A new tool for modeling materials

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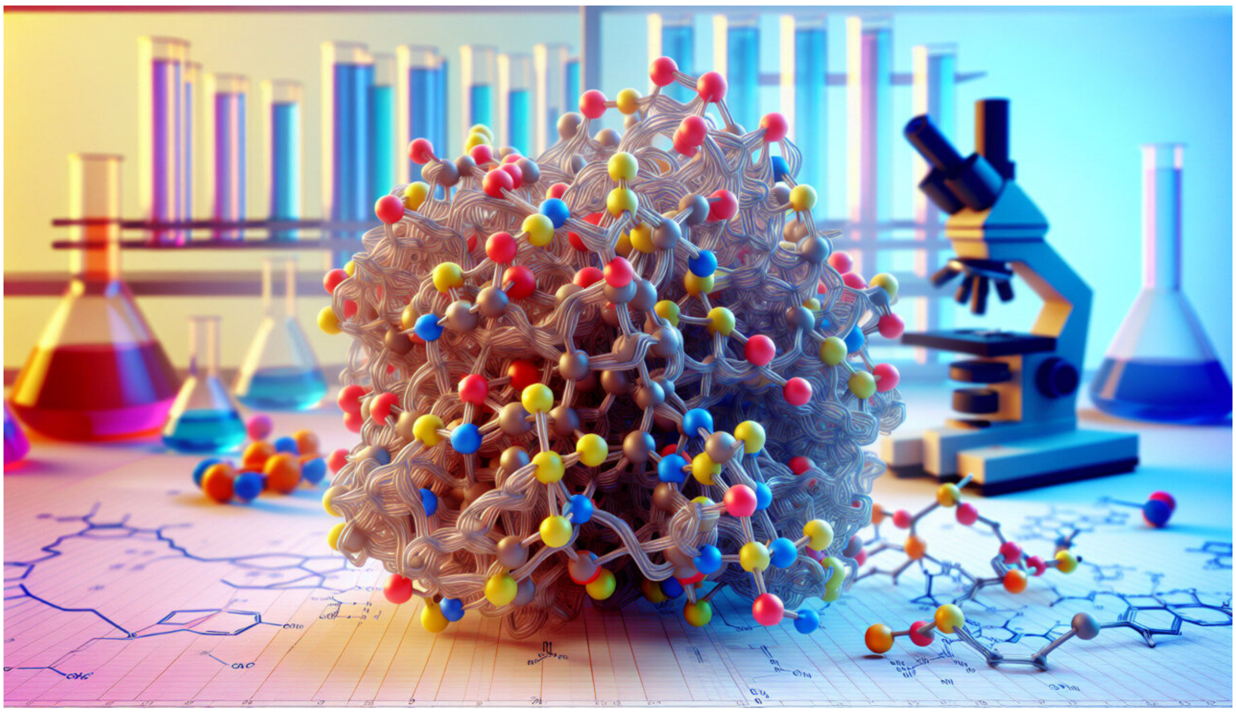

Credit: AI-generated image

Thermoset polymers made with composite materials give us everything from concrete bridge reinforcements to jet airplane wings to fiberglass boat hulls, and Philippe Geubelle's mission is to make these composites using methods that are faster, cheaper, and more energy-efficient than traditional methods.

Geubelle, Ph.D., Bliss Professor of Engineering at the University of

Illinois Urbana-Champaign and Executive Associate Dean of the Grainger College of Engineering, works with the interdisciplinary Autonomous Materials Systems Group at the university's Beckman Institute to model frontal polymerization, a technique that turns liquid monomers into solid polymers using a chemical reaction.

"Whenever we do a simulation, it takes a while because numerically, it's very hard to capture this front that propagates through the structure," he said. "There are a lot of parameters that define this process. We want to know—what will happen if I change the chemistry or if I change the temperature at which I'm doing this? What if I change the environment?"

The team already was creating computer models of the process, but Geubelle thought utilizing machine learning could speed up the modeling. He turned to NCSA, home to experts in machine learning and artificial intelligence, and to Illinois Computes, a program that matches NCSA computing and data storage resources, technical experts, and support services with researchers across the Illinois campus.

"We took advantage of this great program called Illinois Computes. The primary objective of that program is really to pair researchers on campus with researchers at NCSA, and NCSA has a very good group that focuses on machine learning and artificial intelligence, including using machine learning to solve partial differential equations, which is what we are doing," said Geubelle, Ph.D., Bliss Professor of Engineering at the University of Illinois Urbana-Champaign and Executive Associate Dean of the Grainger College of Engineering.

Geubelle and post-doctoral research assistant Qibang Liu were paired with Seid Koric, Ph.D., NCSA's technical associate director and research professor of mechanical science and engineering, and Diab W. D. Abueidda, NCSA research scientist. Koric leads projects at the forefront of using the latest advances in artificial intelligence and machine learning to help scientists run models and find answers more quickly and accurately.

They created various advanced AI models to run on high-performance computers by first training an artificial neural network, an ML-based deep learning process that uses interconnected nodes in a layered structure that resembles the human brain. By feeding neural networks different values of training data, the model learns by example and can be trained to recognize patterns in data, find connections, and predict outcomes.

"Training these networks typically requires lots of data generated by classical numerical methods to reduce the prediction errors, which is computationally costly," said Abueidda. "But when these networks are properly trained, they can infer results orders of magnitude faster than classical computational methods for new input data."

A breakthrough in training neural networks

Koric and Abueidda developed a novel way of reducing the amount of data needed to accurately train the neural network by monitoring the evolution of an error defined directly from the underlying partial differential equations. By focusing the ongoing training for the network on the error measure obtained from the physics (governing equations)—the team was able to find and train the data from the areas in the model that were least accurate—and thus greatly reduced the training data needed to develop an accurate model.

"Being able to pinpoint and focus on the areas where you need improvement can result in a lot of speed-up in the entire process," said Koric. "By choosing data with large errors obtained from physical insights to feed into the system, rather than blindly generating a large amount of data, we've found a way to reduce the need to generate lots of training data."

Geubelle added, "if you do this randomly, I would say maybe 40% of the training examples you're solving are useless because they don't really improve the system very much. You put all your efforts into training the network in the region where the error is large. That is the adaptive nature of the process."

The team used NCSA's Delta supercomputer to run its models. The system offers both CPU and faster GPU processors, and one of Liu's efforts has been to work with NCSA to adapt codes written for CPUs and GPUs. So far, the collaboration has led to a paper in *The Journal of Physical Chemistry*. The team also won another round of support from Illinois Computes to continue their work.

"We are breaking down silos and really effectively collaborating under Illinois Computes. Everybody's bringing their own expertise to the plate, and we are solving challenging or unsolvable problems by the power of machine learning, AI and high-performance computing," said Koric.

"I generate the data from a CPU machine and then transfer that data to a GPU machine," said Liu. "It actually takes a little time, but with the neural network we want to be using GPU machines because they are so much faster,"

The ML approach to modeling frontal polymerization has also enabled the team to much more efficiently examine and solve the inverse problem in manufacturing, that is, to find the set of process conditions—determined by variables such as initial temperature, degree of cure of the resin, heat loss and more—that lead to a prescribed pattern of manufacturing. Solving the inverse problem, said Geubelle, is crucial for processes such as 3D printing because it is then possible to feed microstructures into a printer that result in a completed macrostructure.

"If you tell me what microstructure I need in order to do this, I can send it and have it made," he said. "But to solve this inverse problem, you need to be able to solve the forward problem really, really fast and that's where machine learning comes in."

Machine learning and AI, and the new adaptive deep learning processes developed in collaboration with NCSA allow Geubelle and his team to model the frontal polymerization problem in seconds rather than hours. That speed is essential for inverse design because of the enormous number of parameters involved. Geubelle said his group had worked on speeding up the process of inverse design using conventional methods, but the process was still too slow.

Novel contributions and a cycle of innovation

The new project will allow the team to continue addressing the challenges of multiscale modeling of composite polymers using novel artificial neural networks, including generative AI methods. It will also delve deeper into work that uses the target design of a material as the input and gives the design variables as a return. This "one-shot" inverse model is expected to be substantially more efficient than more conventional inverse modeling methods, according to Koric.

As ML models and AI continue to mature, the adaptive training framework developed by NCSA could be applicable to many other areas of science, including various engineering disciplines, medicine, geology and seismic research, Koric said.

Volodymyr Kindratenko, director of the Center for Artificial Intelligence Innovation (CAII) at NCSA, noted that the work with Geubelle and the larger research group at Beckman Institute puts the

University of Illinois at the forefront of innovative, collaborative AI/ML research.

"This work is an excellent example of what we call translational AI research," said Kindratenko. "Koric's team takes an existing ML methodology and uses it in new ways to solve problems in a science domain where nobody even thought it was possible. In doing so, the team advances the ML field with novel contributions and creates a cycle of innovation in both the ML and computational science fields. The work can then serve as a blueprint for other researchers to follow in their respective domains."

Koric said the project also breaks down the barriers that continue to keep technology and science experts working separately.

"If you look at this kind of research, people are generally in two camps," he said. "You have computer scientists, on one hand, doing their fundamental computational research in AI and machine learning, and on the other hand, you have applied scientists and engineers who are using traditional computational methods but aspire to advance their research to the next level with AI/ML methods.

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Brendan McGinty, director of NCSA's Industry Partner Program, noted that the private sector is eager to jump on the AI bandwagon, and NCSA's work takes AI's impact a step further.

"Dr. Koric and Dr. Geubelle take incorporating AI in modeling further, more specifically, to address polymer production," said McGinty. "They are showing that deeper and faster improvements to models are possible by combining AI, modeling, and domain expertise with HPC to maximize uplift. On the corporate end, this translates into improved competitiveness and return on investment."

Provided by National Center for Supercomputing Applications

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