Reliable, fast simulations of complex events Virginia Tech mathematician's goal

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Timely, accurate prediction or control of complex phenomena – such as predicating the path of a hurricane or controlling a jet -- is the goal of Serkan Gugercin's National Science Foundation Faculty Early Career Development Program (CAREER) research.

Gugercin, an assistant professor of mathematics affiliated with the Interdisciplinary Center of Applied Mathematics at Virginia Tech, received the five-year CAREER grant worth $400,000 to do "Reduced-order modeling and controller design for large-scale dynamical systems via rational Krylov methods." The award is NSF's most prestigious for creative junior faculty who are considered likely to become academic leaders of the future.

Gugercin explains that there is a mathematical model behind every physical phenomenon. For instance, one can write down mathematical equations to represent both the physical aspect and the time sequence of heat transfer in the sterilization step of food processing. Data produced by simulating the resulting model would allow you to produce a safe, palatable product.

"We always want more detail and more accuracy in mathematical models, which leads to a large number of coupled equations in the resulting model," Gugercin said. "For example, if you want to predict the path of a hurricane in half-mile increments for a 1,000-square-mile area, your model will have millions of coupled equations. That is a computational challenge because you cannot create an accurate prediction in a timely manner. It would take days. And it would require a supercomputer, not a simple lap top or desktop."

For a "reduced-order model," Gugercin determines how many equations in a model are very important to the entire process, and then solves just those equations, which significantly shortens the computation time. "But we can't be arbitrary. It has to be an accurate representation of the full model so that we have confidence in the prediction," he emphasizes.

The process is important to the technology we use everyday. The computer chip is a prime example. In 1971, the Intel 4040 model of an integrated circuit (IC) contained around 2,300 components. Compare that to the 2001 Intel Pentium IV chip, which contains some 42 millions elements with more than a mile of interconnectivity, according to N.P. van der Meijs of Delft University of Technology. Such complexity can result in significant delays and interference, Gugercin said. Therefore simulations are needed to discover where delays might occur, for instance. This is done by modeling the interconnection. A typical mathematical modeling of such physical process easily results in anywhere from hundreds of thousands to millions equations. "But simulating a million equations is a formidable task. So we reduce the number of equations to be used in the simulation and make predictions based on that model," Gugercin said.

Another application for model reduction is control. If you are manufacturing steel, you need to control the speed at which it is cooled. Too fast and it will be flawed. Too slow and the steel will still be hot when it arrives at the next manufacturing step. Some 80,000 equations represent the mathematical model for cooling steel, according to Peter Benner of Technische Universität Chemnitz. "In this case, you are not trying to predict a process; you are trying to control the process," Gugercin said. "You wouldn't want to design a mechanism to control a process that is based on 80,000 equations. It would be too complex and would not be able to act quickly and accurately. So you design your controller based on a simple model so it can act quickly."

Two other applications where you want a reduced order model so a controller can respond quickly to conditions are in airplanes and the international space station. Because there are so many fields where large-scale simulations and computations are crucial – from research on molecular dynamics to vibration suppression in structures – Gugercin's goal is to develop mathematical tools and high-quality software that scientists and engineers can use to create reliable, rapid simulations of complex systems.

In obtaining reduced-order models, Gugercin employs the so-called "(rational) Krylov subspace methods" heavily used in numerical linear algebra when dealing with large-scale problems. Krylov-based methods are among the most successful tools currently available in numerical linear algebra; hence making them the perfect candidates for model reduction of large-scale dynamical systems. The concept of Krylov subspaces is named after the Russian mathematician and naval engineer Alexei Krylov based on his 1931 paper "On the numerical solution of the equation by which, in technical matters, frequencies of small oscillations of material systems are determined".

For the Career award's educational component, he will offer a graduate level course on reduced order modeling and interdisciplinary seminars on scientific computing. With Joseph Ball, Christopher Beattie, Reinhard Laubenbacher, Ekkehard Sachs, and Craig Woolsey from Virginia Tech., Athanasios Antoulas from Rice University, and Tryphon Georgiou from University of Minnesota, Gugercin is organizing the 18th International Symposium on Mathematical Theory of Networks and Systems in Blacksburg in July 2008. His research projects also provide experiences for graduate and undergraduate students in high-performance scientific computing.

Source: Virginia Tech