STRATEGIC PARTNERSHIP PROGRAM

Vision Report

Georgia Tech Computational Science and Engineering

Whether you're involved in creating new products, detecting intruders, treating patients, or boosting national security, you're only as good as your team. That means you not only have to have the talent in-house, but you have to constantly be on the lookout to nurture and acquire new talent. When you work with the **Strategic Partnership Program at Georgia Tech**, you'll expand your team and partner with people who can help you conquer the grand challenges you face today and in the years to come.

The **Strategic Partnership Program, from the School of Computational Science and Engineering**, is made up of computer scientists, engineers, and other scientists whose research, in one way or another, involves uncovering the rules, patterns, and relationships of the world. By understanding these principles, we can astronomically increase our chances of success, whether that's curing the disease, stopping the bad guys in their tracks, or building world-changing solutions.

How we can help you

Joining the **Strategic Partnership Program** gives you access to the world's top thinkers, the people who have the skills, imagination, and expertise to help you solve the world's most daunting challenges today and make the right predictions that will put you in the driver's seat for tomorrow.

In looking at the world we can see that we are moving toward a data-rich economy. We're experiencing computation at scales never before seen and every sector, whether it be health, national security, environment, manufacturing … you name it, is looking at data science and what it means for their company. It's critical to figure out how to integrate new data and technology into your business so you can remain at or rise to the top of your field.

By working with and supporting the Strategic Partnership Program your company will have a vibrant link to the world's best talent in computational science and engineering, high-performance computing, and big data. Whether you're in industry, government, or research, when you join our program you'll have the opportunity to build relationships with our faculty leaders and gain access to their research to help you advance your organization's goals.

In addition, you'll gain direct access to our diverse pool of graduate students. You'll also get the opportunity to shape the next generation of computational and data scientists by giving feedback to the Computational Science and Engineering academic program curriculum.

At the Strategic Partnership Program, the word, partnership, is key to the kinds of relationship we're focused on growing. That's because we can develop more knowledge and solve more problems more quickly when we work together than we can alone.

What's more through our annual partners' meeting, you will have an opportunity to exchange ideas, and even collaborate with other partners — competitors as well as peers.

We harvest the strongest minds in the field to take part in the Strategic Partnership Program. Our faculty has the ingenuity to help you understand where advancements are heading so you can have the right information when you're deciding where to invest your resources. Not only that, but we can help you validate decisions you've already made, or give you the knowledge you need to redirect your investments.

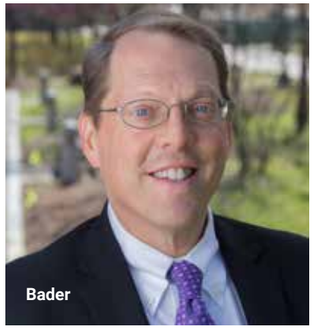
We've identified roughly five areas where we can increase your chances of success.

We can help you …

1. **Measure, predict, and shape the behavior of your customers, employees, and competition.**
2. **Discover hidden relationships, connections, and results by using visualizations to connect people to your data.**
3. **Rapidly investigate the natural properties of materials and bio-organisms.**
4. **Increase the power of investigations and the amount of available knowledge by connecting the cloud and isolated databases.**
5. **Create novel computing solutions for your particular needs.**

When you harness our expertise in high-performance computing and big data, we can uncover the information you need to triumph in your next endeavor. ■

Finding tomorrow's best talent


Bader

Any business or agency lives or dies on the quality of its talent. When you take part in the **Strategic Partnership Program**, we not only connect you with our stellar and diverse faculty, we also introduce you to the next generation of superstars, our graduate students. Coming from all corners of the world, with a vast variety of experiences and outlooks, our students are the cream of the crop.

You'll have the opportunity to learn from them at hosted lunches and informal gatherings where you can intimately get to know them, their ideas, and their skills. You'll also be able to review recruiting prospects through our resume book and connect directly with them through email.

You'll be able to tell us in-person exactly what skills and talent you need from prospects so that we can create the kind of educational experience that is most fruitful for our students as well as their employers.

We're looking for a true partner, not a mere funder. We believe if we're going to tackle the big mysteries and grand challenges of the future, we need to work together with the people who are on the front lines. We need to cooperate in order to explore the big questions as well as their consequent unknowns. We have to discover the relationships between, as well as predict and even shape, a host of human behaviors and their outcomes. We must be able to connect the data we have access to and use the cloud to investigate physical and chemical properties, even identifying new affiliations. By linking our expertise with your ambition to solve your organization's challenges, we can unveil a new world filled with hope, promise, and prosperity for all.

David Bader
Professor and Chair
School of Computational Science and Engineering
College of Computing, Georgia Institute of Technology

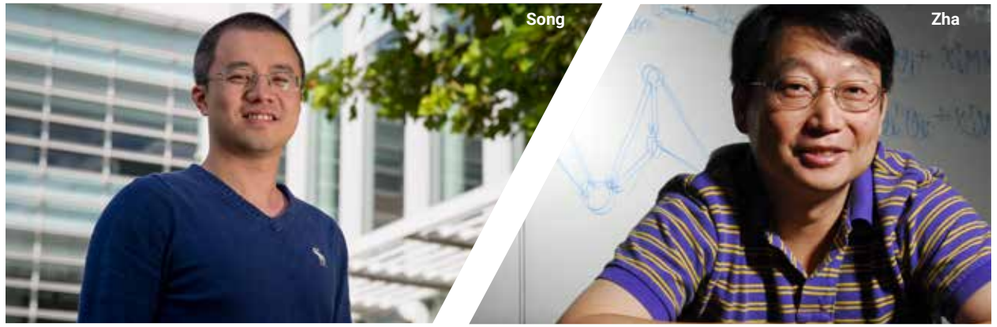
The Strategic Partnership Program allows partners to:

1. **Forge research relationships with faculty and attend an annual partners-only meeting.**
2. **Keep up with the latest research through our seminars, events, and news.**
3. **Get to know our faculty and graduate students face-to-face in school-hosted lunches and informal meetings.**
4. **Shape the kinds of computational and data scientists you want to hire with invited feedback on the Computer Science and Engineering (CSE) graduate program curriculum.**
5. **Connect directly to your workforce recruitment pool through email access to our students.**
6. **Review the most promising recruitment prospects with the Graduate Student Resume Book.**
7. **Extend your brand to the wider CSE community through placement of your corporate logo on the CSE website and Strategic Partners Wall.**

We can help you … Measure, predict, and shape the behavior of your customers, employees, and competition

Perhaps nothing is as fraught with risk as trying to understand and predict human behavior. Yet so many avenues of business and government, whether it's the retail industry, law enforcement, or just plain and not-so-simple traffic engineering, require being able to first understand, then predict, and even steer human behavior into desired domains.

Using computer intelligence in this realm has largely been a matter of developing algorithms that work well enough in most circumstances. However, this method breaks down when the network you're investigating gets too large. There are just too many factors that influence behavior. One area that's fraught with complications like this is when you're trying to understand and predict the behavior of customers.


Song

Zha

"It's complicated," says **Le Song**, associate professor in CSE. "We don't observe every single detail of how a customer decides what to do. We don't know if there's a single formula that can help us determine their behavior, so methods that are based on predetermined rules aren't good. Deep learning is far more flexible in learning complex human behavior."

Because deep learning focuses on recognizing patterns instead of a straight formula, intelligence systems using deep learning can adapt to factors as they change. So, to take the retail customer as an example, there are many different components that can influence customer behavior from advertisements, sales, political leanings etc. Each of these has different levels of influence depending on the time of day, the season, what's going on in the world, the customer and their mood. A deep learning method can better account for the diverse and changing array of influences.

Having already helped Alibaba Group improve its prevention and detection of financial fraud on its system from an accuracy of 70 percent to 95 percent, Song is now working with Lexis Nexis to help their systems determine which loans to grant.

Helping systems make decisions in real time is key. **Hongyuan Zha**, professor in CSE, looks at modeling, predicting, as well as shaping behaviors of things like metals, humans, and groups of humans, such as nations.

"This is the right time for machine learning," says Zha. "Industry and government can really benefit by leveraging these techniques which are

constantly being developed. It's an exciting time."

Credit scoring is one area Zha's work in deep learning has been used. Continuing this theme he's also looking at scoring, not only economic data but behavioral and social data about people.

His techniques work well in the inorganic market too, like his efforts to determine how to move from one state of a material, in particular metals, to another. He examines modeling the microstructure of a specific material in terms of how porous cracks are distributed, how lines crystalize, and how all of this impacts the properties of the material.

"We also study collective behavior of populations, such as countries, and how their drive to optimize defense gives rise to certain behaviors," says Zha.

Almost anything from how people will use mass transit, finding good matches for marriages, a labor pool, a medical school residency program, or the probability of disease spreading can be analyzed to predict and even shape outcomes using these deep learning techniques.

"Over the next few years we anticipate being able to have deep learning models that benefit from being combined with human knowledge so they can be adapted to new environments more easily and use less data," says Song. ■

We can help you ... Discover hidden relationships, connections, and results by using visualizations to connect people to your data

Data is a numbers game. It's what computers are best at. But it takes people to see what it all means and how it's related to the real world.

"Visualization allows humans to detect what computers can't. We're much better at spotting visual data than computers are," explains **Duen Horng (Polo) Chau**, assistant professor in CSE.

Finding hidden relationships or even ones that are intentionally deceptive is often tricky for computers. But if we can teach them to route their attention to the proper areas, to learn which data is important and which should be ignored, then they can become better at a host of tasks from self-driving, to tracking terrorists, to intrusion detection.

"When some hackers get into a system they lie low and map out the people, or the routes with the best information. This avoids triggering the alarms before they commit their massive leak and disappear," says Chou.

In the next three to five years, Chau anticipates we'll be much better at teaching computers to spot which of the weak signals they're detecting are truly random and which are a result of subterfuge from intruders.

Ümit Çatalyürek, professor in CSE, works on visualization systems and graph algorithms in bioinformatics as well as tracking terrorists and the spread of pathogens. He says that separating the wheat from the chaff is also vital for medical applications. As digital pathology gets even more powerful, not only will processing these images become more intensive for computers but managing the data and separating it from the noise will be a challenge.

In the next few years, Çatalyürek sees us having better systems for handling the large amounts of data and more mobile methods for reading it.

"This will change the game by giving us far more insight on diseases like cancer and others," he says. "We'll be able to identify more genes that cause these diseases as well as more treatments and cures." ■

Add the Strategic Partnership Program to your team and you add:

15 tenure-track faculty • **16** research scientists • **150** masters students • **100** doctoral students

We can help you ... Rapidly investigate the natural properties of materials and bio-organisms

The continued growth of computing power will mean that reading and investigating the building blocks of materials, whether biological or inorganic, will be easier, cheaper, and more mobile. It will make disease investigation more nimble and allow medical professionals to discover more quickly how and why diseases arise.

One of the big questions to come out of this progress, according to CSE professor **Srinivas Aluru**, will be how to best store, analyze, and use the data in medical research and treatment. A huge challenge in and of itself because he currently harnesses 100 million to several billion base pairs compiled from human genomes. He figures out how to store and control all of this data so researchers can compare genomes, as well as sequence the genomes of pathogens like bacteria and viruses, in order to uncover how disease arises, spreads and is best controlled.

Inherent in this quest are other huge questions, Aluru says. How can you protect all this human data from prying eyes and misuse by rogue actors? What constitutes misuse and what right do people have to their own healthcare information? In addition, since genomic data is inherited, how can you preserve the rights of children, grandchildren and the like, to their genomic data when their ancestors have given their data to researchers, or have had it taken without their consent?

"Sequencing human genomes will be so easy and cheap, we'll have to create privacy rules and guidelines to protect people and their progeny," Aluru says. In addition, we'll have to continuously improve our cybersecurity to keep this information out of the hands of

anyone who doesn't have a right to see it. That includes not only cybercriminals but terrorist organizations and states.

Researchers are also moving toward being able to predict the structure of polymorphs, which will make the drug manufacturing process a lot more predictable and cost-effective.

Computer-aided drug design is already a burgeoning field, but one of the setbacks has been that it's still a big surprise when a drug maker is producing a pharmaceutical and, through some unknown and unforeseen circumstances, the drug creation process begins forming different molecules with the same chemical composition. Not only can it mean huge losses for the manufacturer, but it can also result in drug shortages for sick patients. **David Sherrill**, professor of Chemistry and Biochemistry as well as CSE, believes that in the next three to ten years they will be able to predict with good accuracy when the manufacturing will produce the desired particles and when it will form errant molecules.

Quantum computing promises to make child's play of the currently complicated calculations for simulating molecules, says Sherrill. Psi4, the computational chemistry application he developed is already being adapted using algorithms for quantum computing.

Using machine learning to create algorithms that can investigate all of the possible properties of molecules is something else we'll be able to do in the next five years. This promises to both accelerate these investigations and give us a more exhaustive understanding of the characteristics of molecules, according to Edmond Chow, associate professor in CSE.

On the inorganic side of life, Professor of Materials Science and Engineering and CSE **Surya Kalidindi** anticipates the Materials Genome Initiative, a federal effort to discover and use innovative materials, will devise solutions for stronger, safer, and cheaper materials for use in applications from aerospace to medicine to defense. ■

We can help you … Increase the power of your investigations and the amount of available knowledge by connecting the cloud and isolated databases

The cloud offers a tremendous opportunity for industry and the government to use the insight of academic researchers to the advantage of all parties. One example of where this will be done in the near future is in the fossil fuel industry, according to **Felix Herrmann**, Georgia Research Alliance Eminent Scholar Chair in Energy at Georgia Tech.

It used to be the case that a company would need to own and operate extremely large supercomputers in order to run the calculations designed to find and evaluate potential locations for oil and gas deposits. Now thanks to the enormous growth of high-performance computing and big data, academics can leverage the resources of the cloud to develop the algorithms in partnership with industry.

Herrmann's research group is currently creating algorithms for this purpose. He plans to start a public-private partnership with companies who need his group's expertise and intends on using the profits to fund his students and his research endeavors.

With implications far beyond the fossil fuel industry, this business arrangement can extend into any industry with a need for new algorithms. By employing the cloud's immense computing capabilities to fuse academia's prowess for research with industry and government's need for novel solutions, Herrmann envisions a sustainable method for driving innovation.

While connecting to the cloud offers a tremendous opportunity to boost the processing power and speed of calculations, connecting multiple simulations to work cooperatively presents the potential to understand how different scenarios may play out together.

Richard Fujimoto, Regent's Professor in CSE, already uses this method when looking at how land use and transportation issues affect the growth of cities. He imagines going beyond his current work forecasting how rideshare will impact urban environments to investigating how autonomous vehicles stand to change traffic patterns and commuting options.

Connecting sims stands to increase the possibilities for understanding, not just the likely impact new technologies will have on city life, but can also be used to foretell how any phenomena that can be simulated may interact with each other. For example, how a change in the demographics and financial resources of the nation might affect the healthcare system, or how the increasing growth of online retail may affect communities' use of land, employment options, and regional planning.

Perhaps the area where computing may have the biggest impact on people's lives day to day is in medicine. Whether it's large medical records databases held by different providers, health apps, smart mattresses, and other devices that collect information on an individual level when these disparate sources are linked it can result in better clinical care for patients as

well as valuable analytical data for the industry.

"Georgia Tech is very strong in translating data from diverse sources into harmonized data sets," says **Jon Duke**, director of health informatics in CSE. "The big challenge for the future of medicine lies in being able to manipulate larger, more complicated sets and assemble and deliver the information in a way that's useful for doctors and researchers so we can conduct precision medicine," he adds. ■

We can help you … Create novel computing solutions for your particular needs

Being able to predict and explain everything is one of the noble goals of science, yet one that will forever remain out of reach. No matter how far we progress, there will always be some facts that stay unknown and some things that are worthy of investigation. New methods and new systems will be needed to solve new problems.

That's one area in which, **Richard Vuduc**, associate professor in CSE, thinks high-performance computing can help.

"The idea of high-performance computing has been neglected by large swaths of industry," says Vuduc. "There have been periodic upgrades in speed from time to time and it's been fast enough for demand, but if we want to be mobile then we have to use less energy. One way to achieve energy efficiency is making faster running systems."

Vuduc thinks a good way to make systems faster and use less energy is to switch from the general purpose processors the majority of industry is using to customizable processors. Creating chips and tailoring algorithms specific to the job will use a lot less memory, allowing more complex calculations to be computed on much smaller devices, which in turn will lead to more mobile solutions to help solve ever more intricate problems.

However much processing power, or custom computing we are capable of, uncertainty will always persist. **Tobin Isaac**, assistant professor in CSE, is interested in being able to take those unknowns into account. He's working on creating an "uncertainty quantification" that allows scientists to calibrate how much trust they have in a scientific prediction given that some quantities are unknown. He's interested in helping researchers discuss not only what they know, but what they still don't know and may never know, so that scientists and the public will have the appropriate amount of faith in whatever prediction is being made. ■

Building a better way to find tomorrow's talent

Whenever a new employee is hired they undergo training at their new job to learn the specifics of what they'll be doing, but they also undergo a "detraining" program as well. That's where they learn, either formally or informally, that the way they learned it at graduate school is not the way it's done at their new employer. It may not even be the way it's done anywhere.

Detraining costs companies and their employees not only time and frustration but money. That's because every minute an employer has to spend teaching their new workers how not to do the job is a minute they aren't spending getting the work done.

But what if you could bring new employees on board knowing they're ready from day one? Impossible? Not if you have a hand in what and how they're taught.

When you join the Strategic Partnership Program you'll get the opportunity to share with our faculty what skills and talents you're looking for in new employees. You'll get to tell us —in-person —what works and what doesn't at your place of business so that we can better prepare our students for success after they graduate. When you hire them, they'll come to you ready to go on day one and help your outfit be the best it can be.

You'll also gain the advantage of meeting our students long before they come seeking employment, so you'll know who they are before they even knock on your door. Through a series of lunches, informal gatherings, and talks, you'll hear from them about their skills, talents, values and what they're looking for in terms of their career and life experiences.

In addition, you'll get to know our graduate students' work experiences through our CSE Graduate Student Resume Book, and you'll be able to contact them directly through email, so you can get to know them online or set up face-to-face meetings.

Every research university does these things in part, but too often they are ad hoc and highly dependent on existing connections between specific faculty members and particular areas of the company. When you're part of the Strategic Partnership Program you'll be involved in an organized, holistic enterprise that's well positioned to grow and change as your organization does.

Connect with us

Your work is vital. Doing your part every day to transform the world, you need the best minds in computer science alongside you helping you enrich the world and making your organization stronger. When you join the Strategic Partnership Program at Georgia Tech, you'll work with forward-thinking people at the top of their field who are fervent to share their expertise with you.

You'll get the opportunity to build relationships with our eminent and inquisitive faculty in high-performance computing and big data who can help you boost your chances of success when you're determining where to focus your efforts. You'll be in the best position to interact with our first-class graduate students as you build your next-generation workforce. With a wealth of resources at your fingertips, you'll be better connected and more prepared than your competition because you'll have the foremost researchers uncovering solutions that anticipate the needs of tomorrow.

Become one of our valuable partners and we can help you clarify your path to success today and illuminate the future.

CREATING THE NEXT®

Georgia Tech Computational Science and Engineering

cse.gatech.edu

Georgia Tech College of Computing
266 Ferst Drive NW
Atlanta, Georgia 30332-0280

cse.gatech.edu