Data Crunch
UCI Research Cyberinfrastructure Center is moving to CALIT2

Tactical Pivot
Startup faces turning point; finds new customer opportunities post-pandemic

Thermal Performance
Squid skin-inspired insulation material has myriad applications

Efficiency Hunters
New program will train students to conduct energy-efficiency assessments of local manufacturing businesses

Problematic Proteins
Researchers model the good, the bad and the ugly in protein aggregation

Curious Mind, Compassionate Heart
Computer science professor is committed to improving lives beyond the classroom
CALIT2’S NEWEST TENANT PROVIDES SUPPORT FOR COMPUTATIONAL CHALLENGES

Sharon Henry
A new resident is setting up shop in the CALIT2 Building.
The UCI Research Cyberinfrastructure Center (RCIC) serves hundreds of scientists and helps to make much of their breakthrough research possible.

The RCIC defines and maintains infrastructure for high-performance and high-throughput computing, research data storage and analysis, and scientific software tool integration for academic research at UCI. “You could look at us as a small supercomputer center,” says Philip Papadopoulos, RCIC director.

Papadopoulos, along with a team of six staff members, also provides support for researchers using the center’s resources, such as the HPC3, a high-performance community computing cluster that enables users to have access to a larger computing/analysis system.

Much of RCIC’s specialized work involves developing scientific software integration, he says. This software can have a multitude of purposes from analyzing gene sequences to first principles computational chemistry to statistical analysis.

“Complications come in when a piece of software from physics has a different set of requirements than a piece of software from chemistry, which has a different set of requirements from software in computational biology,” he says. “It isn’t worth the time of a domain scientist to try to figure out all of the details. We try to do much of that for them.”

Another challenge for RCIC is managing their computing resources. Research demands vary. One user may need to run 10,000 jobs, with each job fitting on a single physical node. Another will require one job with 1,000 cores – all at the same time, Papadopoulos says.

WE’RE USING A LOT OF COMPUTERS

“I think we’re one of the larger users of compute time,” says David L. Mobley, professor of pharmaceutical sciences and chemistry at UCI. Mobley uses computer methods to help guide pharmaceutical drug discovery. “We’re using a lot of computers for a long time, relatively speaking – 10 to hundreds of computers for a day or days.

“We do simulations or modeling that tries to predict binding,” he says. For a drug to work, it must bind to its target to trigger a biochemical change. This phase of drug development is largely trial and error and typically long and costly. Mobley accelerates the process by using physics-based algorithms, computers and powerful processors to predict interactions.

“We’re working on a system that’s been previously studied to make sure that our methods are working well enough that they can be used to discover new drugs,” Mobley says. The COVID Moonshot, a nonprofit, open-science effort to develop a patent-free COVID antiviral therapy,
“uses techniques that we work on and test on HPC3,” he adds.

**A COG IN THE RESEARCH MACHINE**

Papadopoulos joined UCI about four years ago, coming from the San Diego Supercomputer Center (SDSC), one of the nation’s first supercomputer centers. “The last machine I built there was about 10 times the size of what we have here,” Papadopoulos says. However, “once you get up to a certain level of complexity, it’s all the same. The size of our resource is a scaled version of what you would see at NCSA (National Center for Supercomputing Applications) or Texas (Texas Advanced Computing Center at the University of Texas at Austin). We all have the same problems. We build the same kind of software and have the same management infrastructure.”

The main difference with being part of a supercomputer center is the proximity to users, Papadopoulos notes. At SDSC, users might be across the country. “What I like about being at UCI is that we’re closer. Here, all our users are essentially local. Prior to COVID, I could go visit them in their office. In San Diego, I couldn’t sit down and have a cup of coffee with them.”

It’s that contiguity that bolsters Papadopoulos’ enthusiasm for relocating the RCIC to CALIT2 from its current location in the UCI Multipurpose Science & Technology Building. “Faculty members never step foot in that building,” he says lightheartedly, adding “I miss talking directly to people who are doing research.

“I feel like I have this place as a cog in the research machine where I help provide specialized infrastructure to assist in research. It’s not nearly so satisfying if you can’t talk to the people who are trying to discover the next drug, do machine learning, or doing chemistry calculations and need good people to make sure that the infrastructure is well run and well done from the software side.”

**LET ME TELL YOU ONE STORY**

Wei Li is an expert in cancer bioinformatics and endowed chair and professor of bioinformatics in the UCI School of Medicine.

Li harnesses big data to develop better diagnostics and therapies for disease. High-performance computing and data storage that can collect and manage huge-scale datasets and perform real-time data analyses are critical for his work. The RCIC’s capabilities are a major reason he decided to move to UCI, he says.

“Let me tell you one story about how they helped me,” Li explains, leaning forward to make his point. “We started our lab in 2020. Then one year later, with Philip’s support, we were able to publish a landmark paper in Nature Genetics.” The paper presents a new way to understand the human genome and why certain mutations in our genome will cause disease. “That paper is really data heavy,” he says. “We have data on 46 tissues from 467 individuals – more than 600 terabytes of data. It is a very important paper that would not exist without RCIC’s support.

“We’ll continue in this direction for diabetes, prostate cancer and primarily ALS. This is our ongoing work – all using the RCIC. We cannot do the job without their support,” he affirms.

**HAMMER OUT IDEAS**

When the renovation is complete, the RCIC will be housed on the third floor at CALIT2. Each of the seven offices will have floor-to-ceiling glass partitions and be configured into a U-shape. An open area in the center is designed to be a gathering place.

“When people need to work on something, they can close their door and it stays quiet,” Papadopoulos says. However, the visibility, “creates a place that’s open, where people routinely sit and talk with each other and hammer out ideas. My experience is a lot of the best ideas and germinations for new research proposals come from chatting with somebody, and a light bulb goes off in your head, or their head, and you say, ‘Hey we should do X. That’s a really good idea,’ and you go from there.

“We work with everybody on campus, but I think there’s a lot of things that we can do for various people who are in the CALIT2 building, and they just don’t know us yet. We’ll be much more visible over here.”
TECH STARTUP STRATEGICALLY PURSUES NEW MARKETS TO STAY SUCCESSFUL
“Startups are full of surprises,” says Aditi Majumder, CALIT2 researcher, professor of computer science, and founder and CEO of Summit Technology Laboratory (STL). “Perseverance and optimism are the key.”

Majumder started her company in 2015. With expertise in computer graphics, visualization and virtual reality, she developed a novel display technology that allows anyone to create collaborative reality experiences by precisely controlling the light emitted from multiple off-the-shelf projectors on objects and surfaces of any shape and size. The multiprojection mapping software creates a high-resolution, scalable plug-and-play display system and has applications in varied environments: education, trade shows, training simulations and entertainment.

With a National Science Foundation Phase I Small Business Innovation Research (SBIR) grant in 2017, STL was making good progress in growing its small business. It had presented collaborative reality experience displays at multiple venues, including the Seattle Museum of Pop Culture in 2018 and the Discovery Cube children’s science museum in Orange County in 2019, and began pursuing applications for tradeshows. It had grown from three employees in 2017 to nine in 2019. However, when the pandemic hit, this sector completely shut down, forcing the young company to pivot.

What could have been a serious slump for Majumder and STL turned into a fortuitous juncture. Her team had recently entered xTechSearch, a U.S. Army nationwide competition for nondefense businesses and startup technology companies to award and accelerate new technologies that could help solve Army challenges. Majumder made it to the top 50 and walked away with three free passes to the 2020 Association of the United States Army annual meeting and exhibit.

“This was a turning point for STL. We were able to explore many federal agencies and defense contractors at the conference and find the pain point for defense visualization needs,” says Majumder. Afterward,
Top: STL installed a multiprojector display at the Discovery Cube science museum in Santa Ana, simulating a helicopter cockpit for multiple users to experience a high-resolution video about the various sources of energy.

Bottom: The Seattle Museum of Pop Culture featured a Holodome exhibit, using STL technology to create a shared 360-degree immersive experience for users, without virtual reality headsets.

Left: Aditi Majumder’s company has received six Department of Defense contracts over the past three years for a total of $4.2 million in funding to develop projects, such as the Panalytics Pod, an almost 360-degree surround interactive visualization environment for multiple users to navigate through data analytics while engaging in face-to-face discussion.
Top: STL participated in an advanced battle management system exercise at Nellis Air Force Base in September 2020. The Decision Pod, a portable, large, high-quality interactive display, impressed the users.

Bottom: STL creates transportable interactive displays that can be used to enhance situational awareness and collaborative decision making in many different applications such as emergency response and disaster recovery.
she made an important contact through LinkedIn: retired Major General Stephen Clark, who has since joined STL as chief business officer. He was impressed by the STL technology and was able to apply his own experience to understanding the possibilities of projected collaborative displays for tactical field operations or in command and control centers.

“During any crisis, be it a war or natural disaster, first responders rely on critical data in order to make lifesaving decisions,” explains Clark. “With the proliferation of sensors and data analytics, the mass amounts of information available to operators can become obfuscated by the limited format available to display it. What we can absorb and understand through a 15-inch laptop is very different than when viewed on a 150-inch display.”

Clark notes that in defense and disaster management industries, millions of dollars are invested annually in digital visualization tools that combine artificial intelligence with Internet-of-Things sensors to speed overall decision making but very little to advance how it is displayed. “Since STL’s product is ruggedized and highly portable, it is perfect for tactical units that have to pack up and change locations often, as the system sets up in under 30 minutes with two people and breaks down in about 15 minutes,” he says.

After identifying the fact that its collaborative reality technology can enhance an important function within the defense industry, STL has attained six contracts to develop products with the Department of Defense Air Force. In the past three years, they’ve received two SBIR Phase 1, two SBIR Phase
2, one SBIR Direct to Phase 2 and one Small Business Technology Transfer (STTR) Phase 1 contracts, for a total of $4.2 million in funding.

Many of these products center around transportable interactive displays that can be used to enhance situational awareness and collaborative decision making in many different applications, such as command and control, base operations, emergency response, disaster recovery and intelligence analytics.

The STL team showcased one such product, the Decision Pod, to Air Force personnel in September 2020 at an advanced battle management system exercise at Nellis Air Force Base. The Decision Pod is a portable, pack-and-go, large, high-quality interactive display that can be either flat or curved (for greater immersion). It can be deployed by two people in under 30 minutes and requires no special power or audio-visual equipment. It was used as part of the exercise to visualize and explore data analytics created by 3D remote virtual ops platform Immersive Wisdom. According to Lieutenant Colonel Adam Chitwood, who led the exercise, “The tech demonstration exceeded all expectations. The big display was easy to see and was preferred by all users over VR goggles. After a few nights of reduced sleep, we found the big display much easier to use than a laptop screen.”

In 2021 with the STTR funding, STL explored the feasibility of using a hand gesture-based interface to not only control the data projected on their collaborative display by a UAV but also to fly the UAV. “We wanted to answer the question: Could we fly a small drone with our hand, as opposed to a joystick?” says Clark.

STL is piloting the system with an electric-powered, vertical takeoff and landing (eVTOL) aircraft. This would allow simultaneous visualization of terrain conditions and other areas observed by the UAV as its path is continuously manipulated – all controlled by the user’s hand gestures.

“This is much more lucid,” explains Clark. “As the user, from the time I see and know what I want to do, my hand is already moving there naturally. I don't have any man-machine interfaces that cause delays. This will provide key decision-makers rapid, precise understanding of salient terrain features, spatial relationships between assets and target areas, time-and-distance challenges for logistics, in addition to air traffic density.”

Even with seven patents issued, three pending and recent funding successes, Majumder is looking toward
future markets for the next growth opportunity. “Our immediate goals are to take the products we have built for the defense sector and apply them to the emergency management and disaster recovery and risk mitigation market. In the long term, we want to address other markets with the same technology,” says Majumder.

She thinks medical could be next. The team is working on a product to project surgical stencils that could be used by plastic surgeons for guidance, training and remote collaboration in underserved areas of the world. It would allow a surgeon to project guidance directly onto the body part that needs surgery, for instance a child with a cleft lip. The system projects light, conformal to the surface area, to indicate incision points rather than the current practice of inking.

Muhammad Twaha Ibrahim, a UCI graduate student in computer science, is working on the stencils as an STL intern. He’s shadowed a few surgeons to understand the current practice. “These incision points mark important facial landmarks. Ultimately, the position of these points tells the surgeon where to make the incisions and then stitch the lip so the reconstructive face looks correct. Obviously, it’s really important to get it right.”

Ibrahim says that these surgeries typically occur when children are very young, under 1 year old. Their skin is tender. The STL surgical stencils could be safer and allow for more online collaborative consultation. The company has submitted a fast track grant proposal to the National Institutes of Health for funding the project.

“Building a good team is hard and takes perseverance,” says Majumder. “It is the biggest hurdle that a startup faces. It took me years to build the solid team of 10 that we have today. A blend of experience and dynamism is what makes the magic.”

She also says that having her Visualization Lab located in the CALIT2 building is helpful, as it’s in the midst of the UCI ecosystem on campus, which is critical to fostering collaborations with researchers in other schools.

“I am forever grateful for the space that CALIT2 provided us during those early years and the connections it brought for us,” explains Majumder. “CALIT2 connected us with a vibrant student community, helping us to give back as well. We have multiple interns who are getting exposed to our new company and technology, which is a huge blessing.”
Researchers in CALIT2’s Lab for Cephalopod-inspired Materials have invented a squid-skin inspired material that can wrap around a coffee cup to shield sensitive fingers from heat. They have also created a method for economically mass producing the adaptive fabric, making possible a wide range of uses.
UCI ENGINEERS DEVELOP A METHOD FOR ECONOMICAL MASS PRODUCTION OF INSULATING MATERIAL

In the future, you may have a squid to thank for your coffee staying hot on a cold day. Drawing inspiration from cephalopod skin, researchers in the CALIT2 Building invented an adaptive composite material that can insulate beverage cups, restaurant to-go bags, parcel boxes and even shipping containers.

The innovation is an infrared-reflecting metallized polymer film developed in the first-floor laboratory of chemical and biomolecular engineering Associate Professor Alon Gorodetsky. In a paper published in Nature Sustainability, the research team describes a large-area composite material that regulates heat by means of reconfigurable metal structures that can reversibly separate from one another and come back together under different strain levels.
“The metal islands in our composite material are next to one another when the material is relaxed and become separated when the material is stretched, allowing for control of the reflection and transmission of infrared light or heat dissipation,” says Gorodetsky.

“The mechanism is analogous to chromatophore expansion and contraction in a squid’s skin, which alters the reflection and transmission of visible light.”

Chromatophore size changes help squids communicate and camouflage their bodies to evade predators and hide from prey. Gorodetsky says by mimicking this approach, his team has enabled “tunable thermoregulation” in their material, which can lead to improved energy efficiency and protect sensitive fingers from hot surfaces.

A key breakthrough of this project was the UCI researchers’ development of a cost-effective production method of their composite material at application-relevant quantities. The copper and rubber raw materials start at about a dime per square meter with the costs reduced further by economies of scale, according to the paper. The team’s fabrication technique involves depositing a copper film onto a reusable substrate such as aluminum foil and then spraying multiple polymer layers onto the copper film, all of which can be done in nearly any batch size imaginable.

“The combined manufacturing strategy that we have now perfected in our lab is a real game changer,” says Gorodetsky. “We have been working with cephalopod-inspired adaptive materials and systems for years but previously have only been able to fabricate them over relatively small areas. Now there is finally a path to making this stuff roll-by-roll in a factory.”

The developed strategy and economies of scale should make it possible for the composite material to be used in a wide range of applications, from the coffee cup cozy up to tents, or in any container in which tunable temperature regulation is desired.

The invention will go easy on the environment due its environmental sustainability, said lead author Mohsin Badshah, a former UCI postdoctoral scholar in chemical and biomolecular engineering. “The composite material can be recycled in bulk by removing the copper with vinegar and using established commercial methods to repurpose the remaining stretchable polymer,” he says.

The team conducted universally relatable coffee cup testing in their laboratory on the UCI campus, where they proved they could control the cooling of the coffee. They were able to accurately and theoretically predict and then experimentally confirm the changes in temperature for the beverage-filled cups. The researchers were also able to achieve a 20-fold modulation of infrared radiation transmittance and a 30-fold regulation of thermal fluxes under standardized testing conditions. The stable material even worked well for high levels of mechanical deformation and after repeated mechanical cycling.

“There is an enormous array of applications for this material,” says Gorodetsky. “Think of all the perishable goods that have been delivered to people’s homes during the pandemic. Any package that Amazon or another company sends that needs to be temperature-controlled can use a lining made from our squid-inspired adaptive composite material. Now that we can make large sheets of it at a time, we have something that can benefit many aspects of our lives.”

Joining Gorodetsky and Badshah on this project were Erica Leung, who recently graduated from UCI with a doctorate in chemical and biomolecular engineering, and Aleksandra Strzelecka and Panyiming Liu, who are current UCI graduate students. The research was funded by the Defense Advanced Research Projects Agency, the Advanced Research Projects Agency – Energy and the Air Force Office of Scientific Research. The researchers have applied for a provisional patent for the technology and manufacturing process.
STUDENTS ARE ON THE QUEST TO FIND WEAK SPOTS IN ENERGY PERFORMANCE

The United States’ manufacturing sector is massive — accounting for 12% of the nation’s economy, employing nearly 13 million people (8% of the workforce) and generating 57% of U.S. exports. It also consumes about one-third of all energy produced in the U.S. — a high cost financially as well as environmentally. Industries are facing increasing pressure to make their processes more sustainable but aren’t always aware of potential ways to improve energy efficiency.

CALIT2’s newly launched Sustainable Manufacturing Alliance for Research and Training Industrial Assessment Center (SMART IAC) program aims to help local manufacturers reduce their carbon emissions and cut energy costs by offering no-cost, energy-efficiency assessments. In addition, the SMART IAC will address the growing shortage of engineering professionals with energy and manufacturing-related skills by training students through hands-on participation in these assessments, says G.P. Li, SMART IAC co-director and CALIT2 director.

Last September, UCI was selected as one of 32 universities nationwide to become a U.S. Department of Energy Industrial Assessment Center. IACs provide small- and medium-sized manufacturers with assessments and recommendations on energy efficiency, productivity
Previous page: SMART IAC fellow and UCI electrical engineering and computer science graduate student Rohit Vasu tests a new piece of equipment that the energy auditors will use in onsite assessments.

Top: During assessment training, UCI engineering undergraduate students Hayde E. Abrego Onofre (left) and Meraf Amare gather information on specific systems, processes and equipment.

improvement, sustainability and competitiveness as well as measure the impacts of these recommendations on reducing greenhouse gas emissions. The university will receive nearly $2.25 million of a $60 million investment by the DOE. The grant will also fund energy-efficiency assessments to be provided free of charge to manufacturing facilities in the area.

SMART IAC is housed at CALIT2 and operates along with two satellite centers at California State University Northridge (CSUN) and Cypress College.

BEACON (Building Energy Assessment for Commercial Optimization toward Net Zero) is a collaboration
innovate | integrate | incubate | ignite

By working in tandem, UCI engineering students will have the opportunity to see the process from a technician’s view and, by the same token, technicians are going to say, ‘OK, now we understand what engineers do.’ That is going to be a good collaboration,” he adds.

Since opening earlier this year, SMART IAC has launched a website (smartiac.calit2.uci.edu), recruited students and set up an application process for businesses seeking free energy assessments.

“The SMART IAC will benefit the underserved and underrepresented STEM students at UCI, CSUN and Cypress College,” says Bingbing Li, SMART IAC co-director and associate director of the Autonomy Research Center for STEAHM at CSUN. “And it will improve the energy efficiency and waste management of the small- and medium-sized manufacturers and businesses located in Southern California.”

The center expects to conduct at least 20 assessments of small- and medium-sized manufacturers annually. About 10 SMART IAC fellows will be recruited each year from UCI and CSUN to participate in the training. In the winter quarter, six engineering students (four from UCI and two from CSUN) were accepted into the program.

**FINDING OPPORTUNITIES**

“The first step is training,” says Li Zhao, SMART IAC assistant director and technical director of the California Plug Load Research Center. “Students are introduced to the fundamentals of industrial equipment and processes. They’ll study previous energy assessment reports and learn how to develop an assessment strategy and checklist for an industrial facility. The objective is to prepare students to be energy auditors or energy engineers and find opportunities for improvement in energy performance.”

Meraf Amare, a SMART IAC fellow and third-year electrical engineering student at UCI, says, “My interest in energy efficiency really began because I wanted to learn more about sustainability and how it overlaps with my interest in engineering. There are so many moving parts in just one building,” she adds. “It’s been surprising to learn about just how many different systems have to work simultaneously in order to have clean water, cold air conditioning and things that we normally take for granted.”

**LIKE A TREASURE HUNT**

Prior to visiting a facility to be assessed, students will spend four to six weeks developing a pre-assessment or preliminary analysis. “It’s how we form a strategy,” Zhao says. “The more prepared we are, the more we can find.”

The preliminary analysis defines the scope of the assessment and considers a bounty of criteria submitted by the facility. General information about the building, a list of energy-consuming equipment, operating schedules, energy bills and other materials help the team understand the facility’s current energy situation and may identify simple operational and maintenance improvements. The pre-assessment also helps the team develop a checklist to designate what data will be measured and collected on-site and the types of instrumentation and diagnostic equipment that will be needed.

Armed with a strategy and their checklist, a team of eight SMART IAC members will be ready to conduct the one-day, on-site assessment. “Students will be prepared to go into real-life industrial settings to see the action – motors, compressors, equipment – then identify and measure the problems, and report the data,” Zhao says.

Depending on the facility, the energy assessment team will target specific systems, processes and equipment to find measurable, verifiable and useful energy-efficiency opportunities.

Measurements and a data inventory are usually conducted on different energy systems (pumps, fans, compressed air, steam and process heating). Other common data measured are liquid and gas fuel flows, electrical measurements (such as voltage, current intensity and power), temperatures of solid and liquid surfaces, pressure of fluids in pipes, furnaces, exhaust gases emissions, relative humidity and luminance levels (the measurable quality of light).
“Finding hidden energy savings is like being on a treasure hunt, and the energy assessment team is like a treasure hunter,” he says. “It’s a treasure hunt to find the weak spot where a facility isn’t aware they could save more energy.”

“I wholeheartedly agree,” says Hayde E. Abrego Onofre, a civil engineering sophomore at UCI. “However, we can’t go out and expect to analyze an air compressor, for example, and suggest a change within the machinery itself. Here’s when the treasure hunt plays in – looking around the air compressor for components such as leaks and other details that can deter from maximizing proper usage,” she says. “These tricks to spot details not only optimize energy efficiency, but also impact the people and buildings of the whole manufacturing system.”

Following their on-site visit, the team will work six to eight weeks developing an assessment report containing recommendations for the facility, says Chelsea Choudhary, SMART IAC program manager. “Companies like to save money,” she adds. “The report calculates their energy savings, payback years and potential savings.”

IAC assessments regularly identify more than $130,000 in potential annual savings opportunities, according to the DOE.

“It’s really interesting to see all the small changes that a company or facility operator can adopt and watch it balloon to greater savings,” Amare says. “Sometimes the discourse about sustainability, climate change and other related topics involves a lot of theoreticals, and looking 20 or 30 years into the future. Efficiency audits can provide concrete actions for facilities to begin improving almost immediately,” she says. “I think this is empowering to not only the facility, but to our team as well. It feels like you are making a real difference in the drive toward a greener future.”

“It’s been surprising to learn about just how many different systems have to work simultaneously in order to have clean water, cold air conditioning and things that we normally take for granted.”

Nathaniel Harrison, UCI civil engineering undergraduate, measures luminance levels while training to measure energy efficiency in lighting.
Problematic Proteins
RESEARCHERS EXTEND MODELING TECHNIQUES TO SEEK NEW INSIGHTS INTO CHRONIC DISEASES
Proteins, often called the workhorses of life, are the macromolecules in living cells that do the important job of keeping us alive and healthy. To function well in the human body, these molecular machines must come together in the right ways, at the right times and in the right numbers. However, that doesn’t always happen; sometimes protein aggregation, associated with the formation of numerous diseases, can cause harm.

To better understand how proteins associate and aggregate, CALIT2 researcher Carter Butts turned to the same methods he uses to analyze social networks. Butts, a professor of sociology with expertise in computational statistics and network analysis, joined Rachel Marten, UCI professor of chemistry, molecular biology and biochemistry, to integrate methods from across their disciplines. They are developing computationally scalable techniques for modeling protein aggregation, and then connecting those models with experimental measurements. The goal is to find new insights into the biology that lies behind some of the most serious chronic diseases affecting the country’s aging population, such as Alzheimer’s, Type 2 diabetes, cataracts and others.

According to Butts, in diseases such as Alzheimer’s or Lewy body dementia, proteins self-assemble into highly structured one-dimensional crystals, called amyloid fibrils, which the body is unable to break down. “Over many years, the proliferation of fibrils wreaks havoc on our brains and is ultimately lethal,” he says.

Likewise, in the environment of the eye lens, there is a finite store of special proteins that bend light and allow the eyes to focus. Over time, after exposure to ultraviolet light and other potential harms, the eye lens proteins eventually become damaged and can amass into ever larger molecular clumps. Those clumps result in cataract – the world’s leading cause of blindness. “But not all protein self-assembly is bad: many proteins, like the alpha-crystallins that round up misfolded proteins before they can cause harm, join together in myriad temporary arrangements as they perform their duties,” explains Butts.

So, what do proteins and social networks have in common? Like proteins, humans form complex structures of relationships that evolve over time, where the presence of one relationship can affect others. This dependence between relationships can drive the emergence of social cohesion, centralization and even group boundaries. “While the protein aggregation that leads to amyloid fibrils differs in many ways from the formation..."
of project teams or high school cliques, we have shown that the same methods used to capture dependence in social networks can also be used to model the aggregation process,” says Butts, whose Networks, Computation and Social Dynamics Lab is located on the third floor of the CALIT2 Building.

His research includes both the creation of modeling techniques that can be used effectively with existing experimental data, as well as the collection of new data to validate the modeling work. “This work will result in a collection of novel methods for the study of protein aggregation – the good, the bad, the ugly – that are both statistically principled and empirically grounded, as well as biologically relevant,” he says.

The project is being funded by the NIH, via a joint program between the NSF Division of Mathematical Sciences and the National Institute for General Medical Sciences to support advances in the mathematical and computational sciences that provide fundamental insights into health biology. It represents the next phase in a previous NSF-funded project that the two researchers conducted, which pioneered the use of network models for amyloid formation. The $1.8 million grant will be administered through CALIT2. As an interdisciplinary collaboration between researchers combining innovations from multiple sources, the project exemplifies the vision of CALIT2 as a catalyst that brings together researchers with distinct perspectives to address important problems.

“It is a fascinating problem at a fundamental level, and it has such important consequences for health,” says Martin, who has been working on protein aggregation since 1999, investigating why some proteins are highly soluble, and others are not. “They are all made of the same building blocks, 20 amino acids, but some are much more prone to aggregation than others. I am very excited that this award will enable us to directly measure protein aggregation processes under different conditions and test the predictions our team made in earlier work.”

Butts and Martin hope that the project can substantially transform our ability to predict phenomena related to protein aggregation and model a wide range of protein interactions using a single formalism. This would help address the basic phenomenon of protein association and aggregation that underlies problems of immense social concern. “These include diseases such as Alzheimer’s, cataract, and Type 2 diabetes that are increasingly prevalent in our aging population, as well as economic costs and food security concerns related to prion diseases in cattle and other animals. Our research has the potential to inform the search for solutions to these serious societal problems, resulting in both economic savings and improvements in individual lives,” says Butts.

“Those diseases have serious economic costs, both because treatments are expensive and because of more indirect costs from people becoming disabled due to diabetes or going blind from cataract,” says Martin. “Alzheimer’s and Parkinson’s diseases are even worse, because they are so debilitating and because the underlying causes are still not well understood. I believe our approach to modeling network properties rather than structural properties is unique.”
Face of CALIT2

CURIOUS MIND
DEDICATED COMPUTER SCIENTIST MAPS HIS OWN PROFESSIONAL JOURNEY
Curiosity killed the cat, goes the old adage. But for Sergio Gago-Masague, curiosity created an unexpected career.

The path to becoming a UCI assistant professor of teaching in computer science was winding and uncertain for Gago-Masague. Growing up in Barcelona, Spain, in a working-class family, he found himself more concerned with making a living. His father, an electrician, urged him to find a job – a trade like his. Gago-Masague did just that: “I have always worked since I was 18.”

But his curiosity enticed him to look beyond the limits of a single trade. It also led him to be the first in his family to go to college.

Gago-Masague’s curiosity about computers ignited at his cousin’s birthday party. He was 8 years old and became entranced by his 13-year-old cousin’s birthday present: a new computer. It turned out to be a gift that would give Gago-Masague a lifetime’s focus.

“I didn’t even know what a computer was,” says Gago-Masague. “It was an Amstrad PC1512, powered with an Intel 8086 CPU, no internal hard drive, and two floppy drives to run MS-DOS 3.2.
She told me how to start and operate the computer, and run programs and games.” From that day on, every time he visited, he sped past the cursory relatives’ greetings and made a beeline to the computer. Then he’d lose himself for hours. “It was a new world for me,” he reminisces.

At 12 years old, he received his own computer and would spend days on it, not even stopping for meals, so his parents had to call him for dinner. At 16, he learned how to assemble computers, and at 18, he started working as an IT help desk technician.

Growing up in the 1980s, it wasn’t clear what the future of computers would be. His father urged Gago-Masague to follow his path as an electrician and work in the family business. “At the time, there was a huge rate of unemployment in Spain,” recalls Gago-Masague. It was practical advice that made sense.

After working as an electrician assistant for a while, he decided to “shoot for the stars” and applied to one of the most selective engineering programs in Barcelona: industrial engineering at the Polytechnic University of Catalonia (UPC). The program allowed Gago-Masague to explore many areas in engineering. And the following year, to his delight, the university offered a concentration in computer science for the first time.

“When I finished, I wanted to work in the overlap of computer science and engineering,” says Gago-Masague. “I wanted to see how they could create solutions to real-world problems.”

Gago-Masague continued to work. “I’ve always had one foot in academia and one foot in industry,” he explains. He eventually changed jobs to focus on robotics, and in 2012, his employer co-sponsored him to enroll in the California-Catalonia Balsells Fellowship Program at UCI. Established in 1995 by Pete Balsells and his family, the program’s main goal is to prepare the most talented students from Catalonia in their pursuit of graduate degrees and postdoctoral training in engineering or computer sciences. As a testament to the program’s success, Gago-Masague is now the associate director of the program.

Why UCI? “I fell in love with California,” shares Gago-Masague. “It seemed like a nest of technology with a diverse population. And Orange County seemed like it could become the next Silicon Valley, not vertically, but horizontally.” Even though he had to leave everything behind, and adapt to a new country and culture, he made the leap and came alone, telling his then-
girlfriend, now wife, Susana that he would be back in a year.

During the first year at UCI, Gago-Masague worked as a postdoctoral researcher in the Biorobotics Lab with his adviser David Reinkensmeyer, professor of mechanical and aerospace engineering, and anatomy and neurobiology.

They worked on interactive virtual characters, to help people going through rehabilitation – to engage them and give them real-time feedback about their exercises. “One of the main issues of rehabilitation is that people have difficulty getting and staying motivated,” he explains. “The strategy was both to take patients’ little progress and amplify it so they could see improvement, and to create a human-like interface to provide patients with feedback and encouragement, as a human coach would do. I got really, really excited about what I was doing with Reinkensmeyer,” says Gago-Masague.

“Sergio had an exceptional ability to solve multidisciplinary problems by learning and integrating new fields, and by creating strategic work plans that targeted core bottlenecks,” Reinkensmeyer remembers.

Gago-Masague also started interacting with G. P. Li, CALIT2 director. “I showed him what I was doing, and he said there was an opportunity to continue similar work in CALIT2.” That work led to multiple collaborations, which included principal investigator Michelle Fortier, associate professor in the Sue & Bill Gross School of Nursing. Fortier was looking for support to implement Pain Buddy, a game-based interface to help pediatric cancer patients communicate their symptoms, particularly their pain levels.

“During chemotherapy or other types of therapies, it’s very important to know patients’ symptoms and pain levels. But many times, children can’t communicate well with clinical staff,” says Gago-Masague. “Also, parents may not be as objective as we would wish them to be.”

“Sergio and I began our collaboration many years ago when I was working to establish my program of research to develop and implement innovative means of managing pain in children undergoing treatment for cancer,” says Fortier. “We presented our idea for a mobile health intervention unlike anything available at the time, and Sergio was completely on board and assembled a team of students and investigators to take this plan to fruition.
“Sergio has worked tirelessly over the years to bring his creativity and expertise to our project and has helped us successfully obtain significant funding over the years to reach our goal of a multisite effectiveness trial to demonstrate that Pain Buddy is a helpful intervention for children to manage pain and symptoms during treatment. I am so grateful for this collaboration and look forward to a long future of working together.”

His participation in Pain Buddy and other health-related projects has been recognized by the National Institutes of Health awarding $6.9 million in funding. One of these was Mi Propio Camino (My Own Way), an app developed to help Spanish-speaking patients with hypertension remember to take their medications and encourage lifestyle changes. The project was funded by the NIH’s National Heart, Lung and Blood Institute, and Gago-Masague worked with John Billimek, principal investigator and associate professor and vice chair of UCI’s Family Medicine in the School of Medicine, to build an Internet of Things intervention that addresses a local, medically underserved Latino community. However, the applications can reverberate into numerous areas of health and wellbeing everywhere through its user-friendly interface and thoughtful approaches.

Concurrently, in 2011, Gago-Masague started collaborative research with the California Plug Load Research Center (CalPlug), which seeks to improve energy efficiency in the use and design of plug-load devices.

Gago-Masague also created and heads the CALIT2 Engaging Technology and Application Design (ETAD) Lab. He has been increasingly involved in ICS-focused research such as pervasive computing, user-centric software design, serious games, IoT and active learning. Gago-Masague has received grants for continuing this work, including an NSF-sponsored cybersecurity project now in its second year.

Top: Mi Propio Camino (My Own Way) is an app designed to help Spanish-speaking patients remember to take their medications and make lifestyle changes.

Bottom: In front of graphical presentations of data collected from their PMUI app, CalPlug researchers, from left, Joy Pixley and Gago-Masague, and field-testing coordinator Sabine Kunrath show off the energy monitoring hardware used in their survey.
But all of his varied interests have a common goal: creating interfaces that communicate meaningfully and improve people’s lives.

While continually excited by his own research, Gago-Masague became increasingly interested in helping others. He found he truly enjoyed mentoring students, which led him to consider teaching. He began as a lecturer and from 2015-18, he taught a variety of courses in computer science. In early July 2018, Gago-Masague became an assistant professor of teaching at the Bren School of Information and Computer Sciences.

Even as a full-time faculty member, he continues his lab activities and projects in CALIT2. “It was kind of overwhelming, but I didn’t want to give up anything,” he says. “I have always had a hard time letting things go.”

He also started a family when Susana, who is an engineer with a master’s degree in civil engineering, eventually followed him to UCI. They now have two young children, who are flourishing in University Hills.

However, Gago-Masague is not only concerned about the future of his own children. He’s actively engaged in the future generations of college students.

Above: Gago-Masague celebrates his birthday with some of his students and lab staff. He has become a beloved mentor, teacher and leader on campus.

Right: Gago-Masague’s wife, Susana Anacleto-Lupianez, graduated from UCI with her master’s degree in civil engineering in 2014, when President Barack Obama was the keynote speaker at Anaheim Stadium. She plans to defend her Ph.D. thesis at UCI in fall 2022.
Ten years ago, Gago-Masague uprooted from his hometown in Barcelona and put down new roots at UCI. Now his family tree is growing with his wife, Susana Anacleto-Lupianez, their 4-year-old daughter Norah and 5-month-old son Bruno.

He has been developing a capstone project program in computer science to help fix the "leaky STEM pipeline" and boost employment opportunities. "Underrepresented STEM students don’t always have the opportunities or confidence to compete for highly qualified jobs or to see how their work in the field could help their communities," he explains. "A capstone program with industry-sponsored projects provides students with valuable hands-on experience with real-world problems and allows them to be more competitive for seeking employment."

“It’s a win-win situation,” he adds. “Students get experience and companies have a chance to train and screen excellent potential interns and employees.”

He also serves on the admissions board of the University of California. “It’s given me a good vision of how admissions are handled and the current challenges and opportunities,” says Gago-Masague.

Just as Pain Buddy helps to ease the pain in children, Gago-Masague works to lessen the challenges for those hopeful and curious first-generation, low-income students, as he once was. “I’m very sensitive to students who don’t have easy access and all the struggles that come with that,” he says.

Through his research, teaching and service, Gago-Masague is paving the way for students to succeed in their programs and realize their dreams, whatever path they may take.
In January, UC Office of the President announced the expansion of CALIT2 to include UC Riverside (pictured) as a third campus partner in the multidisciplinary research institute, joining founding members UCI and UCSD.

“We have focused research areas that are complementary to existing research and faculty strengths at San Diego and Irvine,” noted UCR Chancellor Kim A. Wilcox. “These areas are of critical importance to the future of all Californians, including clean transportation and infrastructure, clean energy and fuels, agriculture technology and food security, as well as natural resource management.”

Faculty and students at UCR will benefit from access to shared-use CALIT2 facilities in Irvine and San Diego, including specialized labs, world-class nanotechnology facilities, wired and wireless infrastructure, and other technical resources. The three campuses will work closely to coordinate joint research and develop projects.
Under the direction of Professor G.P. Li, CALIT2@UCI develops IoT technology-based innovations in a multidisciplinary research environment. By integrating academic research with industry experience, the institute seeks to benefit society, incubate new technology companies and ignite economic development. CALIT2 focuses on the digital transformation of healthcare, energy, the environment and culture.

SPRING IS IN THE AIR . . .

After nearly two years of a remote reality, the UCI campus is coming back to life. Researchers and students are enjoying conversations over coffee or working on assignments together in the CALIT2 Building courtyard. The umbrella tables provide just enough shade to make outdoor networking and brainstorming sessions a comfortable spot for igniting the next generation of bright ideas.

Photo: Sharon Henry