The novel coronavirus has brought about changes that would have been considered inconceivable just a few short months ago. Armed with their trusty laptops, PACE staff took to their home offices with heightened purpose, anticipating that many would turn to computational tools as on-campus work ramped down. Articles on pages 3 and 4 discuss projects to further understand the structure of SARS-COV-2 and model the COVID-19 outbreak in Georgia. I’d also like to congratulate the Medlynk team, including our own Sebastian Hollister, one of three multidisciplinary GT teams amongst the winners of MIT’s COVID-19 Challenge (see page 4).

As academic faculty transitioned their courses for virtual delivery, PACE has likewise been updating our workshops (see page 6). Page 9 contains our schedule for the summer semester. We are also working to communicate a transition plan to move PACE resources to the Coda data center.

In coordination with executive leadership, I’ve spearheaded a plan to refresh all PACE compute and storage equipment currently residing in the Rich data center. This refresh is made possible by leveraging existing PACE budget and commercial financing in order to spread the total cost over five years. Overall, this plan is projected to save the Institute approximately $10M, largely due to more power-efficient computing resources and a reduction in long-term data center costs. Please see pages 6-7, where the Coda migration plan is outlined in detail. One key point of this transition plan is the introduction of a no-cost storage tier. Each PI will be provided with 1TB of project storage for use within the PACE ecosystem. Semir Sarajlic and Dr. Mehmet Belgin will be reaching out to research groups regarding their specific details over the next few months.

Be safe, wash your hands, and remember that while we may be apart, we are not alone. #SwarmStrenGTh

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GEORGIA TECH’S LIGO GROUP FIGHTS COVID-19
BY PARTICIPATING IN FOLDING@HOME

The Laser Interferometer Gravitational-Wave Observatory (LIGO) cluster managed by PACE is now contributing to the Folding@home effort to understand SARS-CoV-2.

The lives of billions of people all over the planet have been completely upended by the impact of SARS-CoV-2. In countries ravaged by the COVID-19 disease, healthcare facilities have been stretched to breaking point, entire nations are confined to their homes, and efforts to contain the virus have seen a complete global economic shutdown and the loss of millions of jobs. In these times of self-isolation, it is easy to feel utterly helpless. While, by far, the most productive way most of us can contribute to this fight is to limit contact and heed the advice of medical professionals, spare computing capacity can be used to further our understanding of the structure of SARS-CoV-2.

Folding@home (FAH; foldingathome.org) is a distributed-computing project that seeks to understand protein structures through numerical simulations of molecular dynamics. Members of the public volunteer to install the FAH software on their own systems, where it then utilizes idle computing cycles (or can be configured by users to run constantly). Proteins are constructed from linear chains of amino acids which spontaneously “fold” into a specific 3-dimensional structure that gives the protein its function. While there are many experimental methods which can be used to determine protein structure, they can only explore a single state; the goal of FAH is to perform simulations which explore protein folding dynamics, potentially revealing new therapies for a host of diseases, including COVID-19. Interested readers can learn more at https://foldingathome.org/covid19/.

Dr. James Clark, a researcher in Dr. Laura Cadonati’s group, in collaboration with Andre McNeill of PACE, has developed a workflow to deploy Folding@home on the LIGO cluster at Georgia Tech. The PACE-managed LIGO cluster consists of 35 compute nodes, each equipped with 24-core Intel(R) Xeon(R) CPU E5-2680 v3 CPUs and 128GB RAM memory per node, which are typically used to search for and analyze gravitational waves from black hole and neutron star mergers in data from the LIGO and Virgo

Above: Illustration of the structure of coronaviruses. Image credit: Alissa Eckert, MS and Dan Higgins, MAMS/CDC.
PACE PROVIDES RAPID SUPPORT TO INCREASE SPEED OF COVID-19 RESEARCH ON HIVE

PACE Research Scientists Dr. Christopher Stone and Dr. Christopher Blanton provided rapid support to Dr. Pinar Keskinocak and Dr. Nicoleta Serban, Professors of Industrial and Systems Engineering (ISYE), and their team, including PhD student Buse Aglar, to assist with their epidemiological modeling of the COVID-19 outbreak in Georgia. The ISYE researchers were on-boarded to the Hive cluster under the sponsorship of Hive PI Dr. Srinivas Aluru. Aluru was given consent by the NSF to provide dedicated access to the recently-acquired, NSF-funded Hive system to the ISYE researchers to accelerate their urgent modeling efforts.

The disease spread model is a detailed agent-based simulation, which requires many runs across different parameter settings and multiple replications for each setting. Since each run is independent of the others, Stone worked closely with the ISYE team to create a parallel processing workflow that launches a large number of concurrent jobs using the PACE launcher tool and accelerates the computations. Launcher, originally created at the Texas Advanced Computing Center (TACC) and adapted to PACE by Blanton, manages high-throughput computing (HTC) workflows on a high-performance computing (HPC) system such as Hive. After each run is completed, the data are combined into a compressed archive. The full set of results is then combined into a single archive that the ISYE researchers can download to their analysis systems using the Globus Hive endpoint. With this workflow on the Hive system, what may have taken a day to run on a local workstation can be completed in less than 30 minutes, a nearly 50-fold improvement, using 384 simultaneous computations. This quick turnaround allows the researchers to rapidly improve the accuracy and reliability of their COVID-19 disease spread model and share results with decision-makers.

PACE has several tools for HTC-style workflows on the system, including launcher and GNU Parallel. The launcher tool used in this work is available to all PACE users. For information regarding launcher, please see http://docs.pace.gatech.edu/software/launcher/.

Below: A model shows how COVID-19 may spread in Georgia under different policies. Image credit: Keskinocak Group.

PACE STUDENT’S TEAM WINS COVID-19 HACKATHON

PACE Student Assistant Sebastian Hollister, an undergraduate in the College of Computing, recently joined together with four other Georgia Tech undergraduates (Maximilian Hollister, Akash Moozhayil, Mike Adamo, and Brandon D’arienzo) to participate in the MIT COVID 19 Challenge, a global hackathon with over 1,500 participants, where they won in the Hospital Assets Coordination and Distribution category. After talking with experts, they decided to develop a model that draws from data on the county level to allow hospitals to predict their personal protective equipment (PPE) burn rate. Using the team’s solution, hospitals can see how long their current supplies will last, and suppliers can identify and prioritize hospitals in critical need to better direct their supplies. Their prototype is available at www.ppeburnratecalc.com, and they continue to transition the project into the real world to make an impact.

LIGO

Continued from previous page.

gravitational-wave detector network. This hardware, together with local expertise in containerization and the HTCondor workflow management system, represents a valuable opportunity for the broader scientific community to join this fight. Jobs are already running on the LIGO cluster continuously and are starting to return completed work units to the FAH servers. Georgia Tech researchers now aim to discretize the workflow to better suit a general high-throughput computing environment.

It is hoped that the lessons learned and the HTCondor workflow developed in collaboration with PACE can eventually be scaled up for larger-scale deployment of Folding@home on the Open Science Grid and shared with other researchers with access to similar high-throughput computing resources.
TRANSPORTATION MODELING SIMPLIFIED

The MOVer Vehicle Emission Simulator (MOVES) is the state-of-science model developed by the US Environmental Protection Agency (USEPA) to estimate motor vehicle energy consumption and emissions for transportation projects in the United States. However, running MOVES can be cumbersome and time consuming, given to the complexity of the user interface and input data structures.

A Georgia Tech research team led by Dr. Randall Guensler, including Dr. Haobing Liu, Hongyu Lu, and Dr. Daejin Kim, developed the MOVES-Matrix modeling approach to simplify the MOVES modeling process and increase the analytical processing speeds for complex transportation analyses. MOVES-Matrix is a multi-dimensional energy and emission rate array that is applicable to transportation projects of any spatial (corridor level to regional) or temporal (instantaneous impacts to annual inventories) scale.

MOVES-Matrix is prepared by iteratively running the MOVES model across the entire range and combinations of model input variables. Separate MOVES-Matrix outputs are developed for 117 unique modeling regions, based upon their combination of regional fuel requirements (22 specifications) and inspection and maintenance programs (89 scenarios). For each modeling region, 20 calendar years (2015 to 2030, 2035, 2040, 2045, and 2050), three fuel months (January, April, and July), 23 temperatures (0°F to 100°F, at 5°F intervals), and 21 humidity bins (0% to 100%, at 5% intervals) yields 28,980 runs to obtain the energy consumption and emission rates (CO2, CO, NOx, PM2.5, PM10, SO2, NH3, CH4, VOC, THC, etc.). Each matrix for the 117 MOVES-Matrix regions is composed of more than 5.3 billion on-road energy use and emission rates.

To implement MOVES-Matrix, users need only specify a set of inputs for their modeling scenario (fleet composition and on-road operating conditions), and a series of Python scripts generates the applicable energy use and emission rates from the array. MOVES-Matrix modeling results in exactly the same outputs as using MOVES directly but with a significant efficiency improvement, running more than 200 times faster than using the MOVES user interface. In addition, users no longer need to configure multiple MOVES input files for each scenario.

With the help of PACE, the team processes each MOVES-Matrix region in about 3.5 days. To date, the modeling team has completed more than 1.1 million MOVES runs on PACE, providing energy use and emission rates for 34 of the 117 modeling regions (covering 2,885 out of 3,228 U.S. counties), with 2.2 million more PACE runs remaining to be launched. The team is already collaborating with researchers in Georgia, Texas, Vermont, Ohio, Florida, Maryland, and Washington, D.C., and anticipates that many more users will come online in 2020.

PACE RESEARCH SCIENTIST DR. FANG (CHERRY) LIU SERVES ON PHD COMMITTEE

PACE Research Scientist Dr. Fang (Cherry) Liu served on the thesis committee for CEE Ph.D. student Daejin Kim (see story on this page). The thesis is titled ‘Large-Scale, Dynamic, Microscopic Simulation for Region-Wide Line Source Dispersion Modeling.” All of Kim’s thesis work was completed on PACE, using 331,022 CPU hours of total running time. Liu participated in both the student’s thesis proposal and the defense and helped him with data collection and analysis using PACE. She also provided insights into the thesis direction and structure and offered feedback.

PACE’S INTRODUCTION TO MACHINE LEARNING

PACE’s Introduction to Machine Learning, a hands-on workshop, will cover the basic concepts of machine learning: supervised learning and unsupervised learning, including neural networks and deep learning. It will also cover the basics of using Scikit-Learn and Tensorflow with Keras to train your models. Participants will use Jupyter notebooks, Anaconda, and TensorFlow during the class. The workshop will be offered this summer on May 12, June 10, and July 10, 1:30-4:30 PM.
PACE’S RICH TO CODA DATA CENTER MIGRATION

In March 2019, PACE moved offices from the Rich Computer Center to Coda. Since the move, the Coda data center has been completed, and we deployed the Hive cluster there in September 2019. After a brief ramp-up period, our researchers have kept Hive at nearly 100% utilization. More recently, we deployed the TestFlight-Coda cluster. TestFlight-Coda models the future environment for PACE clusters and includes improvements to the scientific software repository; schedulers; operating system software; and compute, network, and storage equipment. PACE equipment in the Rich data center continues to operate as normal as we begin the process to relocate PACE services to the Coda data center.

Migrating 51,000 CPU cores in over 1,800 compute nodes is not a simple task. Given the importance of computing in research, PACE has done everything we can to best advocate for our research community and to reduce down time during this transition. PACE has developed a strategy to accomplish this goal with four priorities:

1. Reduce or eliminate negative impact to research schedules.
2. Reduce the long-term cost to the Institute.
3. Maximize the utilization of the leased space in Coda in order to make the most cost-effective use of this new resource.
4. Remove HPC equipment supported by PACE from Rich as quickly as possible.

Strategy:

PACE’s director, Neil Bright, in coordination with David Leonard, Director of Academic and Research Technologies, and executive leadership, has spearheaded a plan to refresh all PACE compute and storage equipment currently residing in the Rich data center. As compared to relocating existing equipment, this plan will save the Institute about $10M over the next five years and is enthusiastically welcomed by campus leadership during these difficult times. In partnership with the Offices of Institute Budget Planning and Bursary & Treasury Services, PACE has secured campus approvals and external financing to purchase an entirely new set of hardware. Since the repayment of this financing is completely funded by the existing PACE budget, this equipment refresh will not cause the Institute to allocate any new funding. Following established precedent, we have developed an “equivalent or better” refreshment rubric using the SPECfp_rate benchmark, while accounting for memory, local storage, GPU, and other capabilities that exist in current equipment. PACE’s Team Lead for Outreach and Faculty Interaction, Semir Sarajlic, and Research Facilitation Lead, Dr. Mehmet Belgin, will communicate with individual research groups regarding the refresh details for each PI’s cluster.

Technology PACE will use in Coda:

» Intel “Cascade Lake” 6226 CPUs, totaling 28,744 cores from 1,203 nodes
» Increased local storage performance via NVMe drives
» Increased message passing and storage networking with 100-gigabit HDR InfiniBand

Continued on next page.
Migration
Continued from previous page.

» Similar architecture to the NSF-funded Hive cluster
» Single-precision nVidia RTX 6000 GPUs for AI & Machine Learning workloads
» Double-precision nVidia v100 GPUs
» Software stack highly optimized for this architecture
» 5 petabytes of high-performance storage on a new SFA-18k from DDN utilizing the Lustre file system, as we transition from GPFS
» Red Hat 7 operating system, completing the transition from Red Hat 6
» A five-year warranty on all equipment

After the migration to Coda, the equipment from Rich will be either sent to surplus or used as a trade-in to defray the cost of the new hardware.

Migration Process:
We anticipate the deployment of new hardware and the migration of research groups to the Coda data center to be complete by the end of December 2020. The Rich data center will be decommissioned once this transition is complete. PACE staff will coordinate with individual research groups to ensure a smooth transition.

A PACE Research Scientist will be assigned to each research group as a single point of contact during the migration process. During the process, research groups will continue to have uninterrupted access to their existing resources in the Rich data center. Access to TestFlight-Coda will be provided to ensure workflows run smoothly in Coda. On a per-group basis, the migration process is as follows:

» Testing period on TestFlight-Coda to ensure workflows run smoothly
» New equipment becomes available
» Brief downtime to migrate data from Rich

» Production workflows run in Coda
» Equipment in Rich powered off

Two other processes will occur during this transition. PIs will be asked to confirm user lists to ensure appropriate individuals have access and to determine how to preserve data belonging to former users. The top-level storage organization will be restructured to facilitate easier growth on a per-PI basis. Locations of files within individual user spaces will not be modified.

Introducing Free Tier Storage:
In Coda, PACE will be providing 1 TB of project storage, accessed via user data directories, to each PI at no cost. Additional storage may be purchased by PIs who need more than 1 TB. The cost remains $80 per TB per year.

PACE Archive Storage Service:
PACE is now offering an additional storage option and looking for “early science” applications. The Archive storage tier is intended to house those important datasets that need to be retained but are not in active use. These properties enable a design that is optimized for low cost and reliability, while placing less emphasis on high performance. This architecture makes PACE Archive storage an attractive component of data management plans and is priced at $40 per TB per year.

Please direct any questions related to the Rich to Coda migration plan to pace-support@oit.gatech.edu.

PACE, SCHELLER PARTNER FOR ML
PACE is conducting an 18-hour workshop series on machine learning programming in partnership with the Quantitative & Computational Finance Program (QCF) of the Scheller College of Business. PACE Research Scientist Dr. Nuyun Zhang, has taught the workshops, which have been attended by 68 QCF graduate students, several PhD students, and faculty members. The first sessions, in February and March, were taught in the classroom and covered TensorFlow and Scikit-learn while averaging 40 questions and answers per session. April workshops, covering TensorFlow and Text in Deep Learning, moved online with recorded video accompanied by real-time discussion. The workshops will be continuously developed and published as online training materials. QCF and PACE are also planning to publish a paper or book on the topic of machine learning programming and application in QCF in the near future.

NEW PACE STAFF
PACE’s cyberinfrastructure (CI) team welcomed two new members in April 2020. Deirdre Womack joined as Systems Support Engineer II and will work in system administration. Greg Beyer joined as Systems Support Engineer Sr. and will work to improve tools, processes, and procedures. In addition, CI team member Peter Wan has taken a new role as Systems Support Engineer Sr., where he will focus on security.
SEARCHING FOR THE NEEDLE IN THE HAYSTACK:
HOW RARE GAMMA-RAYS ARE IDENTIFIED IN
CHERENKOV TELESCOPE DATA

The universe is home to some pretty violent and extreme places. Prominent examples are matter sucking black holes, exploding stars (supernovae), colliding neutron stars (gamma-ray bursts), and rapidly rotating neutron stars (pulsars). It is in these places where nature does alchemy and creates the elements that fill the periodic table. A necessary ingredient for cooking elements is the presence of particles of extremely high energies. Because these particles — cosmic rays — are captured on Earth, scientists know that processes must take place through which a particle can acquire energy equivalent to that of a speeding bullet. Finding out how these particle accelerators work is the objective of the research carried out by Dr. Nepomuk Otte’s group.

Otte and his group do this by observing these objects in very-high-energy (VHE) gamma-rays, which is light that is a billion times more energetic than light from the sun. Because only interactions with at least one high energy particle can produce VHE gamma-rays, VHE gamma-rays are ideal for probing cosmic particle accelerators. But VHE gamma-rays are scarce, and it requires the right technique to detect them. From the available methods, Cherenkov telescopes have emerged as the most sensitive instruments. The way Cherenkov telescopes work is very peculiar. When a VHE gamma-ray impacts with the atmosphere, it starts a cascade of thousands of charged particles, mostly electrons and positrons, called an air shower. The particles in the shower emit bluish Cherenkov light, which a Cherenkov telescope detects as a flash that lasts only billionths of a second. By projecting the light onto its camera, the telescope thus takes an image of the air shower. VERITAS, an array of four Cherenkov telescopes located one hour south of Tucson, AZ, records shower images.

The image resolution is only 0.1 degrees, which by astronomical standards is very coarse. For comparison, the diameter of the moon is 0.5 degrees. But it is good enough that appropriate algorithms can reconstruct the event from the image, identifying a measurement of the arrival direction and the energy of the gamma-ray. The reconstruction algorithm also determines if the air shower was initiated by a gamma-ray or by a charged cosmic ray. That is important because there are a lot more cosmic rays than gamma-rays. In some cases, one needs to sift through hundreds of thousands of cosmic-ray images before one finds one gamma-ray image in the data - the literal search for the needle in the haystack.

Simulations play a vital role in the reconstruction. Because an image only provides information about its brightness, shape, and orientation, researchers have to somehow infer from that the energy and the type of particle - cosmic ray or a gamma-ray - that started the air shower. Ideally, one would compare the recorded image with images where the particle type and its energy are known. Unfortunately, it is not feasible to place an artificial VHE gamma-ray source outside the atmosphere and use it to calibrate the recorded images. Instead, physicists do the next best thing and perform computer simulations.

These simulations include a broad range of effects, which is why the simulations are very computationally intensive. The level of detail in some of the simulation steps is indeed mind-boggling. Not only does the physics need to be modeled accurately, but so do the environment and the telescope. Defining the simulation models sometimes takes years of measurements in the laboratory and the field. The simulation of an event starts by releasing a gamma-ray or a cosmic-ray outside of a virtual atmosphere. The particle is followed until it interacts, and an air-shower develops. At that point, the computer code tracks thousands of shower particles and simulates the
PYLAUNCHER TOOL DEPLOYED ON PACE FOR HIGH-THROUGHPUT PERFORMANCE COMPUTING

High-Throughput Computing (HTC) solves problems where many calculations are independent of each other. These types of problems are common in many fields, with many cases in the computational biological disciplines. A natural outgrowth is the addition of parallel processes in an HTC-like manner. High-Throughput Performance Computing (HTPC) is a combination of High-Performance Computing (HPC) applications in the style of HTC. For example, materials scientists work to screen many materials for particular properties, requiring the use of multiple processors to find the solutions in a reasonable amount of time. Currently, the tools to perform HTPC calculations are more limited than those for HTC.

TACC scientist Victor Eijkhout’s pylauncher is an evolution of the idea of the TACC’s launcher tool, which was recently modified for use on PACE and deployed by PACE Research Scientists Dr. Christopher Blanton and Dr. Kevin Manalo. Pylauncher provides a more feature-rich means to do HTC-style workloads, at the cost of more complexity in creating individual jobs. Launcher provides a simpler workflow at the cost of being restricted to serial jobs. Seeing the benefits of pylauncher, Blanton sought to allow the software to run at PACE and other HPC sites which use a PBS-based scheduler. Towards that goal, he has developed the required components and has offered the modifications to the official TACC pylauncher GitHub (https://github.com/TACC/pylauncher).

Pylauncher adds the ability for the user to do large numbers of tasks, which can be single-processor computations, shared-memory parallel computations, or distributed-memory parallel computations. It gives a great deal of flexibility to researchers in how they structure their computations, since it uses the Python scripting language. “With the rapid growth in our HTC user community at Georgia Tech, PACE is expanding our support of HTC and HTPC that will continue to further our Institute’s goal of providing our researchers with the tools to “create the next,” said PACE Team Lead for Outreach and Faculty Interaction Semir Sarajlic. “Our supported HTC tool, Launcher, recently helped accelerate COVID-19 research for Dr. Pinar Keskinocak and her team [see story on page 4], which highlights the type of rapid support and facilitation that our PACE Research Scientists, Dr. Chris Stone and Dr. Chris Blanton, provide.” The advancement in technology to support HTPC is just one way that PACE will continue to “Create the Next!”

TELESCOPE

Continued from previous page.

emission of Cherenkov photons. The simulation then ray-traces every photon through the atmosphere, and in case a photon hits the mirror of a telescope, it is further followed until it encounters the focal surface of the camera. The last step simulates the camera response, which includes the photon detectors, the electronics, and the digitization of the signals. The simulation output is the same as in real observations, and it is also processed in the same way as actual data. The only difference is that for each simulated event, the researchers know what type of particle started the air shower and what its energy was.

Simulating events is a Herculean effort. Luckily, once produced, the simulations are reused in the data analysis for many years. For VERITAS, the collaborators have just finished the simulation of some 100 million gamma-rays on the Open Science Grid, which took two years to complete. It would have taken a desktop computer 2,000 years to achieve the same task. The data volume of the simulation exceeds 300 TB.

The researchers not only use simulations for data analysis; they also heavily rely on them in design studies of the Cherenkov Telescope Array (CTA). CTA will be ten times more sensitive than VERITAS and will be its successor. CTA achieves its better sensitivity with two arrays with tens of Cherenkov telescopes. One array will be installed on La Palma in the Canary Islands and one in Chile. In the U.S., a novel Cherenkov telescope is being developed for CTA, a prototype of which was completed last year in Arizona.

SUMMER 2020 PACE WORKSHOPS

PACE continues to offer regular hands-on training workshops during the Summer 2020 semester. Each workshop is developed and taught by PACE Research Scientists and is designed to help PACE users make greater use of PACE resources.

- Linux 101 by Dr. Aaron Jezghani: May 13, June 9, July 9
- Linux 102 by Dr. Aaron Jezghani: May 27, June 23, July 23
- Python 101: Intro to Data Analysis with NumPy by Dr. Michael Weiner: May 29, June 25, July 22
- Optimization 101 by Dr. Chris Blanton: May 21, June 11, July 8
- Applications of Machine Learning: Your First ML Project by Dr. Chris Blanton: May 28, July 21, August 5
- Introduction to Machine Learning by Dr. Nuyun Zhang: May 19, June 10, July 10
- Introduction to Deep Learning by Dr. Nuyun Zhang: May 26, June 17, July 17
- Git 101 by Dr. Chris Stone: June 18, July 14
- PACE Orientation by Semir Sarajlic: alternate Wednesdays, beginning May 20

Please note that registration closes 1 day prior to each class to ensure that we may provision all the necessary training accounts and materials needed for the hands-on portion of the class. For more information, visit pace.gatech.edu/training.

We also continue to offer PACE Consulting Sessions on alternate Tuesdays, beginning May 19. Consulting sessions are a great opportunity to drop in and get one-on-one help from the PACE Research Facilitation team with any problems impeding your research using PACE. Consulting Sessions do not require registration, and users are invited to join any session.
TRANS-NEPTUNIAN OBJECTS SIMULATED

Are we alone in the universe? This is an age-old question that has long piqued the interest of mankind. Thanks to the thousands of exoplanets — planets outside the Solar System — that have been discovered over the past decade, we are in a golden era to answer this fundamental question. To better predict the habitability of these exoplanets, the team led by Dr. Gongjie Li extends the study on the spin axis variations of our own Earth and quantifies the changes in the spin-axis orientation of exoplanets. Large variations of the spin-axis can lead to atmospheric and climatic catastrophes. PACE allows Li’s lab to run a large number of high-precision simulations to evolve the planetary systems and to characterize the spin-axis variations of the planets. This helps them better understand the habitability of planets orbiting other stars.

Closer to home, many puzzles remain in the vast outskirts of the Solar System beyond Neptune. Minor objects known as trans-Neptunian objects (TNOs) reside outside of Neptune, and their orbital architecture reveals unexpected features and challenges our understanding of the way in which the outer Solar System works. For instance, some of the minor objects’ orbits are greatly tilted from the ecliptic plane where the planets reside, and this hints at the possibility of outer planets inside our solar system, which are far away and too faint to yet be detected. These discoveries motivate the study of the dynamical processes in the outer solar system which govern TNO orbits. Thanks to the computational support from PACE, Li’s lab simulates the influence of a possible outer planet (Planet Nine) as well as past stellar flybys around our solar system which could explain the distribution of the TNOs.

Below: Snapshots of TNOs during a stellar flyby. Image credit: Moore et al./Li Group.

TEAM PHOENIX PREPARES TO COMPETE

Georgia Tech’s Center for High Performance Computing (CHiPC) and PACE have recently initiated a new undergraduate Student Cluster Competition (SCC) team to compete for a spot in the cluster competition at Supercomputing 2020 in Atlanta. Team Phoenix is run as part of an undergraduate research class through the Vertically Integrated Projects (VIP) program, and enrolled students learn about the ins and outs of high performance computing and supercomputing cluster hardware, software, and applications.

The course is led by instructors from Computational Science and Engineering (CSE) and PACE. The team leads and co-instructors, Dr. Rich Vuduc (CSE, CHiPC director), Dr. Aaron Jezghani (PACE), Will Powell (CSE), and Vijay Thakkar (CSE graduate mentor) have led students through discussions of challenging topics, including application optimization, cluster storage, and networking configurations. Team Phoenix students have also been able to hone their skills in CUDA programming and have tested running the standard Top 500 benchmark, Linpack, on the PACE instructional cluster, PACE-ICE. These students have also benefited from the PACE Linux 101 and 102 workshops, taught by Jezghani, which have given them a head start in using PACE cluster resources and tools.

Team Phoenix students are currently working on their application for the SCC, and vendor partners Penguin Computing, Nvidia, and Intel have agreed to join Georgia Tech’s proposal push as the official vendors for the team. Through this robust collaborative effort, Team Phoenix hopes to be a strong home-town contender when SC comes to Atlanta in November.
IMPROVED TRANSUDCERS OFFER SOLUTIONS

Capacitive micromachined ultrasonic transducers (CMUTs) have been gaining significant traction in the last decade as a viable alternative to traditional bulk piezoelectric transducers, which have been the dominant transducer technology for nondestructive evaluation, medical imaging, medical therapeutics, and many other applications. CMUTs use flexible membrane structures as a moving electrode of a variable capacitor which can be used as an electroacoustic transducer. By utilizing flexible membranes, CMUTs demonstrate a closely matched impedance with water and do not require the complex matching layers associated with bulk piezoelectric transducers. Moreover, these silicon micromachined membrane-based designs enable wafer-level microfabrication, broadening the available design space, especially for applications that require small size and high element density.

Membrane-type arrays such as CMUTs are particularly susceptible to acoustic crosstalk, which can impact their performance especially in terms of bandwidth. Accurate simulation of acoustic crosstalk and modeling of full arrays are therefore required to evaluate the performance of CMUT arrays. Full CMUT arrays can be comprised of several hundred to thousands of membranes, which would require considerable computational effort to simulate using standard 3-D finite element analysis (FEA). The transient boundary element model developed by the research group of Dr. F. Levent Degertekin reduces the complexity of these simulations by compressing the problem from three dimensions to two dimensions (Satir, Zahorian, and Degertekin, IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, 2013). The acousto-mechanical coupling is solved over a surface mesh, where equilibrium for the mesh nodes are described in terms of lumped mass, damping, stiffness, and radiation impedance. After Fourier decomposition, the full mechanical system forms a matrix equation composed of frequency-independent mass, damping, and stiffness matrices and a frequency-dependent mutual acoustic impedance matrix.

Due to the frequency-dependent nature of the matrix equation, transient performance analysis of CMUT arrays requires solving the mechanical system across a range of frequencies, which is then converted into multi-input multi-output (MIMO) finite impulse response (FIR) filters. PACE clusters significantly reduce the computational effort and time by enabling batch simulation of the system at different frequencies. Batch simulation is also utilized in transient simulations, allowing faster analysis of multiple design parameters, and hence faster optimization of CMUT array design. Furthermore, the increased computational capabilities provided by PACE clusters enable simulation of larger and more complex CMUT arrays, reducing approximation in CMUT array performance analysis.

Above: Effect of acoustical crosstalk on mean membrane displacement of a 1-D CMUT array with 2880 membranes. Figures on the left show the active elements and simulation domain, whereas the figures on the right show the displacement of the membranes at a particular frequency. For the top case, only the edge element of the CMUT array is excited, and the displacement field shows the wave propagation from left to right on the array. For the bottom case, all the CMUT array elements are excited with the same voltage, but the displacement distribution is not uniform due to crosstalk. Image credit: Shieh, Sabra, and Degertekin/Degertekin Group.

INTRO TO DEEP LEARNING
PACE’s Introduction to Deep Learning, a hands-on workshop, will cover deep learning concepts and workflow:
• Practical aspects of Deep Learning: Bias/variance, regularization, optimization algorithm, hyperparameter tuning
• Vision with deep learning (Convolutional Neural Network)
• Text with deep learning (Embedding, RNN, LSTM, Transformer)
• TensorFlow2.0
• TensorBoard
• Pipeline with GPU and CPU
Prerequisite: Basic knowledge of statistics & Python. The workshop will be offered this summer on May 26, June 17, and July 17, 1:30-4:30 PM.