PROPER PARAMETERS

Emmet Cleary uses computing to understand fluid flows. As a California Institute of Technology mechanical engineering doctoral candidate, he works with Tapio Schneider on mathematical techniques to select simulation parameters that produce the most accurate results and to calculate the inherent uncertainty in those choices. They focus on climate models, whose often-unknown parameters can force a researcher to set them manually.

“Cleary says, “Did you get the best parameters? Did you pick the right ones? That leads to a lot of uncertainty.” He tests algorithmic tools to determine the best choices for real-world problems.

STELLAR SCHOLAR

Hannah Kilson explores high-energy phenomena, such as black holes and neutron stars, in which complicated physical properties interact in unusual ways. She’s particularly interested in understanding astronomical changes that occur on a human timescale.

With Elliot Quataert at the University of California, Berkeley, Kilson has simulated neutron star mergers that produce gravitational waves, eject and attract matter around them and launch gamma-ray jets. Kilson uses this model to simulate how light moves through the resulting stellar material, aiming to predict the light signatures Earth-based astronomers should observe from these catastrophic celestial events.

Chan and his co-workers helped Brenner tackle another inefficiency in hurricane storm surge simulations. At the outset, dry areas demand no computational work. But some soon require significant processing as they become inundated. Because no one can predict precisely which dry areas will suddenly demand more computing resources, the computer’s workload becomes imbalanced. “To achieve efficient utilization of the machine, you need to move those patches around on the fly,” Brenner says. “That’s load balancing.”

During the practice, Brenner learned the C++ programming language, then used it to implement task-based parallelism and load balancing. Before incorporating the methods directly into DGSWEM, Brenner created DGSim, a skeletonized version of the program. “We wrote a simulator for our machine, which is bizarre to explain,” Brenner says. “But it allowed us to use a lot of the machine. So I can run the simulation on my laptop whereas normally I would need thousands of cores to do it.”

The group then validated DGSim on Edison, a Cray XC30 supercomputer at LBNL’s NERSC (the National Energy Research Scientific Computing Center), Chan says. “We were able to reduce the number of time steps calculated but still capture the same overall dynamic load profile of the hurricane.” DGSim saved more than 5,000 core-hours compared to running a DGSWEM simulation, and the new algorithms improved hurricane-simulation performance by more than 50 percent. Brenner, Chan and their colleague John Bouchard presented the results at SC12, the international supercomputing conference in Dallas.

Dawson recalls Brenner’s new mastery with DGSWEM after his studies at Cambridge and LBNL. “When he came back, he sort of took over as the lead of that code development,” Dawson says. “He and another student (Kostyuk Kuchykhin) basically rewrite the code from scratch, and they put in a lot of much more modern coding paradigms.”

Today, Brenner finds himself “sitting between those two camps. One is this high-performance computing community, where you have all these people who are trying to figure out how we can get these algorithms to run efficiently on the new computers, and then Clint and his collaborators, who have a very concrete idea of a problem they’d like to solve.”

Dawson and Chan say they admire Brenner’s ability to serve as that bridge. In the summer of 2009, he’ll begin another practicum with Chan’s group, exploring how to make time-stepping not only asynchronous but also locally determined, with each element in a simulation taking its cues from neighboring elements. “We’re excited to have him come back,” Chan says. “I think it will be another good collaboration of him coming with expertise in the domain and us providing expertise in the computer science side.”

EARLY BLOOMER

Stanford’s Carson Kent began working on DOE supercomputers in high school and never stopped.

By Monte Basgall

“Of course the one involving explosives is the one any high school student chooses," recalls Kent, though noting that they didn’t actually blow up anything.

At Stanford, Kent works in the high-demand field of optimization, “the mathematics of efficiency,” as he puts it. “What we’re really interested in are algorithms for computing solutions to problems. That means we define some measure of cost and find a method to reduce that cost as much as possible.”

Kent focuses on optimal transport, which his Stanford advisor Jose Blanchet describes as the cheapest way to move mass from one place to another — sand, for instance, from point A to point B to cover a sinkhole. Optimal transport is a problem that has been around for 250 years, added Blanchet, an associate professor of management science and engineering and an affiliate of Stanford’s Institute of Computational and Mathematical Engineering.

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Kant's an expert, Blanchet says, at "developing and analyzing algorithms for a wide range of problems - complex, large- scale, high-dimensional computational problems." The math can be applied to a variety of other puzzles, such as matching donor kidneys with recipients, linking commercial products with customers in the marketplace, or using machine learning - which feeds known data to an algorithm so it can identify similar characteristics in unknown data - to generate human-looking faces for online advertising.

Kant entered the fellowship after starting at Stanford in 2015. His DOE CSGF practicum work with Argonne National Laboratory's Sven Leyffer exposed Kant to the field that would become the setting for his thesis work in optimization. He also collaborated with Leyffer on a related subject, robust optimization, which Kant describes as "taking optimization and then adding uncertainty." During his practicum "we worked on faster, better methods for solving those types of problems under very difficult constraints and conditions that the Department of Energy cares about."

A poster presented as part of his fellowship described another related problem-solving technique used thousands of times every day in optimization. It works on linear programs, a simple way of expressing a bunch of costs associated with a bunch of decisions. For instance, a linear program can model how Amazon would route packages to customers. The National Football League uses a small modification of a linear program to schedule games each season.

As Kant's CV suggests, it wouldn't be far-fetched to conclude he's among the best-prepared students to enter the DOE CSGF program.

After high school in 2010, his supercomputing challenge experience led to work with other Sandia teams on methods to detect malware in certain Windows files and on using geographic information system web applications to simulate the Western U.S. power grid for ways to detect and prevent failures.

More Sandia collaborations on other real-world projects continued while he worked on a bachelor's of science in mathematics and statistics at the Colorado School of Mines, which he selected for its emphasis on engineering, math, and science. Each summer he interned at Sandia, and for his last three undergraduate years also telecommuted with the lab during the winter while attending classes in Golden, Colorado.

The fruits of those interactions included leading development of a tool called Cyber Shopper. The program sought to model an adversary's actions when attempting gain access to a computer system, he says. This led to a U.S. patent, issued in July 2018, on a method and apparatus for managing such an attack.

Another project applied machine learning to automate something called cognitive radio, which Kant describes as a method for listening in and declassifying wireless transmissions.

While at Mines, Kant also picked up a research interest in uncertainty quantification, which aims to calculate how much trust researchers can put in their computational models of real-world conditions.

That interest began in the summer of his junior year, when Paul Constantine, then a Mines professor, invited him to take a graduate-level short course on the subject at Stanford.

When they returned to Colorado, Kant began a research project with Constantine and a University of Texas at Austin professor that led to a 2016 paper in a Society for Industrial and Applied Mathematics journal on a computational workhorse called the Marquardt chain Monte Carlo (MCMC) method. MCMC is a class of algorithms for sampling among probability distributions. These distributions, for instance, can represent physical quantities of interest in a simulation problem. Some of the authors' calculations ran on MoI, an HPC cluster at Mines.

While an undergraduate, Kant - a veteran of many an elementary and middle school science fair - volunteered as a judge at similar local events. He also taught programming at a Montessori school. Kant says those activities have been rewarding and have helped him recognize how valuable mentors have been in his own career.

One such guide was Sandia's Uzoma Onurkwu, who Kant worked with his senior year at Mines and "was a main cause of my desire to go to grad school rather than industry after undergrad." Onurkwu wrote one of Kant's supporting letters for attending Stanford, as well as one of his DOE CSGF application.

All that happened after Onurkwu and another researcher enlisted Kant to help estimate the effectiveness of error-correcting codes in quantum computation. "It was phenomenal and delivered beyond the tasks we assigned to him," Onurkwu recalls of Kant's performance as a student intern. "We needed a C++ programmer with expert-level experience. He delivered remarkable results for us in that role."

Kant chose Stanford for his doctorate because its programs provide "the right combination of exposure to all the different areas you need if you're going to do computational work." For his Ph.D. work to come, Kant is gearing up to use Stanford's Sherlock HPC cluster to solve some large-scale optimal transport problems.

Kant calls the fellowship "amazing." I've definitely spent a while around the Department of Energy and there are few other programs in it that I value as highly as the DOE CSGF in terms of its ability to build the workforce that the department constantly needs." The same is true if fellows choose to go into industry, he adds.

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AMORPHOUS GOAL

Nicholas Bohli studies soft-matter physics with Harvard University's Chris Rycoff, modeling bulk metallic glasses (BMGs), moldable amorphous metals. BMGs are promising materials for many uses, but they can fail when subjected to certain forces. Bohli has extended Rycoff's computing tools from two dimensions to three dimensions to test a new theory describing how and why BMGs fail. With Jean-Jacques Slotina at the Massachusetts Institute of Technology, Bohli also uses mathematical tools to explore how artificial intelligence algorithms work. He hopes to use algorithms he's developed to extend the BMG models.

A MODEL DESIGN

Michigan State University's Zane Crawford studied finite element algorithms for electromagnetics, but his Sandia National Laboratories practicum - and a discussion with advisor Shanker Balsebaranam - changed that. Now Crawford researches topology optimization - finding the best design for an object to perform a specific task. He seeks novel designs for electrical devices that "best get me from some input signal to some desired output signal."

His algorithms must choose the best orientation and properties to meet that goal. After applying a finite element approach, Crawford uses a topology optimization algorithm to fine-tune selected parameters affecting the system to get the best possible device design.

REALITY: IT'S COMPLICATED

As a Harvard University undergraduate, Ian Dunn realized his chemistry interests focused on physical theory, differential equations and mathematics. He wanted to know not just how molecules react with each other but why. With David Reichman at Columbia University, Dunn wrestles with many-body quantum physics problems, attempting to incorporate more realistic - but complicating - factors into his models. These simulations often require approximations or clever computational schemes to make calculations manageable. His work examines fundamental physics, but someday such models could be used to design and optimize the properties of new materials such as solar cells.
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Several researchers of the papers taken from the first in order optimization algorithms - mathematical techniques for finding puck's most efficient solutions - testing various candidate solutions. These optimization methods refined the tool's objective function (here the property the algorithm seeks to minimize or maximize) on the tool's grid and those optimizations likely are from accelerated first-order methods - even though the authors claim that they take the solution to apex very much more. Credit: Chris Lefler

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