David Bader, who served as chair of Georgia Tech's College of Computing School of Computational Science & Engineering from 2014–2019, takes a selfie with the CoC incoming class of 2017.

In an Interdisciplinary World, Computer Science Education Must Adapt

By Karen Green, *New Jersey Institute of Technology*

Steve Jobs once said that one of his goals as head of Apple was to "bring a liberal arts perspective… to what had traditionally been a very geeky technology and a very geeky audience" [11]. Jobs, of course, succeeded and made personal computers easy, and even fun, to use. A geeky tool went mainstream, and we all benefitted. Although Jobs and Apple changed computing forever, computer science education at many universities has struggled to overcome the stereotype as a home for geeky students more comfortable communicating through algorithms than through speech. Changing that stereotype and creating computer science education that speaks to the needs of today's society is a challenge for those who work to educate future computer scientists. When it comes to academic disciplines, computer science is still a youngster, first appearing at the university level in the 1950s and 1960s and continuing to evolve and expand through the age of personal computing, the internet and the cloud, the creation of massively parallel machines, and the rise of the interconnected Internet of Things, machine learning (ML) and artificial intelligence (AI).

For educators, the challenge has been to match computer science education with the realities of computer science in practice, a challenge complicated by the fact that computing and technology change quickly, while academia does not. As a discipline at the university level, computer science has evolved over the years to incorporate developing operating systems, designing and building high-end distributed systems, network operations, and cybersecurity

The evolution of computer science education continues today, as universities and to some extent high schools, work to give students a background in data science and analytics and developing AI algorithms. But as computers have become ubiquitous in all aspects of life, a complementary discipline called computational science has emerged, which applies computer science and software engineering principles to solving science, engineering, and business problems.

In the simplest terms, computer science is about the science of computers, whereas computational science is about the use of computers to solve science and engineering problems. Computer science majors at universities learn about the theory, design, and implementation of software and hardware components of computer systems. The main goal is to understand the fundamental principles of computing and use that knowledge to develop efficient and reliable computer systems and programs. Computational science brings together computer science, mathematics, scientific principles, and domain scientists to solve complex problems using computational methods. Its focus is to develop and apply algorithms, models, and simulations to understand and predict the behavior of natural and artificial systems. A typical research problem in computer science involves making computing better, such as developing new software or improving computer systems. Computational science, on the other hand, is often used to solve complex scientific problems, such as predicting weather patterns or simulating biological processes [12].

While computer scientists focus on theoretical foundations of computing and the design and implementation of software systems, computational scientists use computational methods to model and analyze complex systems in various scientific domains.

Computational models can be used to predict trends in business, see the possible impacts of storm surge from a hurricane, develop materials strong enough to survive in space, understand the trajectory of a deadly disease, and so much more. Computational science is interdisciplinary in nature, and thrusts computing experts and CS students into a world where diverse collaboration and communication are essential. As Robert Sedgewick, founding chair of the computer science department at Princeton, once said: "Archaeologists write programs to piece together fragments of ancient ruins. Economists apply deep learning models to financial data. Linguists write programs to study statistical properties of literary works. Physicists study computational models of the universe to analyze its origins. Musicians work with synthesized sound. Biologists seek patterns in genomes. Geologists study the evolution of landscapes. Artists work with digital images. The list goes on and on" [15].

While computer science students study a curricula that includes programming languages, data structures and algorithms, computer architecture, operating systems and database systems, computational science students might focus on mathematical modeling and simulation, numerical analysis, data analysis, data visualization and high-performance computing. Computer scientists might develop new algorithms or novel ways for handling large data sets for a scientific endeavor such as climate modeling. In contrast, a computational scientist most likely would work with the climate scientists to create models and visualizations that illustrate a phenomena, such as temperature changes over time.

EDUCATING COMPUTATIONAL SCIENTISTS: THE GEORGIA TECH EXAMPLE

Today, The Georgia Institute of Technology (Georgia Tech) is one of the nation's top schools for computer science education, ranking seventh in the latest U.S. News and World Report [16]. In 1990, however, it was brand new. The Georgia Tech College of Computing (CoC) was launched with the mandate of creating the future of computing and educating new generations of engineers, technologists, and business professionals to apply computing in all walks of life. The CoC quickly became a nationally ranked computer science program and the largest undergraduate degree program at Georgia Tech. But the college was not about to rest on its laurels and understood early on that computational science had to be part of its offerings. Back in 2005, the President's Information Technology Advisory Committee (PITAC) stated, "Computational science's models and visualizations—of, for example, the microbiological basis of disease or the dynamics of a

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hurricane—are generating fresh knowledge that crosses traditional disciplinary boundaries. In industry, computational science provides a competitive edge by transforming business and engineering practices" [13]. Around the same time, some of the brightest scholars, technologists, and scientists came together on the Georgia Tech campus to envision a way to educate not just computer scientists, but computational scientists and engineers capable of modeling real-world phenomena and working closely with domain researchers and business technologists to solve their problems.

In 2004, Richard DeMillo was Dean of the CoC and envisioned new directions for the college that included the creation of a Department of High Performance Computing (HPC) and a focus on computational science and engineering. Behind the scenes, DeMillo had begun talking to potential faculty members who could help fulfill the vision of a new academic division of computational science and engineering guided by two principles.

1. That computational science is its own discipline, separate from computer science, that includes modeling and simulation, computational data analytics, and high performance computing.
2. That by its nature, computational science is interdisciplinary, with scientists in many fields driving computational researchers and engineers to create new computational methods that lead to breakthroughs in science, engineering, medicine, business, and daily life.

This new direction envisioned computational scientists as the glue, or the interconnective tissue, essential in every problem-solving situation and in every discipline and business practice. The age of the stereotypical computer "geek" sitting in a cubical talking to no one, but his computer was rapidly being replaced by the age of computational thinkers, adept at creating algorithms and simulations as part of interdisciplinary problem-solving teams.

As DeMillo recalled, the early attempts by the U.S. National Science Foundation (NSF) to raise the profile of high performance and scientific computing, although well intentioned, ran the risk of marginalizing scientists working at the intersection of computing and other disciplines. Universities simply weren't set up to encourage or reward that kind of interdisciplinary work. Getting recognition required publishing in a specific discipline—not working as part of an interdisciplinary team.

"I was responsible for launching the first NSF interdisciplinary research centers in computational sciences and engineering," said DeMillo. "It was a first step, but I quickly realized that without an academic home, scientists who worked in these centers would have difficulty being rewarded for contributions not directly related to the fields in which they held primary appointments. I watched with dismay as seasoned computer scientists became programmers for biologists while computer science promotion and tenure committees struggled to evaluate their achievements published in Physical Review Letters. My colleagues and I concluded that this new breed of computational scientists and engineers must be welcomed as first-class citizens in their own academic unit and encouraged to pursue career paths that spanned fiercely defended, but artificial, organizational boundaries."

A TRULY INTERDISCIPLINARY ENDEAVOR

In summer 2004, DeMillo was already talking to David Bader, then a faculty member at the University of New Mexico and a lead researcher at the Albuquerque High Performance Computing Center, about the future of the CoC and the role he might play in it. In mid-September 2004, Bader met with a representative of the executive search firm Spencer Stuart about leading the new HPC department. He offered input to DeMillo on expanding the idea of the HPC department into a broader Division of Computational Science and Engineering, and subsequentially came to the Georgia Tech campus for an interview in January 2005. By the end of that interview, he had agreed to give up his tenured position in New Mexico to play a founding role in the new computational science and engineering division.

"When I talked to Dean DeMillo, it was obvious we had similar visions," Bader recalled. "Computational science and engineering had established itself as a truly interdisciplinary endeavor that needed to be acknowledged for its contributions to research and discovery and needed to be taught to computer science students. I wanted the new Georgia Tech computational science and engineering unit to be a home to this new breed of scientists who work hand-in-hand with domain scientists to build models, develop visual simulations, and analyze data using HPC tools."

By the time Bader arrived on campus in summer 2005, DeMillo and Associate Dean Richard Lipton had surveyed the academic, government, and commercial national landscapes in search of potential leaders in computer, engineering, physical, and life sciences. DeMillo concluded that faculty members already at Georgia Tech who understood the culture and aspirations of the College of Computing were the best candidates. He recruited Georgia Tech faculty member Richard Fujimoto—a specialist in large-scale simulations with an international reputation—to lead an effort to bring together resources to create a new CSE unit as part of a reorganization of the CoC. Bader was the first faculty member hired for that unit. In Fall 2005, the unit attracted Haesun Park—another respected computational scientist—who arrived on campus the following spring after finishing her appointment as an NSF program manager. This initial group of Bader, Fujimoto, and Park became the founding faculty members of what was then the Division of CSE and later became the School of CSE.

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The founding of the CSE coincided with a required five-year program review of the College of Computing. Not surprisingly, the formation of the CSE was a subject of much interest to the review committee. Committee members wanted to know how the unit was formed. It was notable that the CSE was permitted to call itself an engineering department in a university that jealously guarded its brand. Georgia Tech's powerful College of Engineering had no objections to COC using the term "engineering" for its new endeavor. In fact, the naming of the new unit had been carefully negotiated by DeMillo and Engineering Dean Don Giddens to send a message about the future of computing at Georgia Tech. Still, the committee wondered whether turf battles would erupt and doom the new venture. DeMillo recalled waiting anxiously for the review committee's report.

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The team that launched the CSE was committed to breaking down departmental silos, so that computer science students could learn to apply their skills in, for example, environmental sciences or molecular biology. They also aimed to dismantle silos so that medical researchers, chemists, and others could work easily with computational science faculty, and both could earn credit for their work. Sometimes, the barriers to truly interdisciplinary education and research were internal. As the Georgia Tech Commission on Creating the Next in Education (CNE) noted in 2018: "Academic disciplines … are the most common organizational silos in a university. Such silos make interdisciplinary programs hard to create and even harder to maintain. Bureaucratic restrictions on course registration, long chains of prerequisite course requirements, and complex accounting rules for allocating a professor's time make it hard for students to take courses outside their major field of study" [7]. The people who built the CSE knew that dismantling silos and establishing a home for their new discipline was vital to their success.

James Fairbanks, a School of CSE student from 2012 to 2016 and now an assistant professor of mechanical and aerospace engineering at the University of Florida, put it this way. "Looking back, I see the benefits of the institutional commitments to the School of CSE. We had a collection of experts with diverse backgrounds and training working together, and without a dedicated home for these faculty, they would've been spread out across many departments. That would've made it hard to dedicate enough resources to creating a comprehensive CSE curriculum. CSE skills are essential to successful research projects, and collaboration between CSE researchers and domain experts is best facilitated when institutional support creates a community of CSE faculty, students, and research staff."

The CoC, with DeMillo as its leader and Bader as executive director of high performance computing, racked up some impressive wins that helped establish its prominence in research, education, and technology transfer through collaborations with industry. In late 2006, the college became the first Sony-Toshiba-IBM (STI) Center of Competence, focused on expanding the reach of the Cell Broadband Engine™ (Cell BE) microprocessor [6]. The Cell BE made its debut in the Sony PlayStation 3. With Bader as its director and funding from the Cell BE industrial partners as well as grants, the STI Center of Competence explored ways to adapt the new technology for other industries, including biotech, finance, and digital media creation.

Bader continued the college's successful collaborations with industry by winning a grant from Microsoft Research in 2006 to investigate the design and optimization of algorithms that fully exploit multi-core processors [2]. Microsoft chose Bader for the award because of his extensive experience designing the world's fastest parallel algorithms for shared memory, symmetric multiprocessor and multithreaded architectures. Bader also received the highly competitive IBM Faculty Award in 2006 in recognition of his fundamental contributions to the design and optimization of parallel scientific libraries for multicore processors [3]. Additionally, in 2007 Bader was awarded Focused Research Program (FRP) funding from the Georgia Tech Office of the Provost. The FRP supported start-up research in high performance computing that required collaboration among different units and that had the potential to evolve into a research center in one to two years.

A FIRST CLASS ACADEMIC CITIZEN

While the national awards meant publicity, respect, and new students for the CoC and the School of Computational Science and Engineering, its founders focused on creating curriculum for both undergraduates and M.S. and Ph.D. students. Bader shared curricula ideas with Fujimoto and presented proposals for M.S. and Ph.D. programs that included collaboration with three schools in the College of Sciences and four in the College of Engineering. Those proposals were approved by Fujimoto, division faculty, and DeMillo in 2007 and the curricula became operative in 2008. The intention, according to Bader, was to develop computational science and engineering at Georgia Tech as a "first class academic citizen" rather than an extra or an add-on program, as many interdisciplinary initiatives at universities tend to be.

Whereas traditional computer science curricula focus on topics such as theory, systems, programming languages, operating systems, networks, human computer interaction, and cybersecurity, computational science teaches students to apply computer science knowledge, often by developing applications for science and engineering disciplines.

The graduate programs in the CSE school were designed for students with undergraduate degrees in computing, a scientific field, engineering, or mathematics. An interest in a science or engineering application area was also essential, according to Bader. To craft the curriculum, the CSE founders reached out to respected senior researchers in academia, at U.S. Department of Energy national laboratories, and in industry. They were the types of innovators that the CSE program aspired to produced, and Bader, Fujimoto and others conducted interviews and held deep discussions with them. In a sense, they worked backwards from their example to create a curriculum that would educate a new generation of computational scientists.

"Perhaps more than other disciplines, interdisciplinary collaboration is essential to practitioners in computational and data science," he said. "Much work in these areas is problem driven, focusing on practical problems that arise in science, business, and engineering. As such, it is imperative that computational and data scientists and engineers have a working knowledge of some domain and its most pressing problems in order to understand how the computational methods might be applied."

With that in mind, Bader and his colleagues made sure to use collaboration in developing the CSE curriculum. They held face-to-face meetings with faculty across the nine disciplinary units that comprised computing, sciences and engineering at Georgia Tech, where they discussed not only course requirements, but culture, core capabilities of computational scientists and engineers, and logistical issues, including how applicants would apply to the program and be reviewed, qualifying exams, and how to evaluate student progress. They created a curriculum focused on teaching five key areas of knowledge.

1. Modeling and simulation to capture the dynamic behavior of systems over time. This includes teaching students to create conceptual models of systems, mapping these models to efficient computer software, verifying and validating the models, designing and executing experiments, and analyzing results.
2. **Computational data anal-ysis, machine learning and visualization.** Data analysis skills are key in most fields today and incorporate ideas from computational statistics, machine learning, data mining, pattern recognition, algorithm development, and data structures.
3. **High-performance computing.** Solving computational problems often requires using powerful supercomputers, and that requires an education that spans computer architecture, programming languages, parallel computing algorithms, and software.
4. **Numerical computing.** Because mathematics is fundamental to most computational models, students must be familiar with concepts such as direct and iterative methods, discretization, generation and propagation of errors, stability, numerical linear algebra, eigenvalue and singular value problems, optimization, and numerical solution of differential equations.
5. **CSE algorithms.** In addition to numerical algorithms, the computational scientist and engineer must be knowledgeable in the wide variety of algorithms that can be applied to problems that arise in practice.

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"Computer science focuses on computing and components and is mostly focused inward," explained Bader. "Computational science and engineering is the collaborative side of computing that looks outward. These are the people who apply core computer science competencies to solve real-world problems."

Fujimoto was named the first chair of the CSE Division and Park the first vice chair, and Bader continued as Georgia Tech's executive director of high performance computing. The CSE M.S. program included an online option, making it the first online degree program offered by the College of Computing. The

CSE would later partner with other units on campus to create new interdisciplinary degree programs such as an M.S. in analytics, a Ph.D. in machine learning, and an M.S. in urban analytics. The new division also continued and strengthened existing interdisciplinary degree programs in bioinformatics and bioengineering. The CSE also established its presence by creating the Computing Research Undergraduate Intern Summer Experience (CRUISE) to bring undergraduate students to campus, especially students from underrepresented minorities, and introduce them to CSE's research programs. The CSE enriched the overall computer science program by establishing courses in modeling and simulation and two undergraduate minor programs.

The founders of the CSE stressed the importance of interdisciplinary research that applied the latest advances in computational methods to research problems in domain sciences. That meant they were well positioned to receive research support from agencies that were recognizing computational science as the catalyst that could accelerate scientific discovery. For example, Georgia Tech was named the lead institution for the NSF program "Foundations of Data and Visual Analytics (FODAVA)," led by Park [8]. FODAVA meant visibility for the CSE and Georgia Tech as well as substantial research dollars. The project included faculty from the other two schools in the CoC and from the College of Sciences and the College of Engineering, thus showing that computational science was indeed its own discipline and interdisciplinary by nature.

Another important win for the CSE was the creation of the Institute for Data and High Performance Computing (IDH) in early 2010 [1]. Bader laid the groundwork for the new institute, first with his multi-year FRP funding beginning in 2007 and then by working with Georgia Tech CTO Ron Hutchins to bring together interested partners within the university and in industry. Bader also developed the vision, mission, goals, and strategies for the new institute. The IDH aimed to enhance Georgia Tech's impact and reputation in the field by focusing on using HPC technologies to develop new applications and simulation codes to solve multidisciplinary problems in life sciences, environmental sciences, energy, material science, and fundamental research. Georgia Tech named Fujimoto as the first director of the IDH.

These early successes led the CSE to become an official school in the CoC in 2010, with Fujimoto continuing as it first chair. Fujimoto stepped down from that role in 2014. The CSE's first external search for a school chair in 2014 led to hiring Bader, who served as chair of the new school from 2014 to 2019. After his five-year term, Bader left to become distinguished professor and the inaugural director of the Institute for Data Science at the New Jersey Institute of Technology.

During his tenure, the School of CSE more than doubled the number of students in the M.S. program, enrolled 71 Ph.D. students by 2019, and launched a Strategic Partnership Program that allowed students, faculty, and business technologists to collaborate to solve business problems. Participants in the partnership program have included Accenture, IBM, Northrop Grumman, NVIDIA, and Sandia National Laboratories. By 2023, the CSE had grown to include 23 tenure track faculty, five faculty with joint appointments, 141 M.S. students, and 81 Ph.D. students. The school hosts two chaired faculty positions and 12 schools across Georgia Tech in CSE graduate programs as home units [14].

Why do students come to the CSE at Georgia Tech? Perhaps because of its hands-on, interdisciplinary opportunities, for example.

- In 2010, a team led by CSE associate professor George Biros won the ACM's Gordon Bell Prize for creating an application that simulated red blood cells flowing in plasma. The simulation of 260 million deformable red blood cells topped the previous largest blood flow simulation by four orders of magnitude [9]. In 2011, a group of students from CSE, mathematics, and biology worked together to understand some of the mysteries of RNA folding, knowledge that is fundamental to understanding how genetic information is stored and passed on—including viruses that cause diseases. The team leveraged multicore computing techniques to enable the biologists to analyze and process large RNA sequences—like the HIV virus—much faster [4].
- In 2015, several CSE students were finalists for "Best Student Paper" at the annual high-performance computing conference (SC15). One paper documented work to create an algorithm that speeds up indexing of bioinformatics data used in biomedical research. The second paper explained the creation of a framework for processing large graphs that are beyond a single device's memory capacity [10].
- In 2019, CSE students worked with faculty in the College of Design's Center for Music Technology (GTCMT), to use deep learning techniques to help a robot named Shimi use gestures to communicate and respond to emotional cues. Before the collaboration, Shimi could communicate only through music [5].

Indeed, graduates of the CSE program—those relatively rare individuals who regularly use their computer science skills in other fields—understand the value of their education. Deepa Nathan earned a master's degree in CSE in 2011 and credits her professors for helping her see how to use her education to help humanity. "Our courses were designed with a high degree of innovation, enabling us to be creative and solve real-world challenges," said Nathan, who has worked in oil and gas, financial services, and big tech. "I am confident that I can say on behalf of my fellow graduates working in fields as varied as cybersecurity, generative AI, biosciences, and many other specialties that the CSE helped us shape our careers to make them impactful."

Kamesh Madduri earned a Ph.D. in computer science in 2008 and is now a tenure track faculty member in the College of Engineering at Penn State University. "Studying computational science at Georgia Tech launched my career in

"Studying computational science at Georgia Tech launched my career in interdisciplinary computing research and helped me secure a post-doctoral fellowship at Berkeley Lab [Lawrence Berkeley National Laboratory]," Madduri said.

interdisciplinary computing research and helped me secure a post-doctoral fellowship at Berkeley Lab [Lawrence Berkeley National Laboratory]," he said.

Fairbanks remembers that producing software was a requirement to earn his doctoral degree—a unique requirement at the time that helped build the School of CSE's culture of creating tools and enabling research in other fields. "As researchers in a computational field, our biggest opportunity for impact is the release of software tools that enable other researchers to succeed. I think the CSE at Georgia Tech understood this from the start."

What started as an idea for a new academic discipline with an interdisciplinary educational focus evolved into a thriving school that occupies an important niche in Georgia Tech's overall educational and research strategy. The school, its faculty, students, and research projects help to accelerate the pace of scientific discovery and business innovation, they provide new opportunities for computing innovations to change lives, and they break down the silos that often separate academic disciplines.

For students, the CSE has meant a chance to apply computer science principles to solve problems and make an impact on issues they care about. They leave the university equipped not only with technical skills, but with the communication and organizational skills that often enhance success. Because computational science and engineering is an applied field, they have the chance to get their feet wet in the most cutting-edge areas of applied computer science, including data science and using AI as yet another tool for discovery. It means that today's CSE student has an interest not only in developing elegant code, but in applying that code in fields as diverse as medicine, climate science, and transportation.

Thirty years ago, DeMillo had a vision, he shared it with Bader, who was so impressed he decided to come to Georgia Tech, and then with Fujimoto and Park. In DeMillo's words, "We never looked back." Together, these creative, resourceful, and inspired professionals shaped a world-renowned School of Computational Science and Engineering and helped establish computational science as its own discipline that, by its nature, intersects with any other discipline that can benefit from computational methods.

As CS education continues to evolve and as AI becomes embedded into the interconnected devices that first appeared in the 1990s, the Georgia Tech example shows that computer science education can step outside its safety zone so that students can match their educational experiences with the real needs of society. ❖

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