series of freely-available computational chemistry lab modules, available through the Psi4Education project, will also be introduced. Visit pace.gatech.edu for the Psi4 workshop schedule.
Computing, and in particular advanced computing, plays a vital role in virtually every aspect of society today, including the U.S. economy, science, engineering, and manufacturing. For example, students pressed by the scale of their scientific or engineering problems are turning to advanced research computing resources to solve their computational and/or data-intensive problems. In doing so, students realize that their course curriculum does not provide them the needed skills to use advanced computing. The Student Program at the Practice and Experience in Advanced Research Computing (PEARC) conference was created to provide an opportunity for students to engage with experts from the field and to quickly learn about best practices in leveraging advanced computing resources.

Georgia Tech PACE research scientist and PEARC ’19 Student Program Chair, Semir Sarajlic, along with the Student Program team, led the PEARC ’19 student program to host a record-breaking 114 student participants. This year’s PEARC theme was the “Rise of the Machines (Learning)”, which Sarajlic suggested would be better termed “Rise of the Students,” given this year’s strong student turnout. In addition to attending the Student Program activities, students participated in the technical program, with 21 accepted student papers and 36 accepted student posters.

Given the costs of travel to a conference, this year’s Student Program success was in part due to strong support from students’ institutions, exhibitor funding, and an NSF grant, through which PIs Dr. Tom Furlani (University at Buffalo), Semir Sarajlic (Georgia Tech), Jay Alameda (NCSA), Alana Romanella (Virginia Tech) and John Towns (NCSA) received $20k from the National Science Foundation to support student travel to PEARC ’19.

One of the key components of the student program was the ability for students to network with like-minded individuals, and the organization provided a strong list of mentors who were willing to meet with students throughout the week and share their insights on the advanced research computing field. This year especially, there was no shortage of mentors, as the over 800 attendees at the conference offered students ample opportunity to network. Visit www.pearc19.pearc.org/student-program to learn more.

Left: Student Program Opening and Student Welcome on July 28, 2019, at PEARC ’19 in Chicago. Credit: Kevin Steven Jackson/sciencenode.org

PACE LAUNCHES UPDATED USER DOCUMENTATION

PACE is pleased to announce an update to our user documentation. This is a major update to our existing guide, with additional sections detailing instructions for various tasks, along with examples such as PBS scripts for submitting batch and interactive jobs. The new site is built using GitHub, which helps us better maintain the documentation and uses a modular design to facilitate future additions and updates. The documentation is available at docs.pace.gatech.edu.

WOMEN IN TECHNOLOGY SUMMIT

PACE research scientist Dr. Nuyun (Nellie) Zhang was on the planning committee and co-hosted the Women in Technology Summit of Georgia 2019 with Georgia Tech colleagues from OIT under the leadership of Cas D’Angelo. The event had more than 200 participants from 26 public institutions within the USG, aiming at improving the diversity gap, specifically in technology and more broadly in STEM-related careers. The success of this event ensured that Women in IT will be a powerful initiative at Tech.
GLOBAL RESEARCHERS STUDY ENVIRONMENTAL MICROBIAL GENOMICS USING PACE

The Konstantinidis lab studies how microorganisms adapt to human-induced environmental perturbations and cause disease in humans and animals. The great majority of microorganisms resists cultivation in the laboratory and thus cannot be studied efficiently. Therefore, another major objective of Dr. Kostas Konstantinidis’ research program is to develop novel culture-independent (metagenomics) approaches to study microbial communities in-situ, in both natural (e.g., terrestrial or marine) as well as human-associated systems. Recent examples of this work include investigations of the role of soil microbial communities in mediating the feedback responses to climate change (Johnston et al., PNAS 2019); new ways to classify microbial taxa and the description of novel taxa (Konstantinidis et al, ISME 2017); the identification of genes and organisms degrading (bioremediating) important organic pollutants, such as disinfectants and crude oil spills (Kim et al., AEM 2018 & Karthikeyan et al, ISME 2019); and new methods for identifying microbial pathogens in diarrheal samples (Huang et al., AEM 2018).

The work also involves the development of new bioinformatics algorithms and pipelines to analyze big (microbial) genomic and metagenomic data (e.g., Rodriguez-R et al., NAR 2018). In fact, the Konstantinidis Lab has put together a science gateway that hosts these bioinformatics tools and allows external users to perform online analysis with their own data (available through the Lab website, enve-omics.gatech.edu). The “enve-omics” gateway currently receives upwards of 3,000 visitors per month (unique IP addresses) and more than 11,000 page views (Google statistics). This usage is remarkable for a new resource (about 5 years since the launch of the gateway). It represents a testament that these tools fulfill critical needs of contemporary research across environmental or clinical settings and bring a lot of attention to the Konstantinidis Lab and Georgia Tech.

Supporting the analysis of these big microbial data and the usage of the bioinformatics tools by external users would not have been possible without the continuous support of the PACE team. PACE not only houses and maintains the computer infrastructure of the Konstantinidis Lab but helps troubleshooting software installation problems and storing and searching large database files (on the order of 250TB currently) in a very timely fashion.

Below: The Konstantinidis Lab, February 2018. Credit: Kostas Konstantinidis

RESEARCHERS GET IN-PERSON HELP AT PACE CONSULTING

The PACE Research Facilitation Team offers consulting sessions to all PACE users every two weeks. These sessions provide an opportunity for researchers to receive guidance with their research computing objectives and get help resolving problems and/or improving scientific pipelines. We strongly encourage our users to take advantage of these sessions, and we welcome any questions ranging from the initial phase of getting the research initiated on PACE resources to more specific questions related to harnessing PACE computing. Assistance is also available for XSEDE, a national network of NSF supercomputers that scientists use to interactively share computing resources, data, and expertise. The times and locations for upcoming consulting sessions are posted on our homepage at pace.gatech.edu.

REVAMPED PYTHON INTRO

PACE’s newly-revamped Python 101 course for Fall 2019 introduces participants to programming in Python 3. The two-hour hands-on workshop covers basic Python programming, NumPy, and Jupyter notebooks, with an emphasis on applying these tools to scientific and engineering data analysis. The times and locations for upcoming Python 101 sessions are available at pace.gatech.edu.
THE INFECTION MICROBIOME: HOW CAN WE BETTER TREAT CHRONIC INFECTIONS?

Infection medicine currently faces two major and growing crises that impact the ability of doctors to treat bacterial infections with our current arsenal of antibiotics. The first is widely recognized – the evolution of antibiotic resistance. The second receives less attention – chronic infections where appropriate antibiotics fail to resolve infections.

Bacterial infections in otherwise healthy people are usually rapidly resolved by effective immune responses, with or without assistance from antibiotics. In some cases, however, infections fail to clear even with appropriate drug treatment, leading to the establishment of chronic (long-lasting) infection, imposing elevated morbidity and mortality on affected individuals. Chronic infections are a rising burden on healthcare systems globally due to increases in populations at risk, including people with diabetes. Deficits in host barrier defenses and/or immune function in at-risk people provide an opening for the establishment of chronic infections, which are then compounded by changes in the mode of pathogen growth (e.g. biofilm formation) that make the pathogen insensitive to standard antibiotic treatments.

To address the global challenge of chronic infections, the lab of Dr. Sam Brown focuses on a particularly well-characterized disease (cystic fibrosis, CF) with very long-duration bacterial infections (decades of infection). CF affects roughly 30,000 people in the US and an additional 40,000 worldwide. People with CF have genetic mutations that result in decreased airway mucociliary clearance and accumulation of viscous nutrient-rich sputum. As a result, CF lungs invariably become colonized by multiple bacterial species in early childhood, leading to life-long infection.

Thanks to computational support from PACE, the Brown lab has developed new experimental and computational approaches to study the infection microbiome of people with CF. Their work combines clinical data with in vitro and ex vivo experimental models to unpack the relationships between microbiome composition, microbial interactions and patient health outcomes. In their first study, they used machine learning tools to define predictors of patient health from both microbiome data and electronic medical records. Unsurprisingly, leading pathogens such as Pseudomonas aeruginosa were predictive of poorer lung function. However, other bacterial taxa predicted better health (Zhao et al., 2019, BiorXiv).

Are these positive predictor bacteria playing an active probiotic role – perhaps by competing with damaging pathogens? Or are they simply bio-markers of a healthier lung? To address this key question of causality, the researchers built an experimental model of the CF lung infection microbiome. The infection model begins with a special 'synthetic sputum' recipe that recreates the biochemistry and viscosity of sputum. The scientists then add defined combinations of up to 12 species that together account for over 90%
The research group of **Dr. David Sholl** uncovers fundamental material properties to engineer the next generation of materials. The group uses atomistic simulations, both ab initio and classical, to provide a glimpse into atomic-level interactions that dictate macroscopic behavior. This molecular modeling approach using PACE resources yields new insights into adsorption and diffusion in porous materials. The group actively works on revealing potential applications of adsorption-based chemical separations. These applications appear in conventional research areas, such as CO2 and hydrocarbon separations in well-studied materials, as well as in emerging fields where it is important to unveil the adsorption properties of a variety of chemicals in new classes of materials (Tang, D. et al., *J. Phys. Chem. C* 2019). The group’s studies of quantitative modeling of adsorbate diffusion through porous materials often require development of force fields (Verploegh, R. et al., *J. Phys. Chem. C* 2019). Besides modeling of adsorption and diffusion, the Sholl group also performs research that provides insights into the characterization of fundamental material properties. A recent example involved using quantum chemistry calculations to study defect propagation mechanisms in porous materials that are degraded by corrosive environments (Han, R. et al., *J. Phys. Chem. C* 2019). The group’s work uses a wide range of techniques, including quantum chemistry, molecular mechanics, Monte Carlo and machine-learning methods. The computationally demanding nature of these methods means that PACE is an invaluable partner in exploring properties of both familiar and novel materials.

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**INFECTION MICROBIOME**  
*Continued from previous page.*

of the observed microbial diversity in patient samples. Half of these species are familiar human pathogens (including Staphyloccoccus aureus and Pseudomonas aeruginosa), while the rest are largely oral bugs that are commonly found in lung samples in people with CF.  

The results to date support the idea that specific oral microbes are indeed capable of suppressing pathogens within the CF lung environment. However, perturbing the community with commonly used CF antibiotics leads to a dramatic and rapid unraveling of pathogen suppression as oral bugs are wiped out, leading to the growth and dominance of antibiotic-resistant pathogens. This pattern is consistent with the ecological principle of ‘competitive release’ – wiping out a dominant species opens a competitive vacuum that will be filled with fast growing, ‘weedy’ species – in this context, pathogens.  

In ongoing work, the Brown lab is using its extensive experimental microbiome data to refine mathematical models of the CF infection microbiome. These models capture information on how each species affects each other – ‘who does what to whom’, together with their direct resistance to antibiotic perturbation. Armed with this information and a mathematical framework to put these pieces together, the researchers are making and testing predictions on how to improve antibiotic therapies. They aim to devise novel and personalized therapeutic strategies combining probiotics and antibiotics that are tailored to the infection microbiome profile of individual patients. More broadly, the work is a step towards ‘prevision medicine’ treatments for the effective treatment of chronic infections generally.

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**PACE USER ORIENTATION**

Every second week, a PACE research scientist offers our orientation session, which is designed to provide new or existing users with all the fundamental information they will need to start using PACE clusters in an efficient way. The covered topics include explanation of the participation model, accessing the clusters, description of PACE queues, submitting and monitoring jobs, and tips for a more productive use of shared resources. The schedule for upcoming orientation sessions is available at pace.gatech.edu. All new PACE users are strongly encouraged to attend.
PETASCALE WORKSHOP HOSTED ON CAMPUS

PACE was one of the host sites for this year’s Petascale Computing Institute (PCI-2019) that took place on August 19-23, 2019. PCI-2019 is a free week-long distributed training event intended for people seeking to enhance their knowledge and skills for scaling their research software to petascale and emerging extreme-scale computing systems. This year’s extensive agenda covered OpenMP, MPI, Hybrid MPI+OpenMP, OpenACC, CUDA, Python in HPC, Debugging, Profiling and Optimization, Parallel I/O Best Practices, Containers, and other topics. Gordon Bell offered a keynote address, “Man vs. Machine: The Challenge of Engineering Programs for HPC.”

PACE participated in PCI-2019 as one of the host sites in collaboration with organizing partners Argonne National Laboratory (ANL), the Blue Waters project at the National Center for Supercomputing Applications (NCSA), the National Energy Research Scientific Computing Center (NERSC), Oak Ridge Leadership Computing Facility (OLCF), Pittsburgh Supercomputing Center, SciNet at the University of Toronto, and the Texas Advanced Computing Center (TACC).

Local students were able to attend all sessions throughout the weeklong workshop, broadcast from sites across North America, from Krone EBB on the Georgia Tech campus. A session on CUDA programming, presented by Dr. Dmitry Lyakh of OLCF, was broadcast from Georgia Tech to the two dozen host sites across the globe.

Dr. Julien Meaud’s research group investigates the mechanics of the mammalian ear, with a specific focus on the inner ear, or cochlea. The mammalian cochlea is a very complicated biological system. It is a fluid-filled organ that includes small vibrating structures, plus hair cells that detect and amplify low amplitude vibrations. When working properly, the cochlea is an amazing sensory system that operates over a wide frequency range and a range of pressure amplitude that spans more than five orders of magnitude. Unfortunately, the cochlea is very vulnerable to many external factors, including overexposure to loud noise, which can permanently damage hair cells and cause hearing loss. The complexity and vulnerability of the cochlea make it difficult to investigate using only experiments. However, a good scientific understanding of how the normal cochlea works is needed to guide the development of novel treatment strategies for hearing loss. Because of the feedback by hair cells, the cochlea is not just a sensory system; it can also generate sounds, called otoacoustic emissions. Otoacoustic emissions are commonly measured clinically to assess the functional status of the cochlea.

Meaud’s team develops computational models that predict how the cochlea responds to acoustic stimuli and the generation of otoacoustic emissions. These nonlinear, time-domain models are carefully calibrated with experimental data provided by collaborators and are based on the finite element method. These highly-detailed models represent with high fidelity the mechanics of the cochlea, including the vibrations of the cochlear structure, the fluid pressure in the cochlear ducts and the biophysics of hair cells. With these models, Meaud aims to advance fundamental knowledge of how the cochlea works and to help improve the diagnosis of hearing loss using otoacoustic emissions measurements. Because the analysis of cochlear function using the model requires analyzing results from a large number of computationally-expensive simulations, Meaud’s team extensively uses the PACE cluster at Georgia Tech in order to speed up the computations.

Dr. Dmitry Lyakh of Oak Ridge Leadership Computing Facility teaches at the Petascale Computing Institute 2019 session, broadcast to two dozen sites worldwide, from Georgia Tech. Credit: Semir Sarajlic/PACE.
Georgia Tech’s Partnership for an Advanced Computing Environment (PACE) recently deployed a cluster to support the Nobel Prize winning Laser Interferometer Gravitational-Wave Observatory (LIGO) project. This project observed the first gravitational waves from the merger of two black holes, and, in doing so, confirmed Einstein’s predictions according to his theory of general relativity. Beyond the addition of new computational resources, this pioneering work is the first step in integrating Georgia Tech into the Open Science Grid (OSG), a national federated computing resource.

PACE started working on building a LIGO resource at Georgia Tech shortly after the arrival of Dr. Laura Cadonati at the Center for Relativistic Astrophysics (CRA) in 2015. The initial proof-of-concept infrastructure was able to accept test jobs from OSG. This initiative yielded great insight into the process of integrating into OSG, and was disseminated to other institutions, including Syracuse University, which subsequently deployed its own LIGO cluster. Based on this successful test, Cadonati procured a new cluster to run production level LIGO workloads. In deploying this cluster, PACE partnered with a team of experts at the University of Chicago led by Robert Gardner to adopt the latest advancements in OSG system and software stack.

**THE FIRST LIGO CLUSTER FOR GEORGIA TECH IS READY FOR RESEARCH!**

**PACE’S NEW LINUX 101 IN DEMAND**

PACE’s new Linux 101 course began in July and continues to see high demand, attracting participants from across the Georgia Tech campus. This course is designed to provide users with fundamental information about the Linux operating system that they will interact with on PACE managed clusters. Topics covered include an explanation of Linux and Bash, command automation via scripting, utilizing environment variables, and customization of Linux sessions. The times and locations for upcoming Linux 101 sessions are available at pace.gatech.edu.

**MACHINE LEARNING TRAINING**

The application of Machine Learning (ML) is allowing researchers of all disciplines to probe the treasure-trove of the ever-increasing data hoard. In these hands-on workshops, attendees will learn the basics of ML with the Tensorflow framework. We will cover the foundation of ML and apply them to leverage this technology for research. Participants are expected to be able to read Python code with guidance. PACE will debut these courses in Spring 2020, and schedules will be posted at pace.gatech.edu.