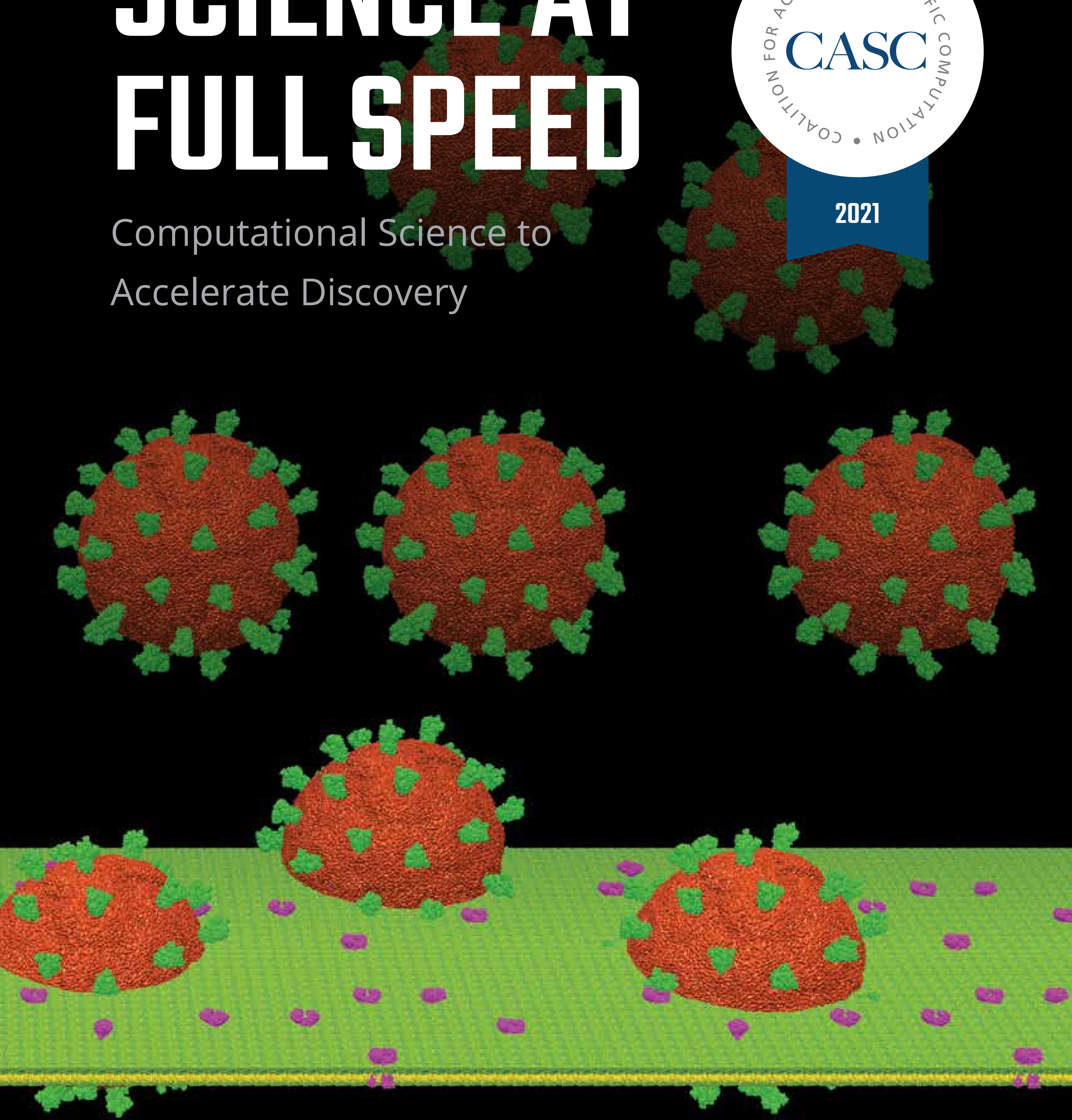
SCIENCE AT FULL SPEED

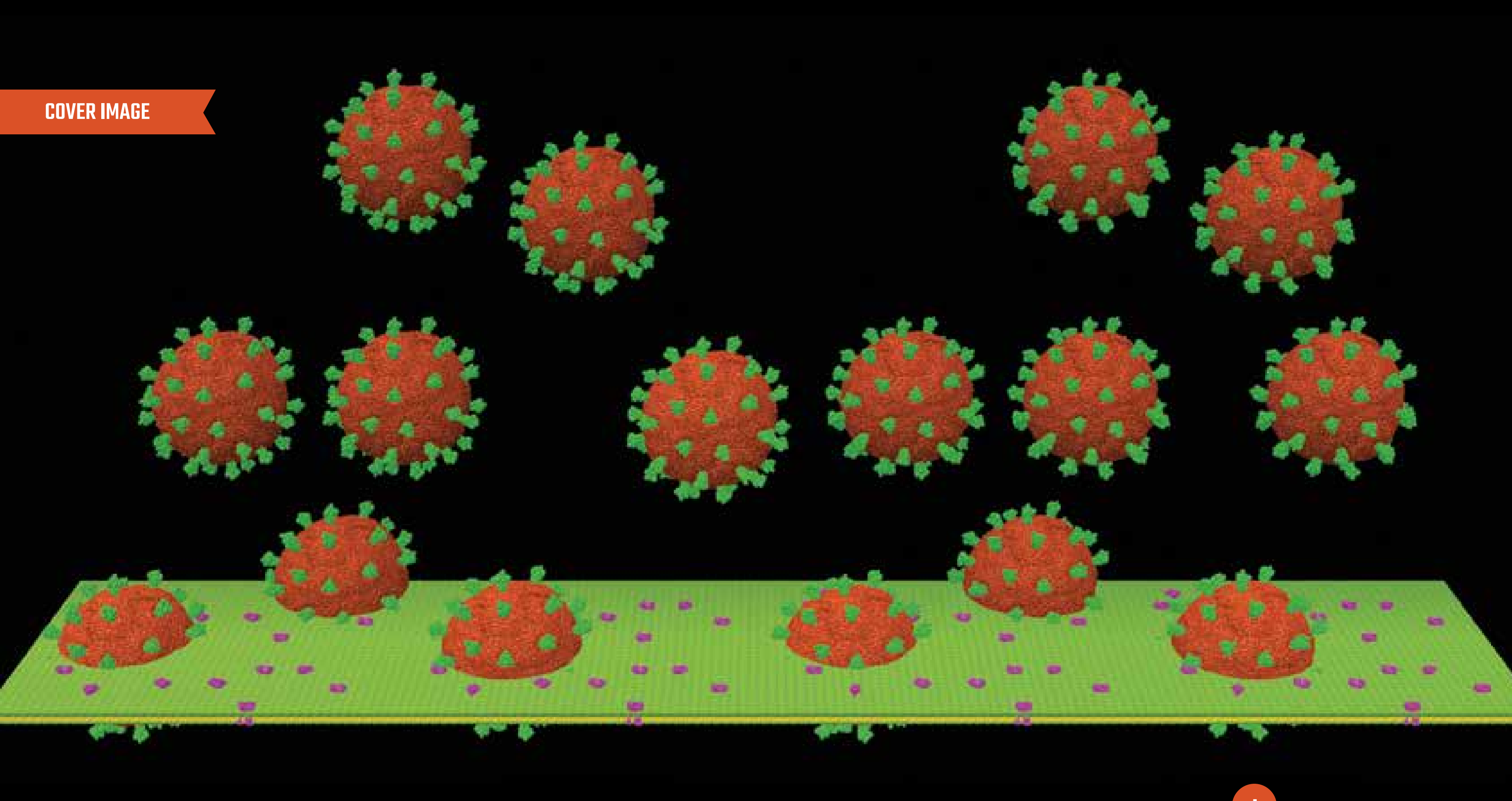
Computational Science to Accelerate Discovery

COALITION FOR ACADEMIC SCIENTIFIC COMPUTATION

CASC

2021





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ABOUT THE COVER

This visualization shows viral particles of the novel coronavirus, SARS-CoV-2, merging with the outer membrane of a human lung cell. Modeling how the virus interacts with the body at the atomic level provides a foundation to inform the design of drugs and vaccines to fight the COVID-19 pandemic. See page 4 for the full story. Image courtesy of Victor Padilla-Sanchez, Catholic University.

ABOUT CASC

Founded in 1989, the Coalition for Academic Scientific Computation (CASC) is an educational nonprofit 501(c)(3) organization with 90+ member institutions. CASC envisions a robust, sustainable ecosystem supporting academic research computing and data services, enabled by a vibrant, diverse community of professionals.

CASC MISSION

- To advocate for the importance of and need for public and private investment in research computing and data services to support academic research.
- To serve as a trusted advisor to federal agencies on the direction of relevant funding programs.
- To actively engage in discussions of policies related to research computing and data services.
- To foster advancement of a robust and diverse community of current and emerging leaders in this field.
- To provide a forum for the community to share strategic ideas and best practices.

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FEATURE ARTICLE

ALL HANDS ON DECK

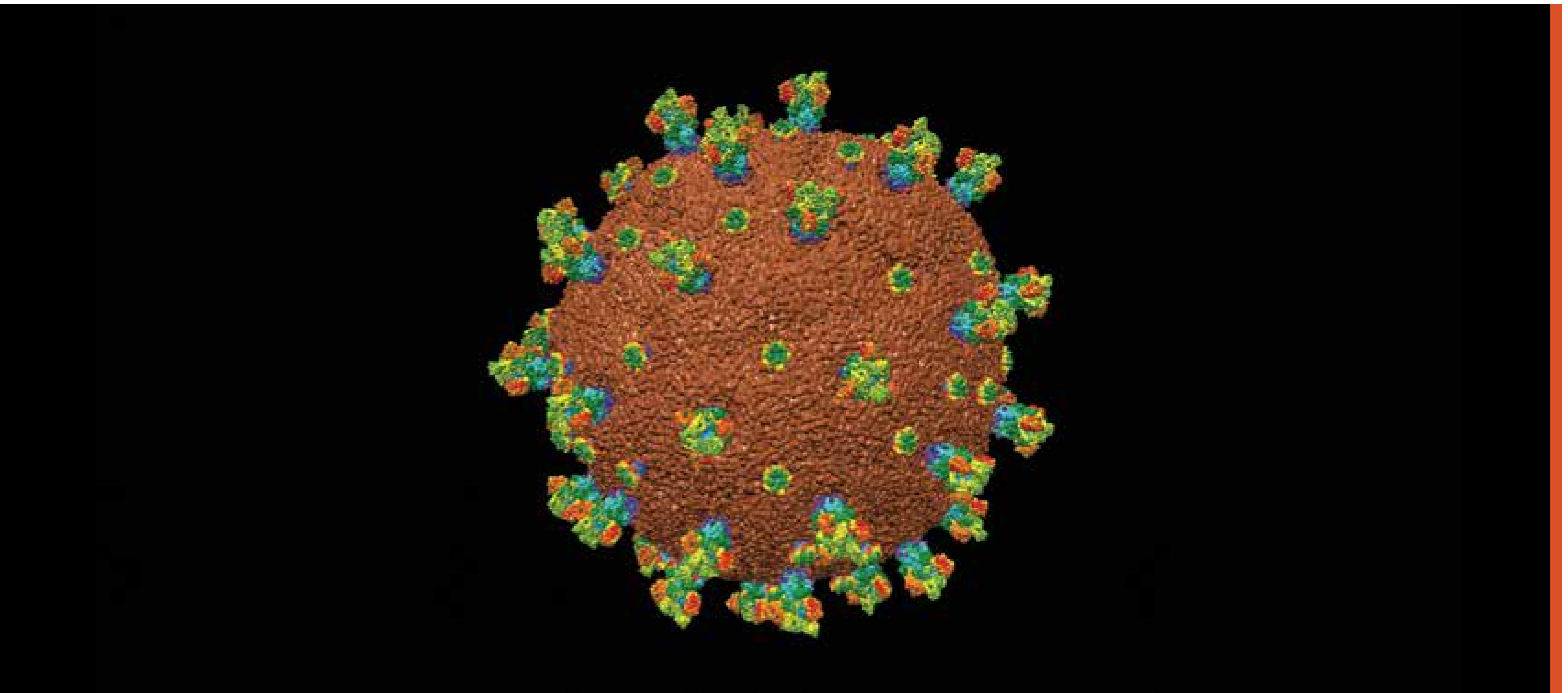
How the computational science community pivoted to the fight against COVID-19

Who can forget the feeling of those first weeks and months as the COVID-19 pandemic swept across the world, an invisible enemy shutting down our communities and igniting our worst fears? But as "normal" life came to a screeching halt, thousands of researchers were just getting started. On quiet campuses across the nation, computers were pressed into action. Amid the shock and devastation, scientists refocused their energies, and hope shined through.

There was much work to be done, and many mysteries to unravel. What was this new sickness? Was it like a cold, like the flu, or like nothing we knew? How did it spread through the body, and through society? Who had it now? Where would it go next? And above all, what could be done to stop it?

In a time of staggering grief and uncertainty, one thing was clear: Science would be more essential than ever. And scientists, across the nation and across the world, answered the call.

While many comparisons have been drawn between COVID-19 and the influenza pandemic that ravaged the world a century ago, the scientific tools at our disposal today are beyond comparison. Complementing and amplifying the talents of our scientific workforce are vast data stores, incredible computational capabilities, and the infrastructure to collaborate on a scale that would have been unattainable even a few years ago. With courage, creativity, and computation, the scientific community has brought great hope in a time of great despair.



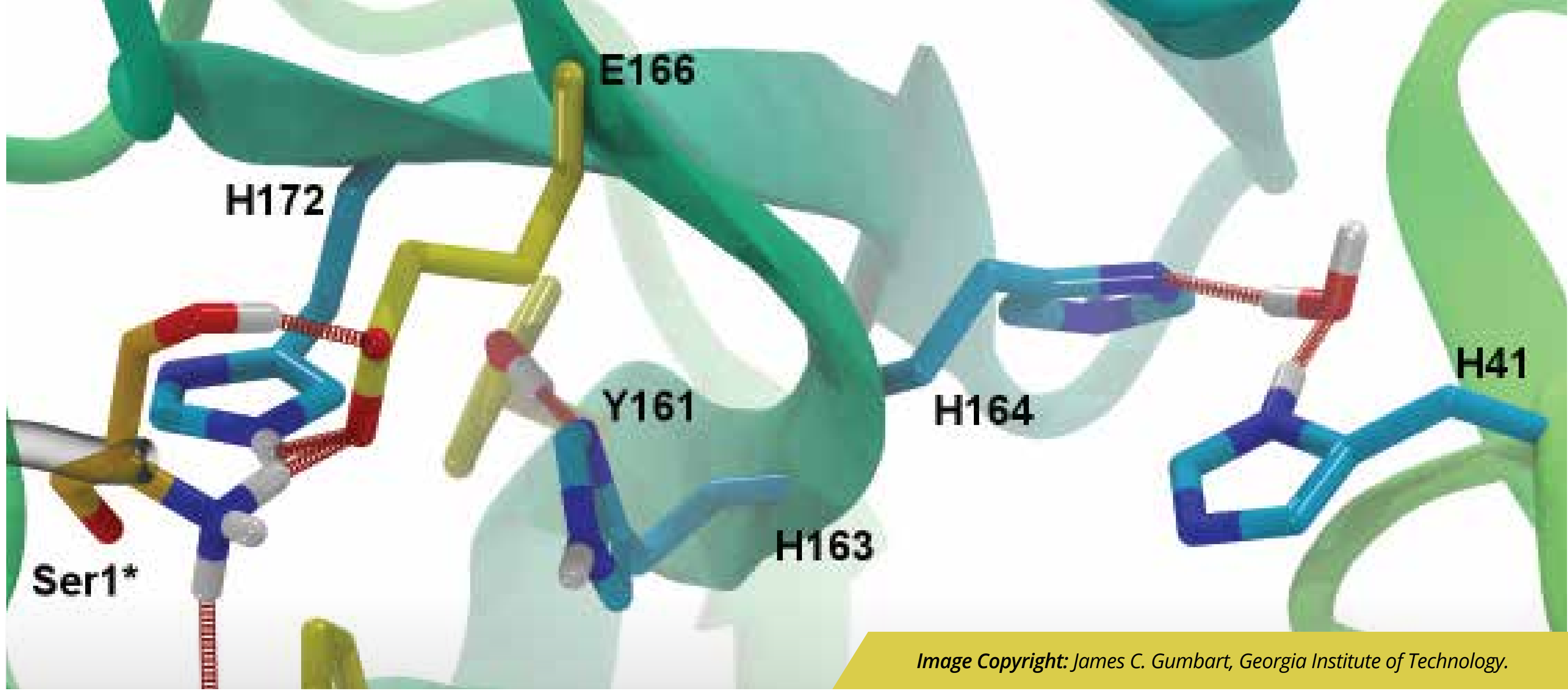


Image Copyright: *James C. Gumbart, Georgia Institute of Technology.*

VISUALIZING THE VIRUS

SCRUTINIZING THE SPIKES

The 46 spike proteins that dot the surface of SARS-CoV-2, the virus that causes COVID-19, are key to its ability to infiltrate and infect the human body. Victor Padilla-Sanchez, a researcher specializing in viral structures at the Catholic University of America, suspected that understanding how those proteins work could prove critical in the search for treatments and vaccines.

Starting with a COVID-19 genetic sequence obtained on February 26, 2020, Padilla-Sanchez constructed a computer simulation of the virus that is detailed enough to show the position of every atom in its spike proteins (seen at left and on brochure cover). To simplify the massive computational task, he used laboratory images of the SARS-CoV virus, which caused the SARS outbreak in 2002-2003, to stand in for the SARS-CoV-2 viral core. This allowed him to direct most of the computational power toward the most critical structures: the spikes.

Padilla-Sanchez then ran the model on the Pittsburgh Supercomputing Center's *Bridges* platform, taking advantage of *Bridges'* large memory nodes. The simulation captures the virus's behavior in stunning detail, modeling the interactions between 300 million atoms as 16 viral particles merge with the outer membrane of a human lung cell. The simulation offers a valuable platform to inform the design of drugs and vaccines.

PROBING FOR WEAKNESSES

Researchers James C. Gumbart, Diane Lynch, and Anna Pavlova of the Georgia Institute of Technology have focused their efforts on the SARS-CoV-2 main protease, an enzyme that plays a key role in the virus's ability to replicate itself. Drugs that inhibit proteases have proved effective against other viruses, so scientists believe the enzyme could be a promising target for potential COVID-19 treatments.

The team used Georgia Tech's *Hive* supercomputer to model the molecular dynamics at the heart of the coronavirus's main protease. The results, shown above, reveal the inner workings of the enzyme's protein-slicing machinery. This up-close view helps scientists understand the virus's life cycle, an important step in the quest to find and exploit its weaknesses.

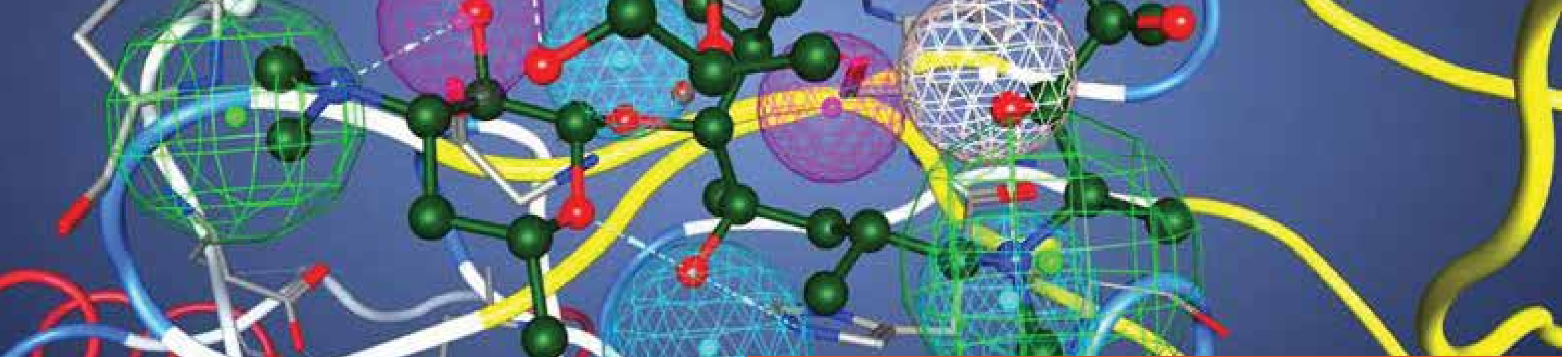


Image Copyright: Valentina Kouznetsova, University of California, San Diego

PURSUING TREATMENTS

MATCHMAKING FOR CURES

What if the cure for COVID-19 already exists? That's the question that inspired researchers Valentina Kouznetsova and Igor Tsigelny of the University of California, San Diego, to design a computational strategy to systematically predict how the novel coronavirus might react to drugs that are already approved by the U.S. Food and Drug Administration (FDA).

To identify FDA-approved drugs that might inhibit the SARS-CoV-2 main protease, the researchers created a model reflecting the features a drug would need in order to target this enzyme, and compared it against the 3D fingerprints of existing drugs. With help from David Huang, a student in the San Diego Supercomputer Center Research Experience for High School Students program, the team used their computer model to virtually "dock" the protease with various drugs and with other random compounds.

The research flagged 64 compounds worthy of further investigation, a collection that includes two HIV protease inhibitors, two hepatitis C protease inhibitors, and three drugs that have already shown encouraging results in COVID-19 studies. The image above shows a model of the antibiotic drug azithromycin, with spheres indicating the drug's functional centers.

STAYING A STEP AHEAD

As scientists pursue drugs to disarm SARS-CoV-2, Arizona State University physics professor Banu Ozkan and doctoral student Paul Campitelli are taking a different tack: thinking like the virus. Instead of searching for weaknesses that can be exploited, they are looking for areas of strength that might help the virus resist drugs designed to destroy it.

The coronavirus's main protease enzyme is seen as a promising drug target, but previous experience has shown that viruses can evolve resistance by swapping in different amino acids that allow the enzyme to continue to function while dodging drugs. This makes drugs less effective over time. Ozkan and Campitelli created molecular dynamics simulations, using ASU's research computing cluster *Agave*, to identify sites on the coronavirus's main protease that could be most "swappable." In this image, the yellow circles are areas of predicted drug resistance. Scientists can use this information to design drugs that anticipate—and evade—the virus's defenses.

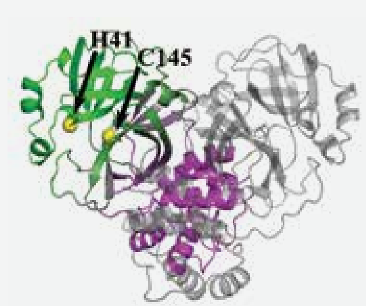


Image Copyright: *Banu Ozkan, Arizona State University.*

INFORMING DECISIONS

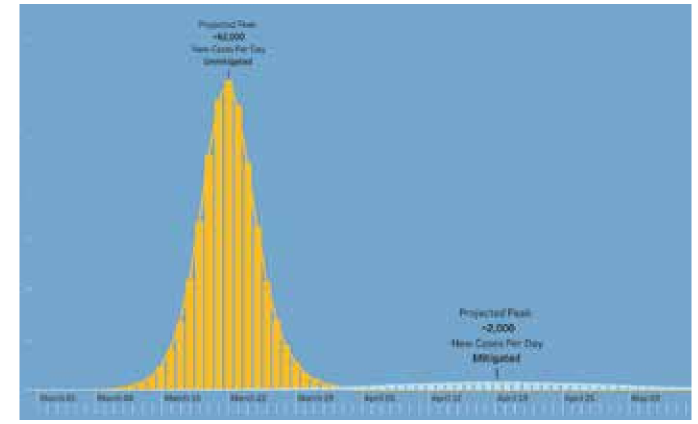


Image Copyright: *Joseph Tien, The Ohio State University.*

CAPTURING THE CURVE

Predicting the course of a pandemic is not like predicting the course of a hurricane. Though both exercises have their challenges, a key difference is that a hurricane will keep plowing ahead no matter what we do, but people's actions directly affect how disease spreads—thus determining, at least in part, the outcome of the pandemic.

Joseph Tien, an applied mathematician and epidemiologist at The Ohio State University, created the image above to capture how different decisions and behaviors could result in a very different experience with COVID-19 in Ohio. The low, flatter line shows the level of COVID-19 infections that would be expected with public health measures such as closing businesses where people congregate and advising mask-wearing in public. The taller curve, in yellow, shows the expected daily infection rate without such measures.

Tien and his colleagues developed these models using the *Owens* cluster at the Ohio Supercomputer Center in partnership with the Ohio Department of Health. While public health research is often conducted in the background away from the public eye, these forecasts were shared widely via daily press conferences, helping to influence people's behavior and inform the state's response.

TRACKING THE SPREAD

The University of Virginia's Biocomplexity Institute has a long track record of studying major disease outbreaks, including the COVID-19 pandemic. The Institute's research team leverages artificial intelligence, high-performance computing, network science, and epidemic science expertise to track hot spots and inform resource allocation. As the threat of COVID-19 became clear, the Institute's team, in close collaboration with Persistent Systems Inc., created two dashboards at the request of federal and Commonwealth of Virginia officials. The first (below, top) tracks the global spread of the disease including active cases, confirmed cases, deaths, and recoveries. The second (bottom) includes forecasts of future weekly hospitalizations in the state of Virginia along with the projected percentages of occupied hospital beds. This information is useful for anticipating future demands on medical resources.

By bringing different data sources together in two easy and digestible dashboards, the work helps researchers study the pandemic and provides a critical resource to help policymakers, healthcare systems, and residents understand key risks and make well-informed decisions.

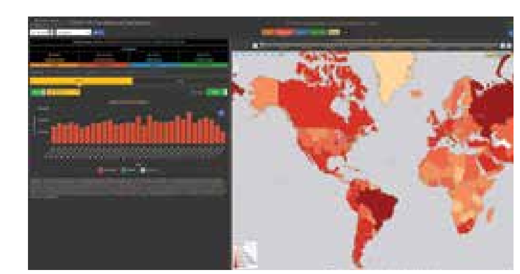


Image Copyright: *Biocomplexity Institute and Initiative of the University of Virginia.*

BOLSTERING BIOMEDICINE

DODGING DEFENSES TO BANISH BACTERIA

How do some bacteria resist even the strongest antibiotics? One important defense is a double membrane of greasy lipids that bacteria form around themselves. Researchers Nicolas Coudray, Gira Bhabha, and Damian Ekiert of the Skirball Institute of Biomolecular Medicine at New York University may have found a clue about how this membrane is formed and maintained.

The image at right shows the 3D structure of a tiny, protein-based machine hidden within bacteria. This machine, LetB (lipophilic envelope-spanning tunnel B), helps transport greasy lipids across the watery environment between membranes, and is critical for bacteria to maintain the integrity of their membrane barrier. That barrier is what protects them against harsh environments and potential stressors—like antibiotics sent to kill them.

The researchers uncovered the atomic structure of LetB using cryo-electron microscopy. They processed the data on *Big Purple*, part of the High Performance Computing Core at NYU Langone Health. In addition to giving scientists an up-close look at LetB's architecture, researchers hope the work can help inform the design of new antibiotics capable of breaching these bacterial defenses.

COMPUTATION AND THE RACE TO CURE CANCER

2019 saw more than 1.7 million new cancer diagnoses and more than 600,000 cancer deaths in the U.S. alone. New immunotherapy treatments could be a game-changer for many cancers, but the success of these therapies varies widely from person to person, requiring a tailored approach.

Immunotherapy works by training a person's own immune system to seek and destroy cancer cells. To find the cancer and ignore healthy tissue, immune cells must be programmed to recognize protein fragments, called peptides, that are unique to that specific tumor. To assist with this step, researchers at Rice University developed Docking INCrementally (DINC), a tool to find peptides that are likely to be recognizable for immune cells. Running DINC on the *Comet* supercomputer at San Diego Supercomputer Center, researcher Didier Devaurs demonstrated how the tool can quickly analyze interactions between thousands of peptides and predict interactions that other tools miss. Researchers hope DINC can help more patients benefit from immunotherapy and avoid treatments that are unlikely to be successful.

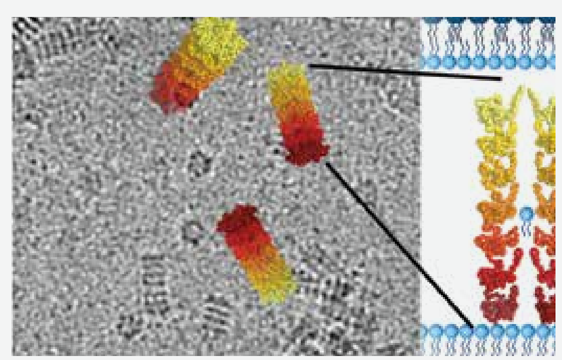
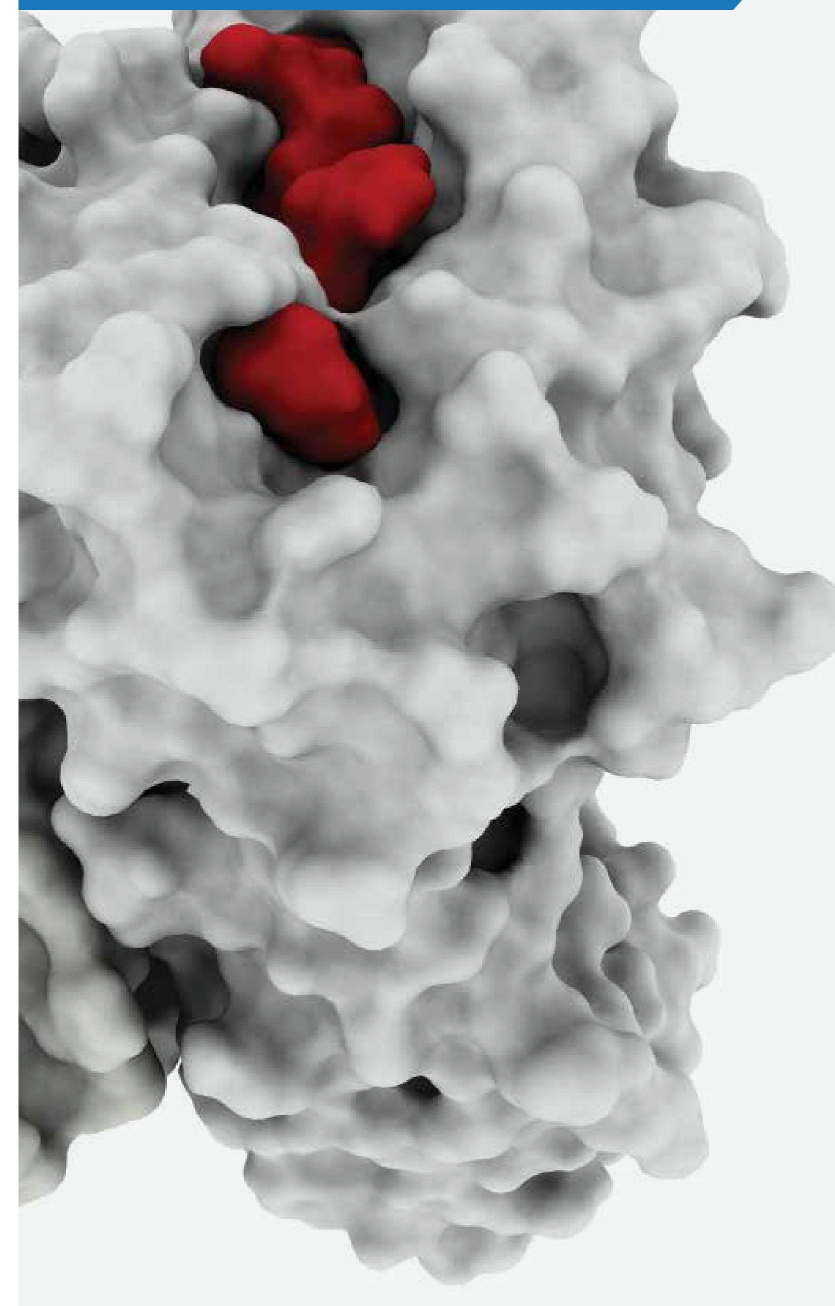


Image Copyright: *Nicolas Coudray, Michael Costantino, Gira Bhabha, and Damian Ekiert, New York University.*

Image Copyright: *Didier Devaurs and Dinler Antunes, Rice University.*



The image above shows a peptide (in red) displayed on the surface of a cancer cell (not represented here) by a receptor protein from the immune system (in gray). If the immune system has been programmed to recognize this specific peptide, the cell will be eliminated.

DEGENERATIVE DISEASE AT THE ATOMIC SCALE

While the root causes of many neurodegenerative diseases remain mysterious, researchers suspect that tiny, liquid-like globs composed of proteins, DNA, and RNA that float around inside cells might play a role. Under normal circumstances, they are responsible for regulating various functions in cells.

The visualization below, created by Justin Drake and Anne Bowen at the University of Texas at Austin and Montgomery Pettit at the University of Texas at Galveston, with computation on the Texas Advanced Computing Center's *Stampede2* supercomputer, simulates the formation of a liquid-like droplet (gray surface) as protein components (green) fuse to it. By studying these processes at the atomic scale, the researchers aim to learn how the behavior of these cellular components may change during disease progression.

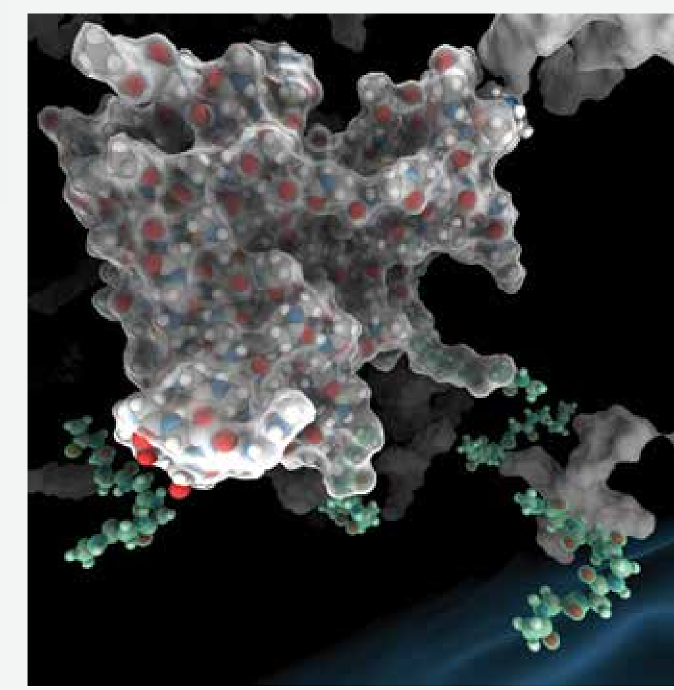


Image Copyright: *Justin Drake and Anne Bowen, Texas Advanced Computing Center, University of Texas at Austin.*

OCEANS OF ENERGY

SEAWEED FOR SUSTAINABILITY

Could the next big biofuel be found under the sea? While the Gulf of Mexico has long been a rich source of energy with its underwater oil reserves, it may also be the perfect place to extract a different slimy source of energy: seaweed. A team of researchers is examining the Gulf's chemistry and currents to see if it's a suitable place to grow seaweed for use as a biofuel, known as macroalgae mariculture.

This visualization shows how nitrate, dissolved carbon, and chlorophyll—important factors for seaweed growth—move around the Gulf of Mexico. The simulations, which were created using the U.S. Department of Energy's Energy Exascale Earth System Model, reflect an enormous number of interacting variables and use sophisticated data visualization techniques to give researchers insights on the region's mariculture potential. The team includes Mathew Maltrud and Phillip Wolfram from Los Alamos National Laboratory, Riley Brady from the University of Colorado at Boulder, Francesca Samsel and Greg Abram from Texas Advanced Computing Center, and Bridger Herman and Daniel Keefe from the University of Minnesota.

***Image Copyright:** Data Courtesy of Mat Maltrud, Riley Brady, and Phillip Wolfram via the Energy Exascale Earth System Model with visualization in collaboration with Francesca Samsel and Greg Abram from Texas Advanced Computing Center and Bridger Herman and Daniel Keefe from the University of Minnesota.*

HARVESTING OCEAN BREEZES

With access to powerful offshore gusts, wind farms at sea can generate more power than those on land. But installing an 800-foot-tall turbine in the ocean is no small feat. Engineers suspected that using a floating platform, instead of fixing the turbine to the ocean floor, could simplify installation in deeper waters, but one important question remained: Would floating turbines work as well?

Hannah Johlas, a researcher at the University of Massachusetts Amherst, modeled the wake of a floating turbine, shown in the image at top right, to help researchers understand how this design might affect power output and turbine lifespan. The computations were performed on two supercomputers, *Comet* at the San Diego Supercomputer Center and *Stampede2* at the Texas Advanced Computing Center. The simulations reveal that the wind wakes of floating turbines are similar to those of fixed-bottom turbines, with only small differences in trajectory and turbulence. Engineers can use this information to design more efficient offshore wind farms with potentially big savings on installation and upkeep costs.

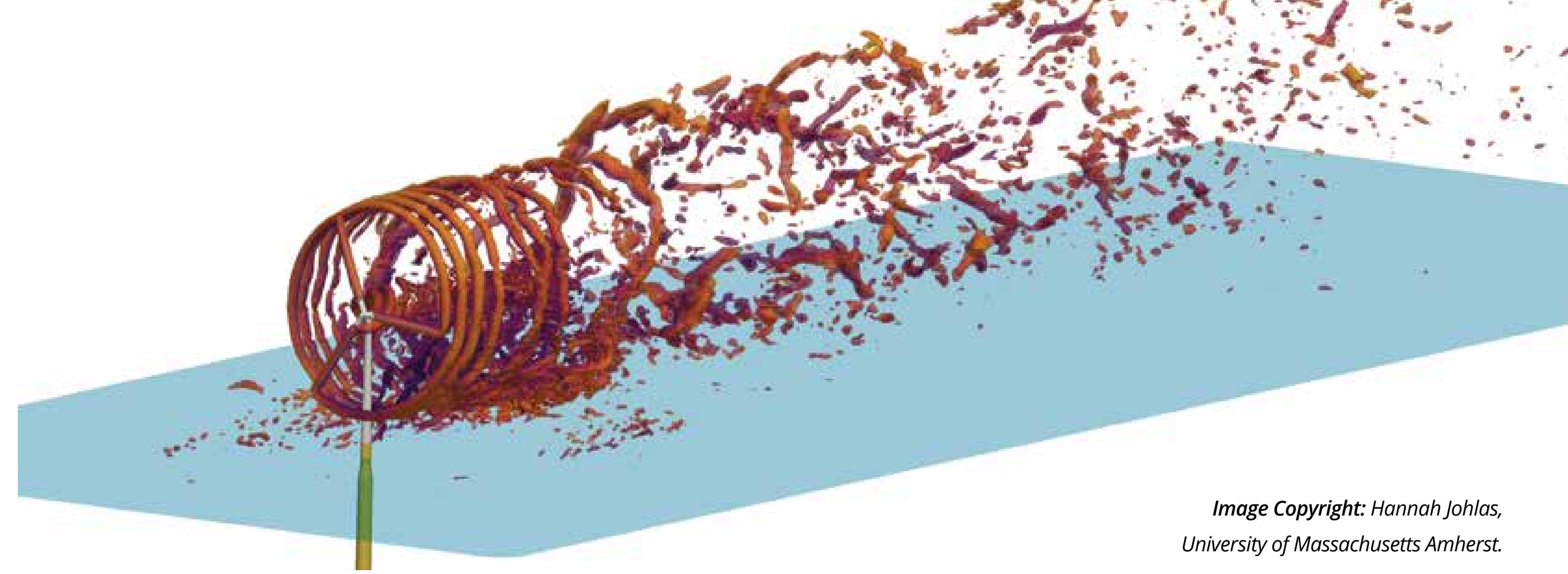


***Image Copyright:** Hannah Johlas, University of Massachusetts Amherst.*

FISH IN THE FORECAST

Accurate water condition forecasts can help fishing boats find the best fishing grounds, reduce fuel consumption, and improve their catch on a daily basis. These forecasts also help officials make quick decisions during crises such as an offshore oil spill.

Researchers Ivo Pasmans and Alexander Kurapov, then of Oregon State University and now at the University of New Orleans and the National Oceanic and Atmospheric Administration, respectively, developed an algorithm to reduce errors in three-day water condition forecasts. The team combined oceanographic observations with forecasts from ocean models using a technique known as ensemble four-dimensional variational data assimilation (DA) and ran their simulations on the *Comet* supercomputer at the San Diego Supercomputer Center.

The image below shows the sea-surface temperature off the coasts of Oregon and Washington on August 1, 2011, before and after DA correction. The black line indicates the position of the upwelling front where warm ocean surface water in the west (red) meets colder water near the coast (yellow). Its location is used by fishermen to find the best fishing spots for the day. By more accurately predicting water temperature, salinity levels, sea heights, and currents, the work can help fishers zero in on the best fishing grounds and conserve energy.

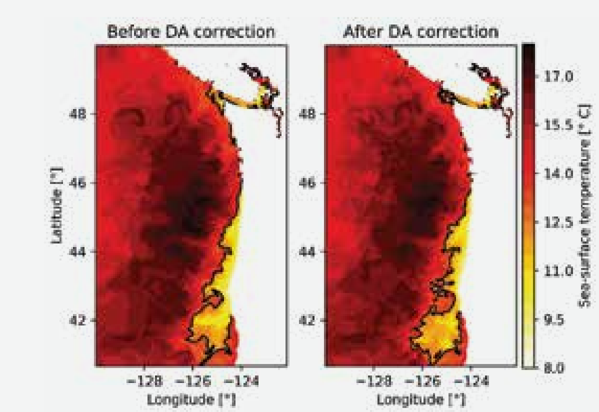


***Image Copyright:** Ivo Pasmans, Oregon State University.*

WEATHER AT THE EXTREMES

FASTER FORECASTS SAVE LIVES

As extreme weather events grow more frequent, it has become increasingly critical for communities to get real-time information on imminent weather risks. To better integrate data and computational resources for hyperlocal forecasting, computer scientists at the University of North Carolina at Chapel Hill, the University of Southern California, and the University of Massachusetts Amherst created advanced workflow management platforms that coordinate and automate the storage, movement, and processing of massive amounts of weather data.

The visualization below, created by researchers Anirban Mandal, Eric Lyons, and George Papadimitriou, displays high-resolution Doppler radar data from Collaborative Adaptive Sensing of the Atmosphere (CASA) during a 2018 severe weather event in Dallas, Texas. On the left, hail (orange) and high winds (red) are shown alongside local GIS information. On the right, data from the workflow performance monitoring system is captured in real-time, showing the modeling computations and data flow happening behind the scenes.

A deeper understanding of local weather risks can enable highly targeted alerts to help protect critical infrastructure, such as hospitals and airports—and save lives.

FEEDING GROUNDS FOR A HURRICANE

Hurricanes get their energy from a warm sea surface. To better understand the fundamental physics that govern the interactions between ocean currents and these massive storms, Daniel Whitt and Matt Rehme of the National Center for Atmospheric Research and Cliff Watkins of Rutgers University used the *Cheyenne* supercomputer to simulate the surface of the sea as it roils beneath a hurricane.

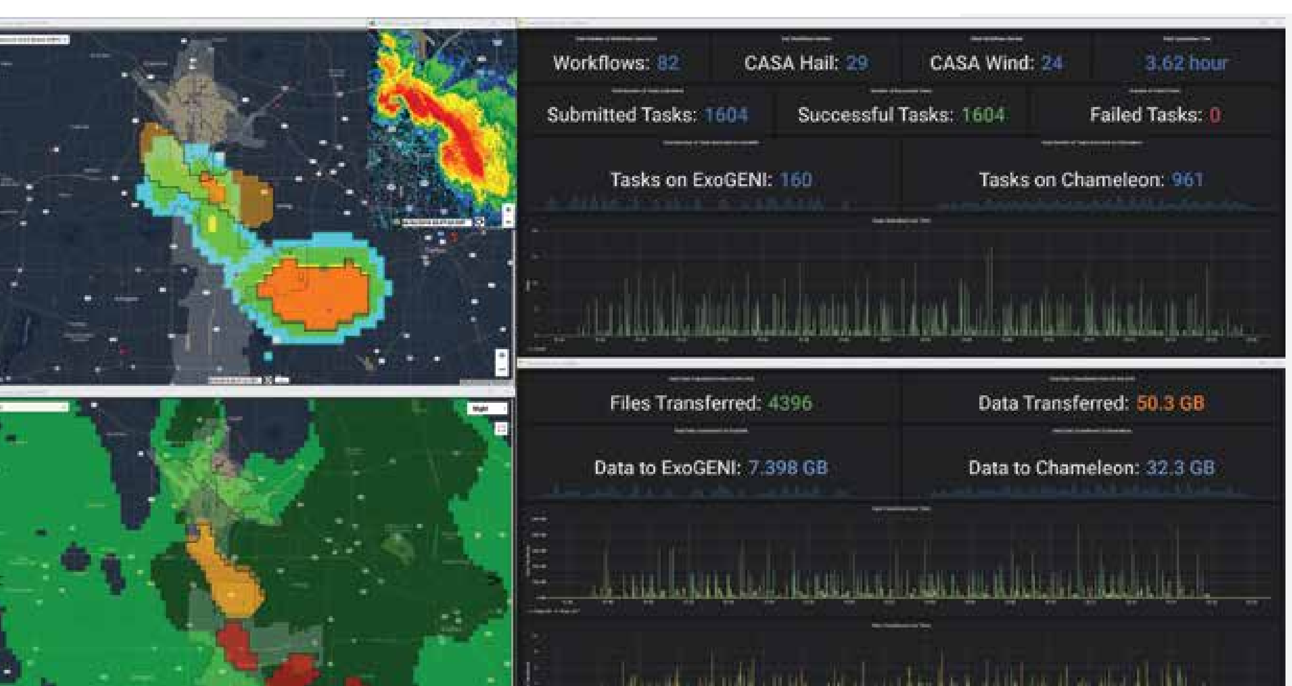


Image Copyright: Anirban Mandal, University of North Carolina at Chapel Hill.

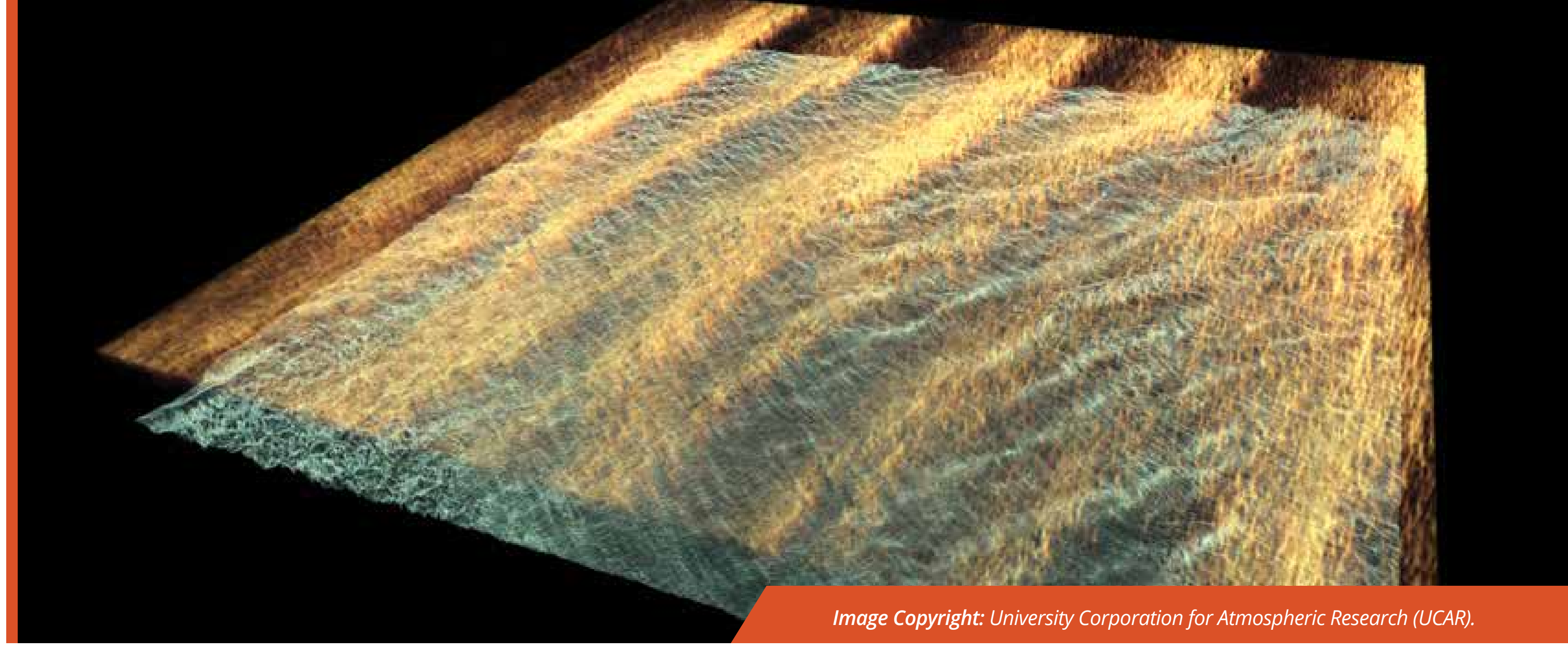
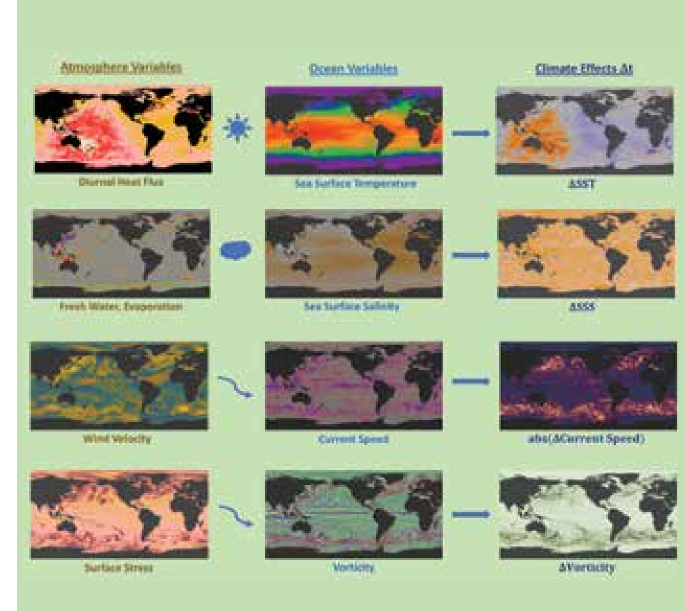


Image Copyright: *University Corporation for Atmospheric Research (UCAR).*

The image above shows a visualization of the simulated upper ocean currents in a 2-kilometer patch of ocean as a hurricane passes above. The orange colors reveal strong near-surface currents that are hundreds of meters wide and kilometers long, but only 10 meters deep. These currents influence the hurricane by affecting the ability for cold water (green colors) to move up to the surface. By helping scientists uncover the physics behind important ocean phenomena, this work can ultimately help improve weather and climate forecasting.



CAPTURING CLIMATE COMPLEXITY

While the science is clear that our climate is changing, there is still much to learn about the intricate interactions between the atmosphere and the ocean that will influence how climate change plays out. To refine our understanding of the enormous number of variables involved and better predict what the future will hold, scientists at the National Oceanic and Atmospheric Administration (NOAA) Geophysical Fluid Dynamics Laboratory developed the Earth System Model. This powerful coupled model simulates both the ocean and atmosphere and can be used to calculate variables such as water temperature, salinity, wind, and vorticity.

NOAA researcher Matthew Harrison and Eliot Feibush of Princeton University used the model to create these visualizations that illustrate how atmospheric variables and ocean variables interact to influence climate, shedding new light on the physical forces at work in large scale climate changes.

Image Copyright: *Eliot Feibush, Princeton University and Matthew Harrison, Geophysical Fluid Dynamics Laboratory.*

EXPLORING SPACE WITH SUPERCOMPUTERS

LIVE LONG AND CLUSTER

On Star Trek, the spacefaring Romulans powered their spaceships with an artificial black hole. While black holes can't power spacecraft (yet), their ability to drive the formation of stars and the evolution of galaxies makes them one of the most powerful—and intriguing—features in the universe.

The University of Washington's "N-body shop" group created a new computer simulation to study black hole

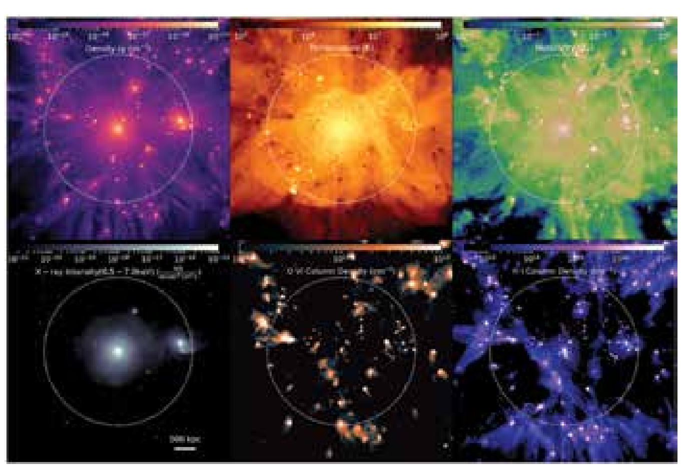


Image Copyright: *Iryna Butsky, University of Washington, published in Monthly Notices of the Royal Astronomical Society, 490(3), December 2019, pages 4292–4306, https://doi.org/10.1093/mnras/stz2859.*

physics, naming it RomulusC after the home planet of Star Trek's Romulans, with a 'C' added to signify a focus on galaxy clusters. Researcher Iryna Butsky and colleagues used not one, but four supercomputers to run the high-resolution simulation: the initial conditions were created at the San Diego Supercomputer Center, the simulations were run on *Stampede2* at the Texas Advanced Computing Center and *Blue Waters* at the National Center for Supercomputing Applications, and NASA's *Pleiades* supercomputer was used for analysis.

The snapshot below shows projections of gas density, temperature, metal content, and other characteristics of a simulated galaxy cluster. These images demonstrate that it is possible to use ultraviolet absorption spectroscopy to study the structures in galaxy clusters that are "invisible" to X-ray emission. Since scientists can't study galaxies in a laboratory, simulations like RomulusC, paired with observations from instruments like the Hubble Space Telescope, are critical to Butsky's expanded understanding of the fundamental makeup of our universe.

FROM COSMIC SOUP TO STARS

The swirling beauty of theimage at right belies the intense drama it represents: a single point in time in the formation of a galaxy. Created by researcher Matthew Turk of the National Center for Supercomputing Applications at the University of Illinois with visualization expertise from Bart D. Semeraro of the Texas Advanced Computing Center, the image captures a step in the evolution of the cosmos.

The variations of color and opacity reflect variations in density, similar to how denser areas of a cloud appear more opaque as light travels through it. As the process continues, gravity will pull the swirling mass of materials together, ultimately condensing into a galaxy that will form stars and light up its surroundings.

Image Copyright: *Bart D. Semeraro, University of Texas at Austin and Matthew Turk, University of Illinois.*

To create the simulation, researchers used data from a test suite of the yt project, a collection of open-source visualization and analysis tools for data-rich astrophysical calculations.

DESIGNING A FAIL-PROOF HEAT SHIELD

One of the riskiest moments for spacecraft is the descent for landing, plunging through a planet's atmosphere at hypersonic speeds. Friction causes the exterior of the craft to grow extremely hot, creating an engineering challenge with no room for failure.

Several space missions have used heat shields made from carbon composites containing carbon fibers and phenolic resin. One of the ways carbon composites relieve heat load is by allowing the phenolic resin to boil away, leaving behind a porous network of carbon fibers, which are oxidized at these high temperatures. University of Kentucky researcher Savio Poovathingal created the image below, which examines how hot gases diffuse through the porous network at the microscale. By examining this oxidation process both at the material's surface and deep in the carbon-fiber mesh, Poovathingal's simulations anticipate potential areas of failure and inform the design of materials that will reliably protect spacecraft as well as the people and instruments inside.

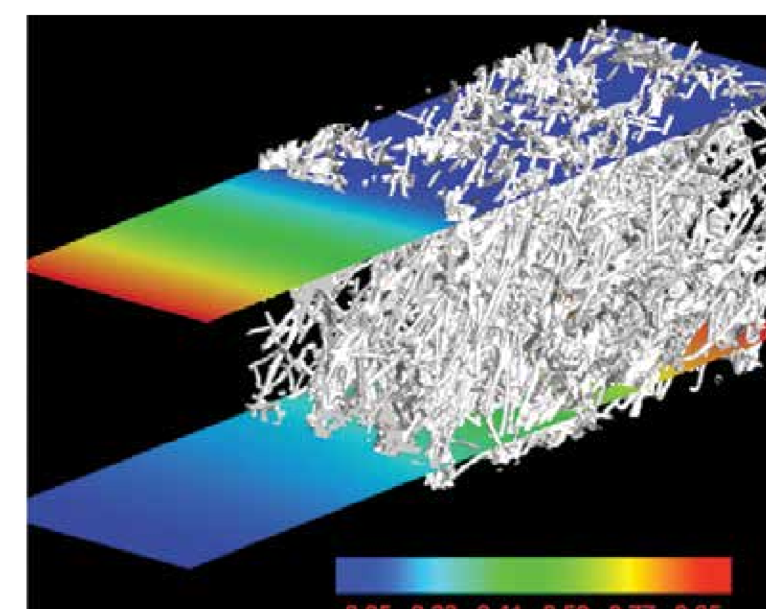
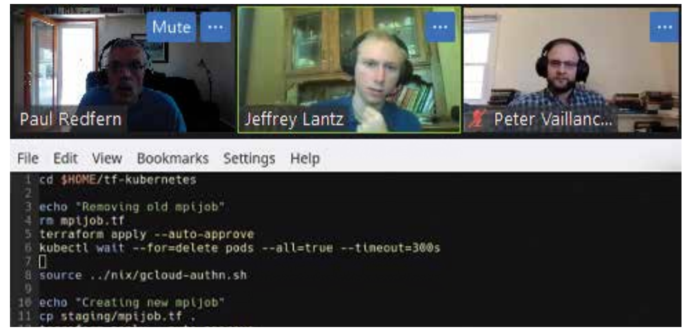


Image Copyright: *Savio J. Poovathingal, University of Kentucky.*

VISIONARY IDEAS FOR VIRTUAL EDUCATION



Cornell University student Jeffrey Lantz's (center) Zoom presentation on how to launch large computations in the cloud. Image courtesy of the Cornell Aristotle Cloud Federation project and copyright Paul Redfern, Cornell University.

REAL-WORLD RESEARCH EXPERIENCE, ONLINE

COVID-19 closures didn't stop students around the country from stretching their minds and gaining valuable research experience—they just did it from afar! While campuses were closed, online internships offered a venue for students to explore their interests and contribute to real-world computational science tools.

The National Center for Atmospheric Research (NCAR) sponsored 14 undergraduate and graduate students for its Summer Internships in Parallel Computational Science (SIParCS) program. Instead of arriving in Boulder, Colorado, ready to learn and socialize, the students were sent laptops preloaded with the software they would need and met virtually with each other and with mentors for professional development, networking, and skill-building sessions throughout the summer. Students contributed to projects in a wide range of areas, from machine learning to Earth science education to 3D printed weather stations.

Interns and program leads gathered online to kick off the National Center for Atmospheric Research (NCAR) Summer Internships in Parallel Computational Science program. Image copyright Virginia Do, National Center for Atmospheric Research.

In a separate program, four Cornell University students immersed themselves in advanced cloud computing technologies through the National Science Foundation Research Experiences for Undergraduates program. Jeffrey Lantz explored and compared the cost-effectiveness of different approaches to launching large scientific computations, while Priyanka Dilip focused on ways to use processing power more effectively to support research applications such as biomedical imaging. Matthew Farnese improved the pipeline used to identify signals of interest in the search for intelligent life beyond Earth, and Sherri Tan helped scientists predict the magnitude of wind gusts at major U.S. airports.

DIGGING FOR ROCKS IN THE CLOUD

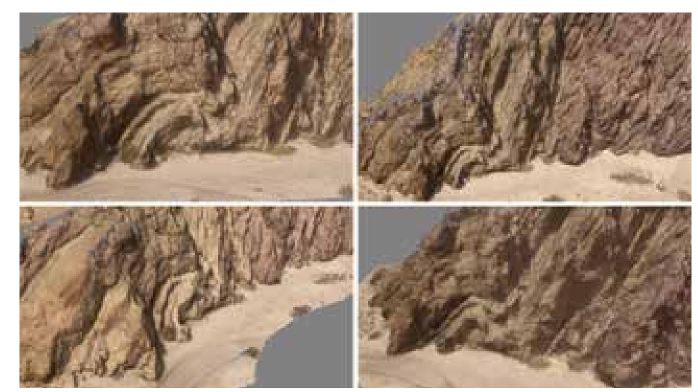


***Image Copyright:** Chelsea Scott, Arizona State University.*

How could students, stuck at home due to the COVID-19 pandemic, possibly get the hands-on skills that are a crucial part of geology education? With existing online tools and a little creativity, Arizona State University researcher Chelsea Scott developed an innovative virtual field camp to teach these skills remotely.

The virtual experience used OpenTopography, a National Science Foundation-funded program that provides online access to topography data and analysis tools at the San Diego Supercomputer Center in collaboration with Arizona State University and UNAVCO. By tapping into this data-rich resource, students virtually collected, plotted, and analyzed rock measurements in a simulated rock fold to unravel the history of the San Andreas Fault near Palm Springs, California.

AN IMMERSIVE EDUCATION

***Image Copyright:** Nicholas Polys, Virginia Polytechnic Institute and State University.*

The Visionarium at Virginia Polytechnic Institute and State University offers students and researchers a perspective they can't get anywhere else: a 360-degree, 27-million pixel dive into their visualization of choice. The 10-by-10 foot room offers an immersive experience complete with a wireless tracking system that lets users explore large-scale interactive visualizations.

Here, users explore the immersive room to compare positive and negative subatomic particles, known as pions. Researchers Jooyoung Whang, Nicholas Polys, and Markus Diefenthaler created the visualization with the multidisciplinary Center for Nuclear Femtography, whose mission is to synergize expertise in nuclear physics, computational science, mathematics, and visualization in order to understand the internal physics of the atomic nucleus. Interacting with massive, multidimensional data through 3D immersive experiences can shed new light on our universe's foundational structures and spur discovery for students and faculty alike.

CREATING FERTILE GROUND FOR COLLABORATIONS

While CASC meetings are an important venue for the research computing community to exchange ideas and information, the personal connections made are just as important, and often pave the way for new collaborations. One such collaboration, between Rutgers University and Durham University in the U.K., came about precisely because of those CASC-made connections.

Kristin Lepping is the Director of Business Operations, Grants, and Workforce Development at Rutgers University's Office of Academic Research Computing (OARC), a CASC member institution. When Dee Magnoni, Associate University Librarian, New Brunswick Libraries, approached OARC head James Barr von Oehsen with a funding opportunity, it became Lepping's job to make it happen. Because the award required U.S.-U.K. collaboration, she immediately thought of her friend Alan Real, Director of Advanced Research Computing at Durham University.

Lepping and Real owe their friendship to CASC meetings, which they both attend regularly. Attendees often say these meetings' small size and social activities set them apart from larger and more anonymous academic conferences. Fun events—like the baseball game where Lepping and Real first met—create space for attendees to form strong and lasting relationships that go beyond CASC meetings.

Thanks to this friendship, Rutgers and Durham University collaborated on a proposal for an award program jointly sponsored by the U.S. National Endowment for the Humanities and U.K. Research and Innovation. The program, New Directions for Digital Scholarship in Cultural Institutions, provides funding for U.S. and U.K. institutions to work together on transformational ways to bring cutting-edge digital methods—like artificial intelligence (AI) and machine learning—to cultural institutions such as libraries, archives, museums, and galleries.

Lepping approached Real, and within a week the two had gathered a team of librarians, archivists, and research computing experts that met regularly to draft the award proposal. When the two university teams came together, they were surprised and delighted to discover that both universities already maintain extensive collections of Japan's Meiji Period (1868-1912), leading them to ultimately propose exploring the use of computational methods in cultural institutions to create new knowledge about the exchanges between Japan, the U.K., and the U.S. using Durham University's Oriental Museum Collection and Rutgers University's similar William Elliot Griffis Collection.

"It was such an interesting synergy, because when all the folks [present on the first call] started talking about collections, it turned out the libraries had similar collections to work on," said Lepping. "All of the chips really fell into place. CASC has been such a great community and network. I go back to their resources on a regular basis."

Whether or not the proposal becomes a formal project, this across-the-pond partnership stands as a wonderful example of how CASC nurtures relationships that can inspire unexpected collaborations, propelling research in new directions.

An image from the Rutgers University William Elliot Griffis Collection depicting Griffis with students who accompanied him to Tokyo in 1871. Photographed by Uchida Studios, Tokyo.

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