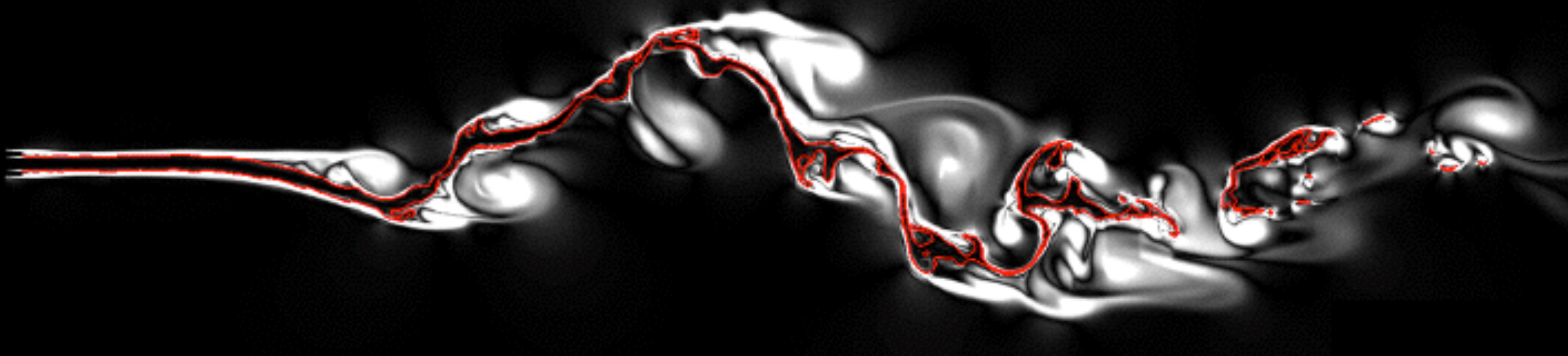
Center for Scientific Computing & Visualization Research



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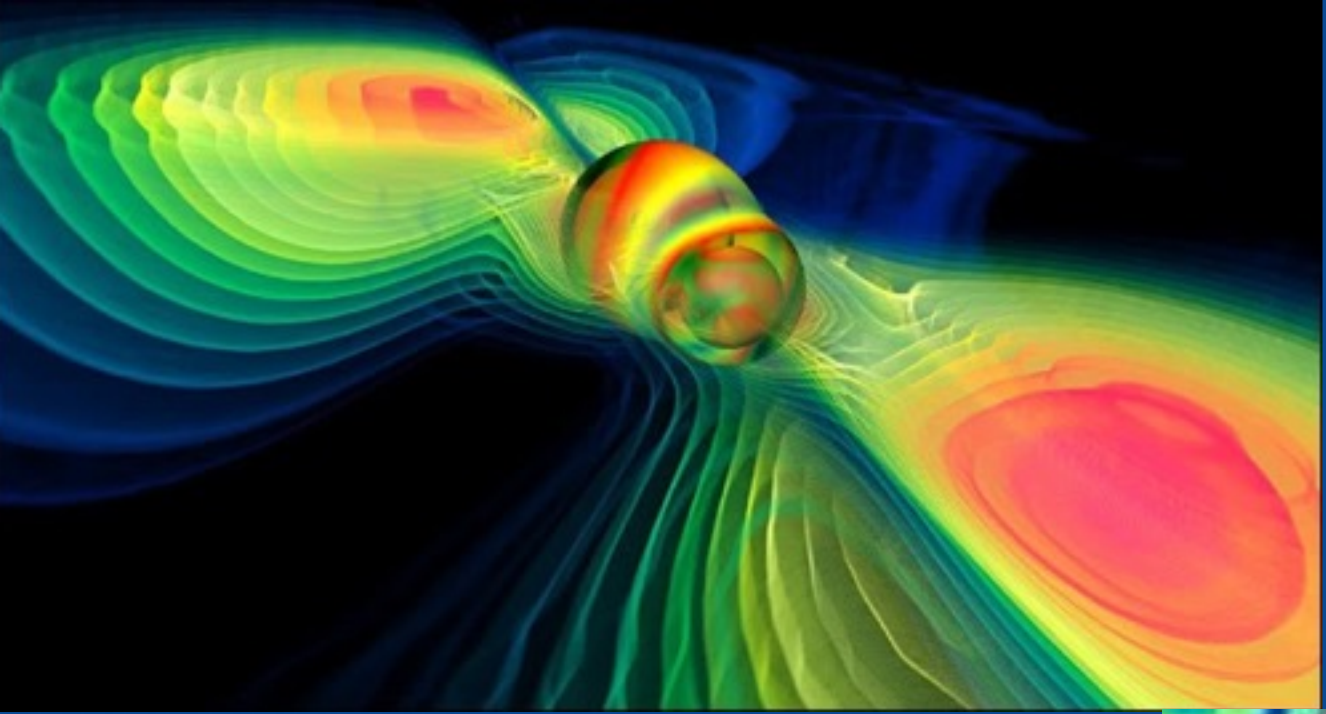
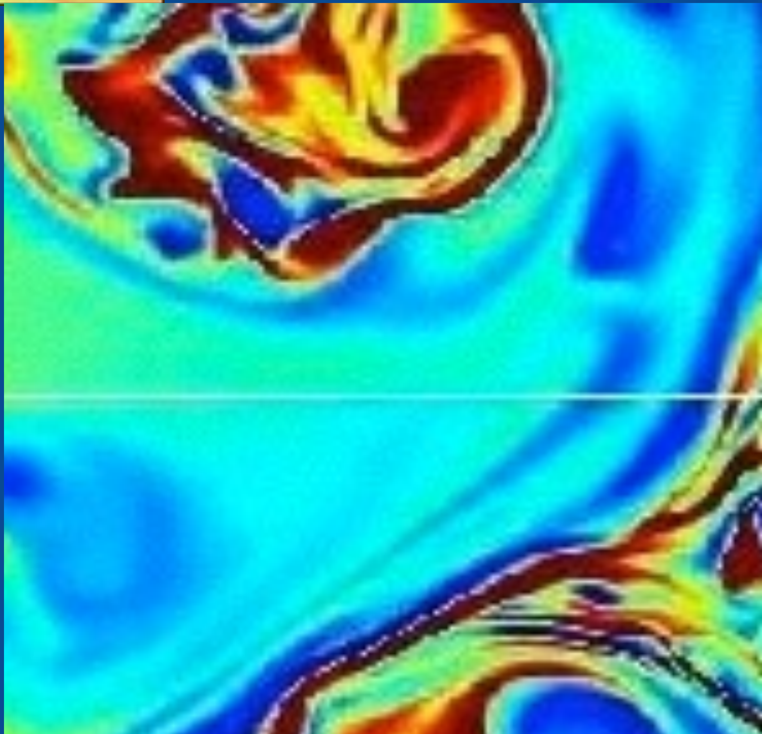
Center for Scientific Computing and Visualization Research

Sigal Gottlieb, PhD
Department of Mathematics
February 2015



Scientific Computing

Developing and using computational methods to solve scientific problems that are otherwise intractable.



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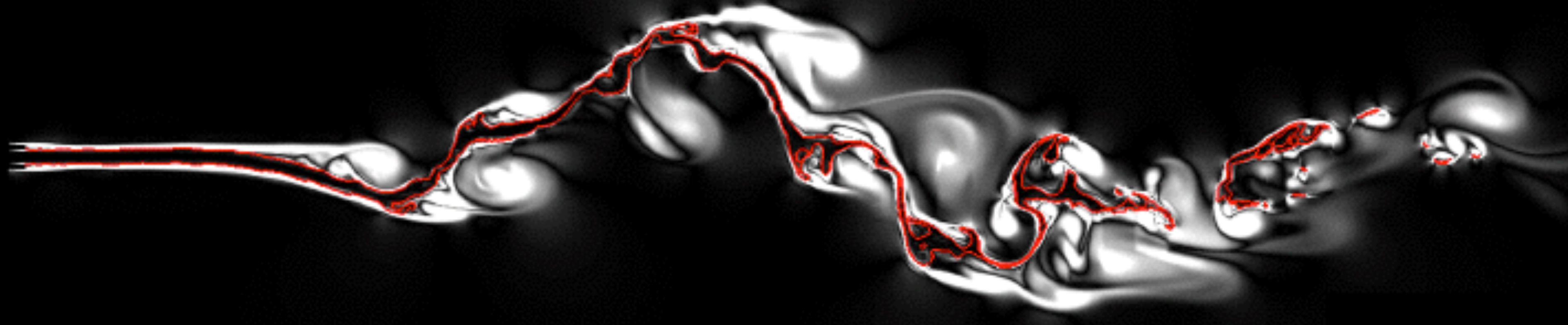
Center for Scientific Computing & Visualization Research



• A fully integrated, multi-disciplinary group of computational scientists
• Working on cutting-edge scientific problems by developing and using state-of-the art computational algorithms on powerful computers.
• Exploring complex problems from a wide range of application areas, as well as novel computational paradigms.

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UMassD scientific computing group

Over 20 faculty members from many departments

- Mathematics
- Computer Science
- Physics
- Electical and Computer Engineering
- Fisheries
- Civil Engineering
- Mechanical Engineering
- Chemistry
- Biology

Our work has been consistently funded by the National Science Foundation, Office of Naval Research, Air Force Office of Scientific Research, and National Air and Space Administration.

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Our activities and accomplishments

- The mission of the CSCVR is to advance the development and application of computational algorithms for scientific discovery
- A major aim of activities is to transcend departmental boundaries and build strong interdisciplinary research collaborations.
- We organized and hosted the first annual UMass system-wide HPCday conference in November 2014. Next year will expand this.
- Senior faculty collaborate with and mentor junior faculty. This mentorship results in increased productivity and success. This past year:
  - Mazdak Tootkaboni (Civil Engineering) received the NSF CAREER award for predictive analysis of stability critical structures
  - Akil Narayan (Math) received the AFOSR Young Investigator Program award for approximations of uncertain parametrized simulations
  - Vanni Bucci (Biology) had a paper published in Nature and was awarded an NSF grant for his work in modeling the intestinal microbiome

Integrating Research and Education

- CSCVR affiliates developed a Computational Science and Engineering track under the umbrella of the Engineering and Applied Science doctoral program. The EAS program has 25 active students, 14 of them in the CSE track. We have graduated one student already.
- Integration of undergraduate research into the mathematics curriculum through a 5-year NSF CSUMS award for $788,985: this endeavor sparked the creation of the Office of Undergraduate Research at UMassD. We want to extend the emphasis on undergraduate research to other disciplines.
- We would like to develop a computational consulting program for students and faculty to work on industrial problems, like in Uppsala University and in Stanford (NSF proposal pending)
- CSCVR affiliates developed new BS and MS programs in data sciences (joint between mathematics and computer science)

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Mathematics and computation is our common language

We were awarded $400,000 from the NSF and AFOSR to buy the HPC cluster, a shared resource we use for our computations. This IBM machine has 448 CPUs and 56 GPUs.

Computational Resources

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High performance GPU computing

The Air Force Research Lab (AFRL) at Rome, NY granted CSCVR four full racks (176 units) of Sony PlayStation 3s for research computing.

UMass Dartmouth pioneered the use of PS3s for astrophysics research back in 2007 when Prof. Khanna of the Physics Dept. created a computer cluster of 16 PS3s and ran his black hole research simulations at supercomputer-level performance.

A new donation of a large GPU-based cluster is now on its way to our campus.

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High performance computing at the MGHPCC

We also have a share in the UMass cluster operating in the Massachusetts Green High Performance Computing Center.

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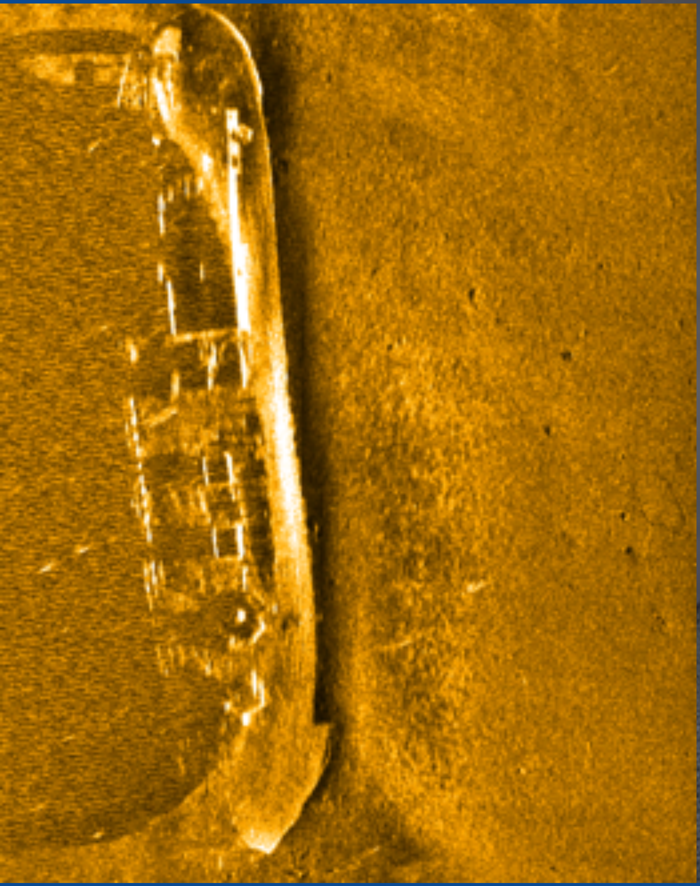
Some CSCVR affiliates and their work

Autonomous mobile robotics



Dr. Ram Bala (CIS) is designing autonomous vehicles, and focuses on sensor fusion to support autonomy. His work is funded by the ONR. This research is supported by the Office of Naval Research and the US Dept of Transportation. He has active collaborations with the Naval Undersea Warfare Center (NUWC, Newport, RI).

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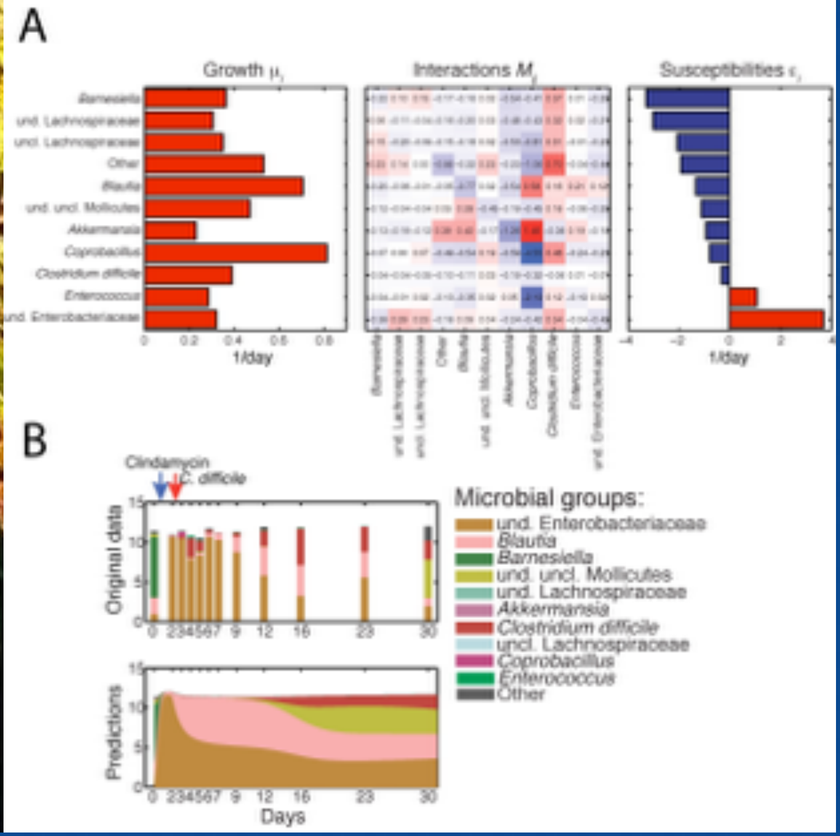
Understanding of the gut microbiome



Dr. Vanni Bucci (Biology) studies the dynamics of the human microbiotic species and their effect on the host immune system.

He recently published a paper in Nature on this work and was just awarded an NSF grant

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Underwater acoustics and whale songs

Dr. John Buck (ECE) has recently been awarded two research grants from the ONR: for his work on “Co-prime Sensor Array Signal Processing” ($743,000) and for “Random Matrix Theory for Adaptive Beamforming” ($404,000)

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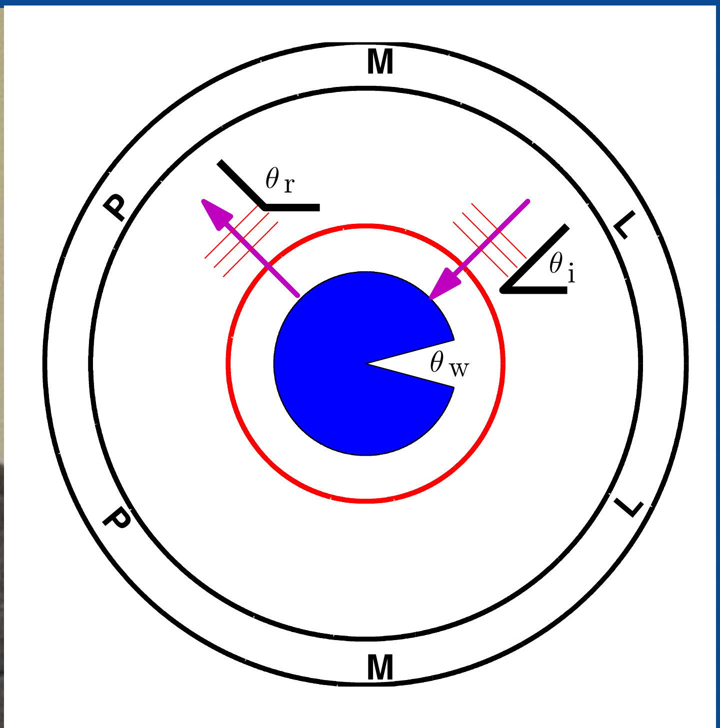
Model reduction methods for multiparameter problems



Dr. Yanlai Chen (Math) works on model reduction methods to reduce the cost of simulation for multi-parameter problems. He is applying his approach to handling large data sets, and working with Southcoast medical systems on problems of mutual interest.

His work is funded by NSF grant "Developing Reduced Basis Methods in the Galerkin and Collocation Framework" ($161,113)

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Model reduction methods for multiparameter problems

Dr. Bo Dong (Math) works on numerical methods for simulation of Korteweg-de Vries type equations, which model such problems as waves on shallow water, tsunami waves, ion acoustic waves in a plasma, and acoustic waves on a crystal lattice.

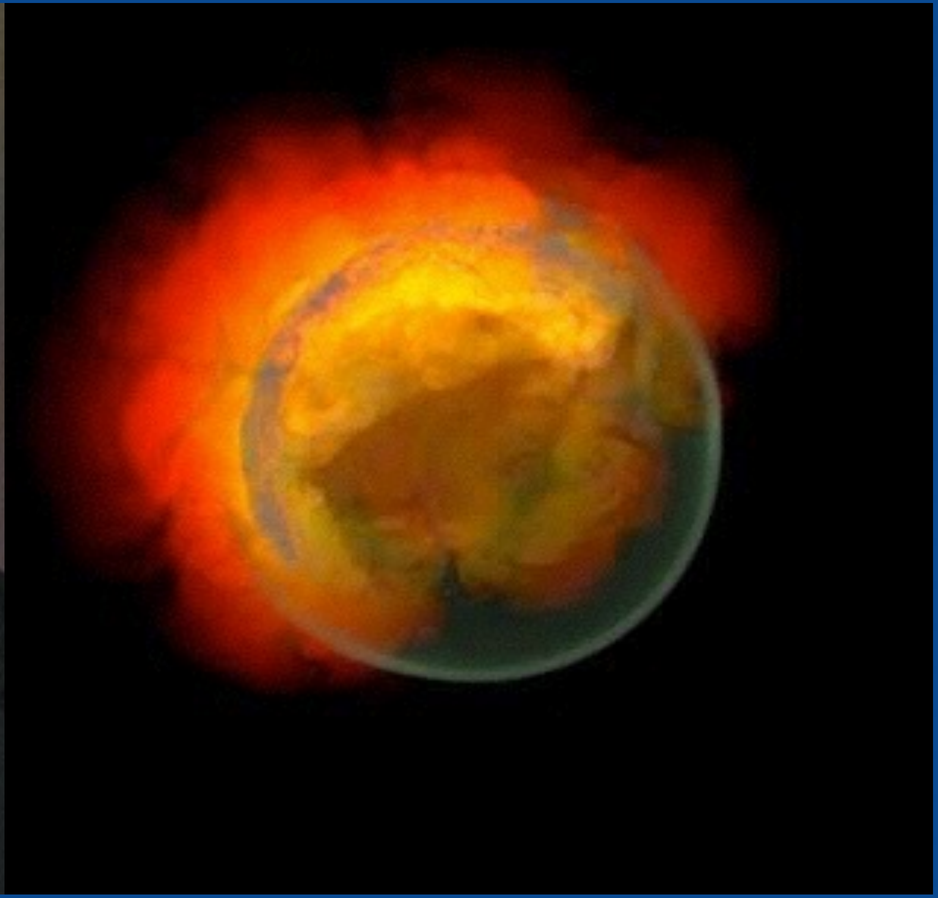
Her work is funded by NSF grant “Development of superconvergent hybridizable discontinuous Galerkin methods and mixed methods for Korteweg-de Vries type equations” ($86,891)

Computational design of wave energy converters



Drs. Geoffrey Cowles (Fisheries), Mehdi Raessi (ME) and Mazdak Tootkaboni (CE) were awarded a grant from the NSF for "A comprehensive computational framework for analysis and optimization of wave energy converters" ($368,221)

Understanding supernovas



Dr. Robert Fisher (Physics) used high performance numerical simulations to conclusively demonstrate a connection between white dwarf stars that fail to completely detonate and a class of oddly dim supernovas.

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Reliability engineering and risk analysis

Dr. Lance Fiondella (ECE) works on models to optimize the reliability of software and systems, including transportation engineering and attack preparedness.

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Time-dependent simulations

Dr. Sigal Gottlieb (Math) develops and analyzes numerical methods that reliably compute how complex flows evolve in time.

This work has been continuously funded by the AFOSR since 2006 ($494,828) and by a grant from KAUST ($202,363).

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Mathematical methods for shape matching in computer vision


Drs. Akil Narayan and Alfa Heryudono (Mathematics) were awarded a grant from the NSF “Computation of geodesics on the universal Teichmuller space for planar shape matching in computer vision” ($325,698)

Dr Narayan (left) was recently awarded an AFOSR Young Investigator Program grant.

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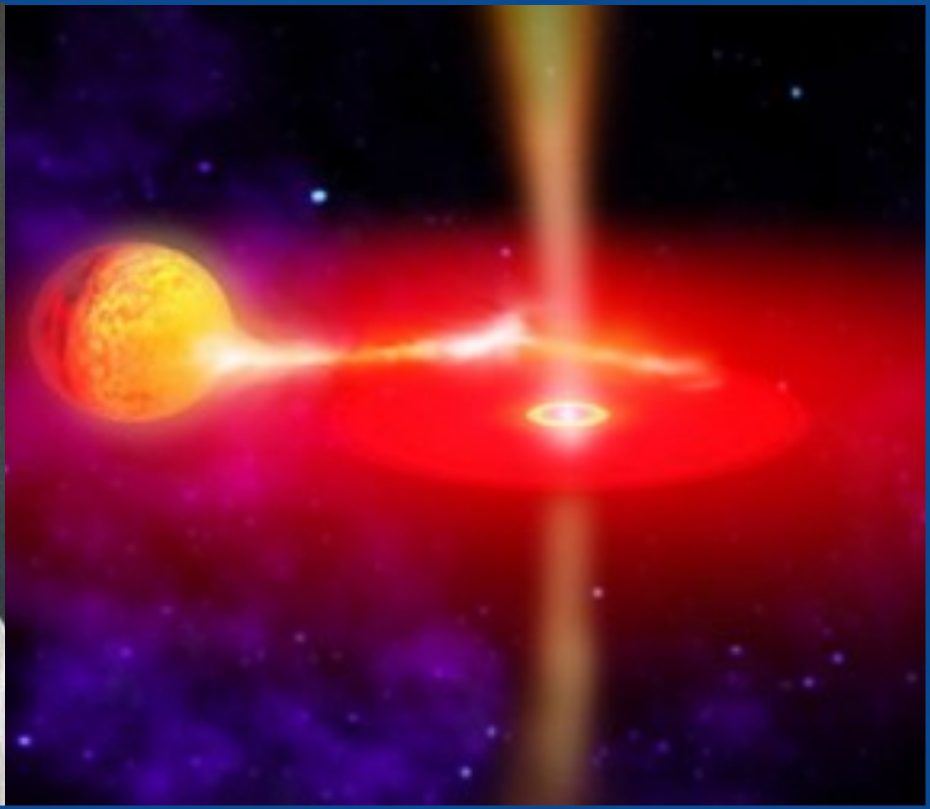
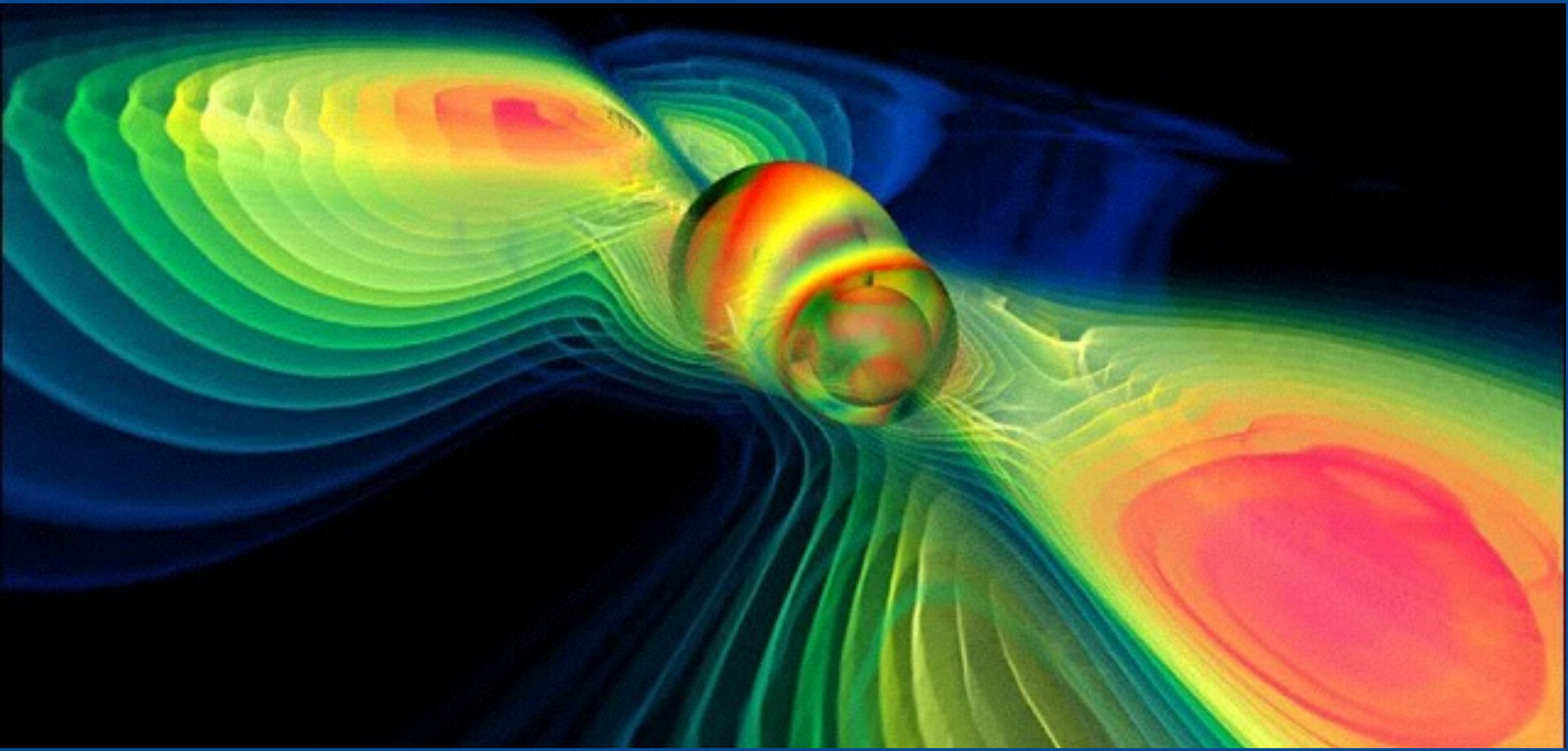
Understanding Black Holes



Dr. Gaurav Khanna (Physics) is funded by the NSF for this work “Gravitation Theory: Numerical Modeling of Large Mass-Ratio Black Hole Binaries Using Time-Domain Perturbation Theory” ($78,000) and for “An Exploration of the Use of OpenCL for Numerical Modeling and Data Analysis” ($167,000).

Understanding Black Holes



This image depicts the burst of gravitational radiation when two black holes merge simulated using the full Einstein general relativity equations.

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An Economical Way to Save Progress

To study gravitational waves, a scientist turned to PlayStations to make a supercomputer.

By LAURA PARKER

This spring, Gaurav Khanna noticed that the University of Massachusetts Dartmouth physics department was more crowded than usual. Why, he wondered, were so many students suddenly so interested in science?

It wasn't a thirst for knowledge, it turns out. News of Dr. Khanna's success in building a supercomputer using only PlayStation 3 video game consoles had spread quickly; the students, a lot of them gamers, just wanted to gape at the sight of nearly 200 consoles stacked on one another.

"It caused quite a stir around here," Dr. Khanna said.

A black hole physicist and associate director of the university's Center for Scientific Computing and Visualization Research, Dr. Khanna first networked 18 PlayStation 3 consoles in 2007 to help model black hole collisions.

His research is focused on finding and studying gravitational waves, vibrations that ripple through space-time. The waves, first predicted by Einstein's theory of general relativity, form after a particularly violent astrophysical event, like two black holes smashing together. Because black holes cannot be observed through telescopes, Dr. Khanna uses supercomputers to create simulations of these collisions.

Supercomputers have become an increasingly important tool for scientists and engineers, who rely on them to crunch large numbers and solve calculations too large for one processor to attempt. According to Dr. Khanna, a supercomputer performs at least 10 times as well as a single desktop computer. He refers to supercomputers as the "third pillar" of science, behind theory and experimentation.

"Science has become expensive," he said. "There's simply not that much money going around, either at the university or the federal level. Supercomputing allows scientists to make up for the resources they don't have."

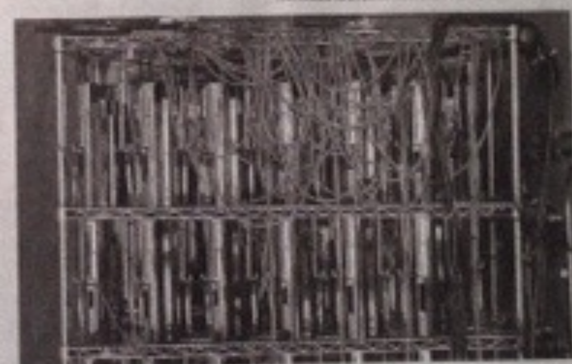
Making a supercomputer requires a large number of processors — standard desktops, laptops or the like — and a way to network them. Dr. Khanna picked the PlayStation 3 for its viability and cost, currently, $250 to $300 in stores. Unlike other game consoles, the PlayStation 3 allows users to install a preferred operating system, making it attractive to programmers and developers. (The latest model, the PlayStation 4, does not have this feature.)

"Gaming had grown into a huge market," Dr. Khanna said. "There's a huge push for performance, meaning you can buy low-cost, high-performance hardware very easily. I could go out and buy 100 PlayStation 3 consoles at my neighborhood Best Buy, if I wanted."

That is just what Dr. Khanna did, though on a smaller scale. Because the National Science Foundation, which funds much of Dr. Khanna's research, might not have viewed the bulk buying of video game consoles as a responsible use of grant money, he reached out to Sony Computer Entertainment America, the company behind the PlayStation 3. Sony donated four consoles to the experiment; Dr. Khanna's university paid for eight more, and Dr. Khanna bought another four. He then installed the Linux operating system on all 16 consoles, plugged them into the Internet and booted up the supercomputer.

Lior Burko, an associate professor of physics at Georgia Gwinnett College and a past collaborator with Dr. Khanna, praised the idea as an "ingenious" way to get the function of a supercomputer without the prohibitive expense.

"Dr. Khanna was able to combine his two fields of expertise, namely general relativity and computer science, to invent something new that allowed for not just a neat new machine, but also scientific progress that otherwise might have taken many more years to achieve," Dr. Burko said.



Gaurav Khanna with a supercomputer he built at the University of Massachusetts Dartmouth physics department using 200 Playstation 3 consoles that are housed in a refrigerated shipping container.

In 2009, Dr. Khanna published a paper in the journal Parallel and Distributed Computing and Systems demonstrating the cell processor of the PlayStation 3 was able to speed up scientific calculations over a traditional computer processor by a factor of nearly 10. The first results of simulations made using the PlayStation 3 supercomputer, detailing the behavior of gravitational waves arising from rotating black holes, were published the same year in the journal Classical and Quantum Gravity.

Dr. Khanna's observations caught the attention of the Air Force Research Laboratory in Rome, N.Y., whose scientists were investigating PlayStation 3 processors. In 2010, the lab built its own PlayStation 3 supercomputer using 1,716 consoles to conduct radar image processing for urban surveillance. "Our PS3 supercomputer is capable of processing the complex computations required to create a detailed image of an entire city from radar data," said Mark Barnell, the director of high performance computing at the Air Force Research Laboratory. The lab later entered into a cooperative research-and-development agreement with Dr. Khanna's team, donating 176 PlayStation 3 consoles.

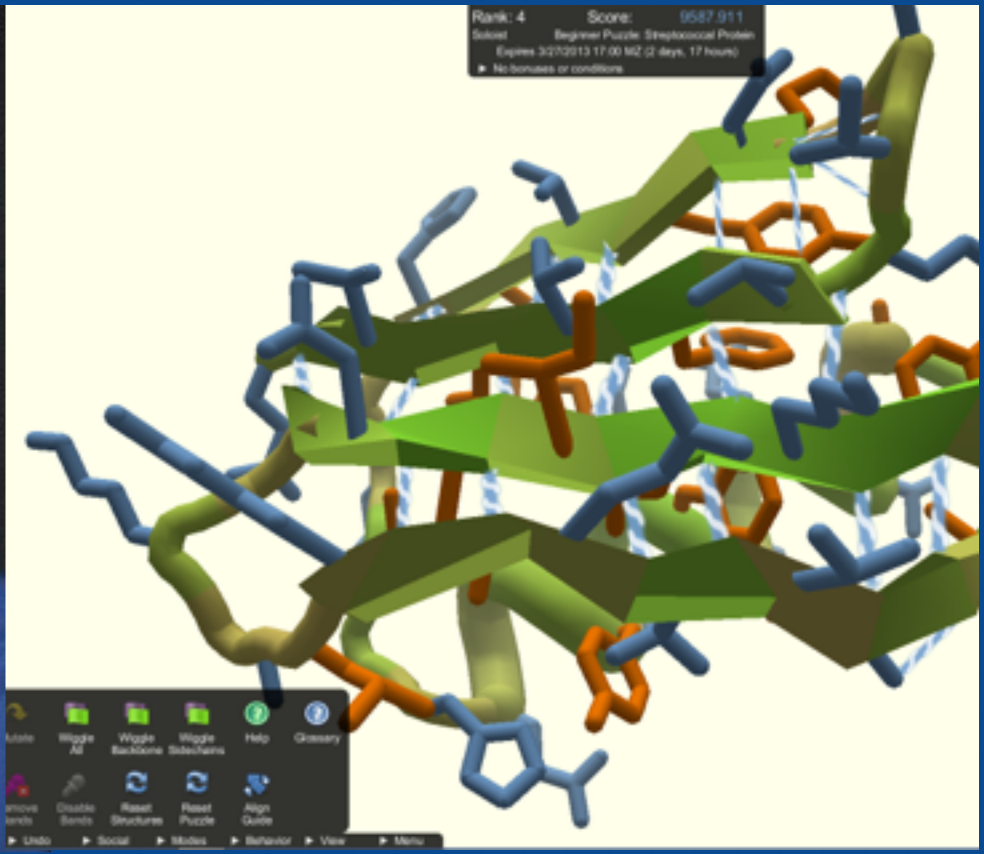
His team linked the consoles, housing them in a refrigerated shipping container designed to carry milk. The resulting supercomputer, Dr. Khanna said, had the computational power of nearly 3,000 laptop or desktop processors, and cost only $75,000 to make — about a tenth the cost of a comparable supercomputer made using traditional parts.

Dr. Khanna has since published two more papers on black hole collisions with results from simulations on the PlayStation 3 supercomputer. Later this year, another 220 consoles from the Air Force lab will arrive. While the plan is to use the consoles to perform more involved and accurate simulations of black hole systems, Dr. Khanna has invited colleagues from other departments to use the supercomputer for their own projects: An engineering team, for example, has signed on to conduct simulations that will help design better windmill blades and ocean wave energy converters, and the university's math department would like to use the supercomputer as a tool to attract students into areas like computational math and science.

But the PlayStation 3 supercomputer isn't suited to all scientific applications. Its biggest limitation is memory: The consoles have very little compared with traditional supercomputers, meaning they cannot handle large-scale calculations. One alternative is to switch to an even better processor, like PC graphics cards. These are also low-cost and extremely powerful — each card is the equivalent of 20 PlayStation 3 consoles in terms of performance.

"The next supercomputer we're going to build will probably be made entirely of these cards," Dr. Khanna said. "It won't work for everything, but it will certainly cover a large set of scientific and engineering applications, especially if we keep improving on it."

Citizen-scientists fold proteins



Dr. Firas Khatib (CIS) is one of the developers of **Foldit**, an online puzzle video game whose objective is to fold the selected proteins as well as possible, using various tools provided within the game.

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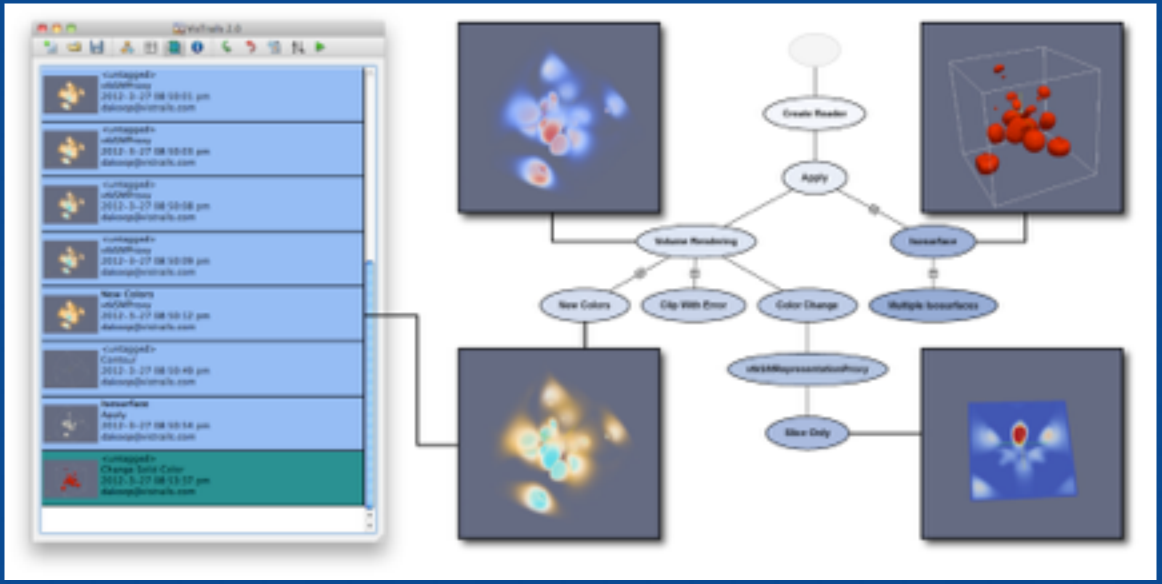
Data Science and Visualization

Dr. David Koop (CIS) is one of the developers of VisTrails, an open-source scientific workflow and provenance management system that supports data exploration and visualization.



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Computational Chemistry

Dr. Maricris Mayes (Chemisty) uses high performance computing simulations to apply quantum chemistry to large systems with thousands of correlated electrons and basis functions.

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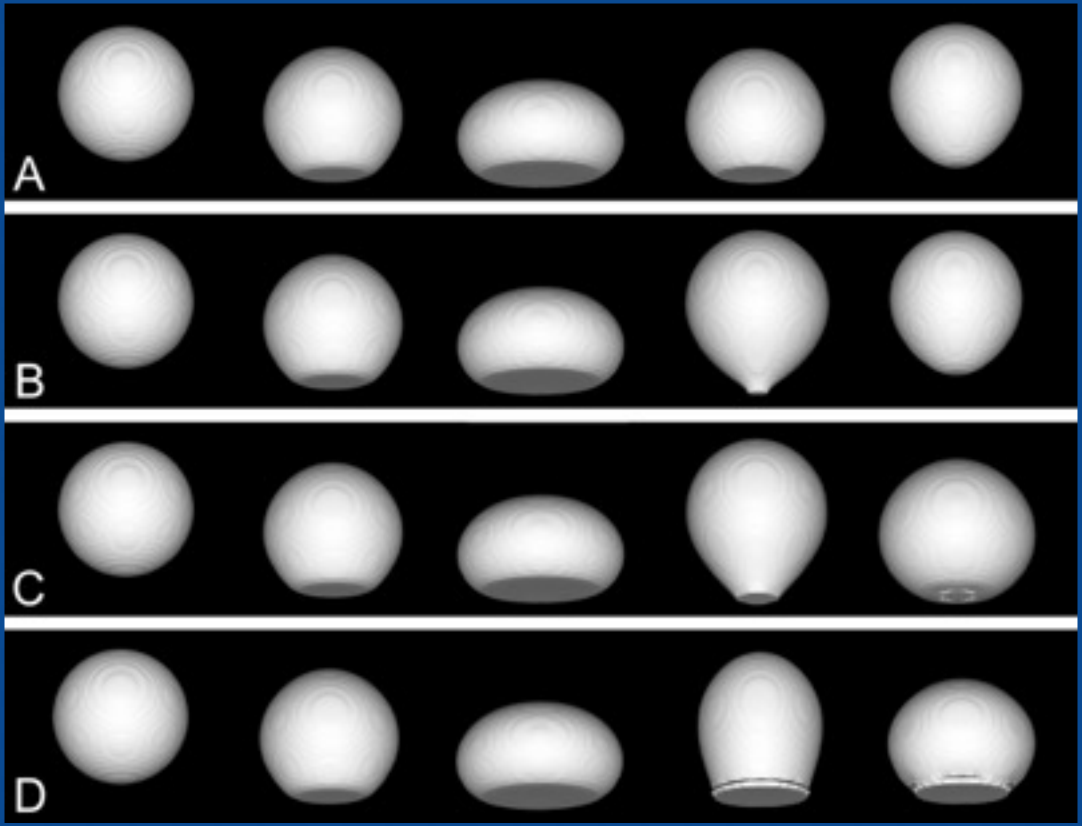
Designing surfaces that prevent ice formation on wind-turbine blades

Dr. Mehdi Raessi (ME) was recently awarded an NSF grant for “Analysis and design of textured super-hydrophobic surfaces capable of preventing ice formation on wind turbine blades.” ($214,583)



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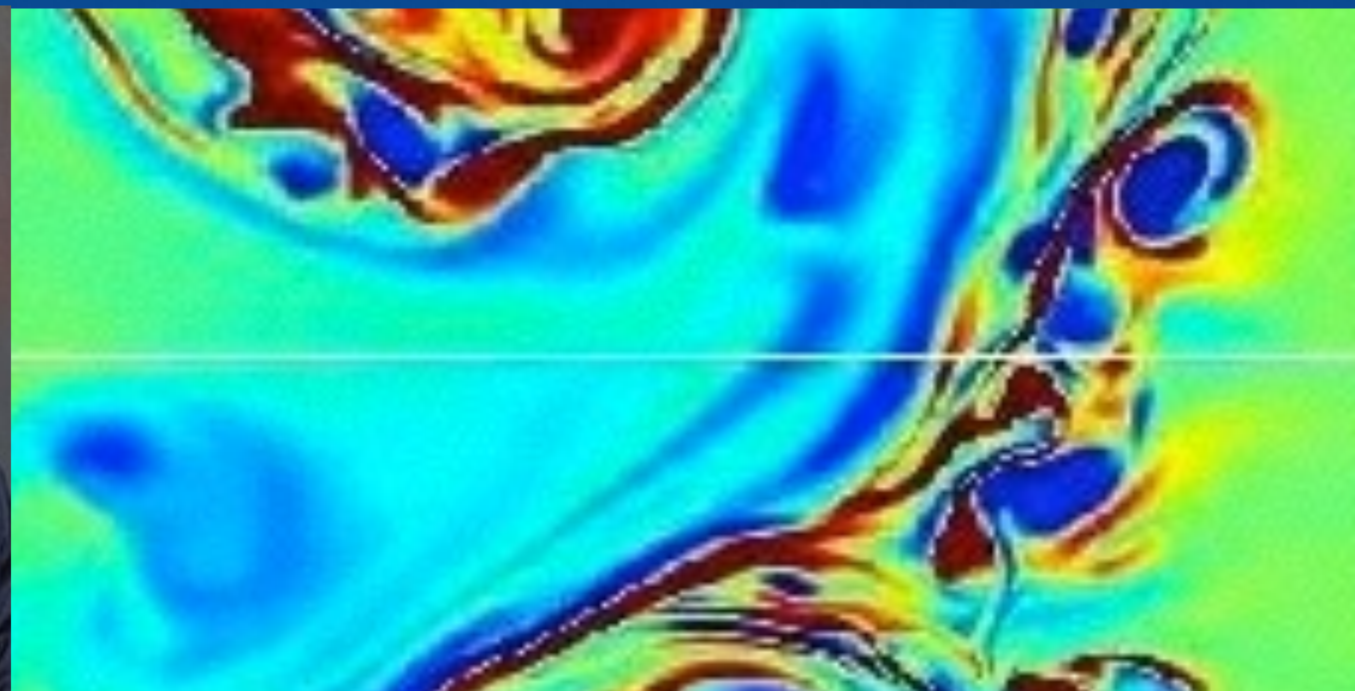
Simulation of ocean circulation



Dr. Amit Tandon (ME) works on ocean mixing and ocean circulation models. His work has been funded by the ONR “Submesoscale routes to lateral mixing in the ocean” ($349,641), the NSF “On the importance of submesoscale processes for ocean productivity” ($328,384), and NASA “Interpreting the ocean’s interior from surface data” ($129,318). Just last month he was awarded a new ONR grant “Coastal and Submesoscale Process Studies for ASIRI” ($647,173).

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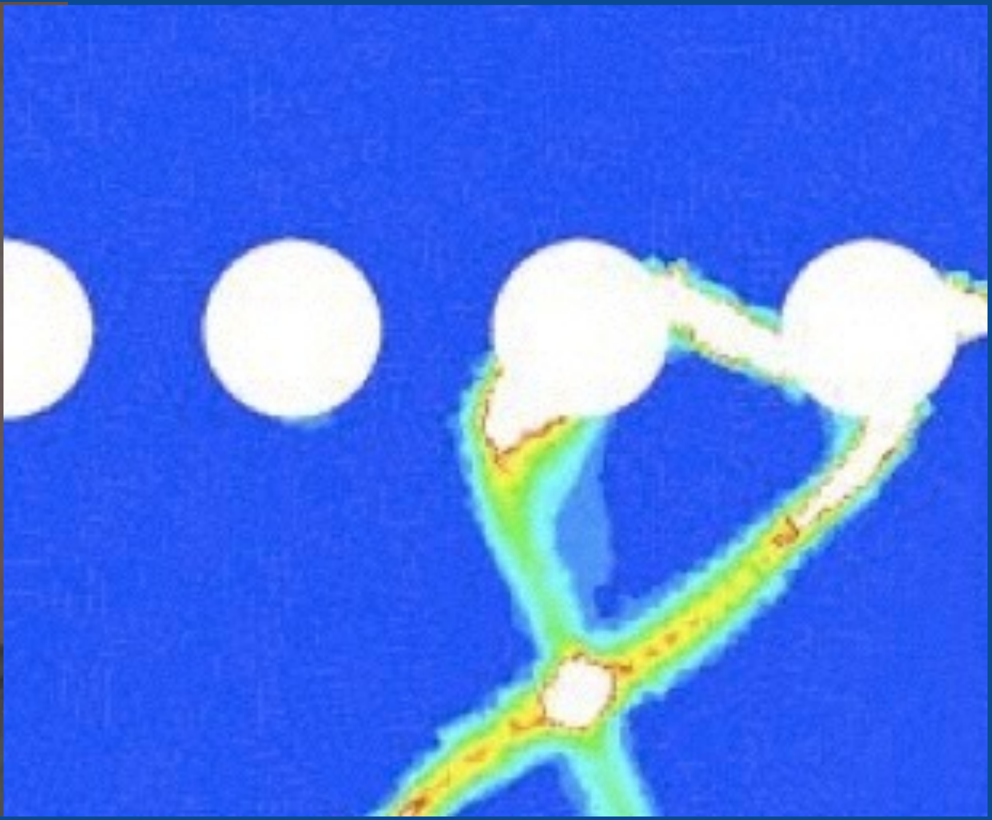
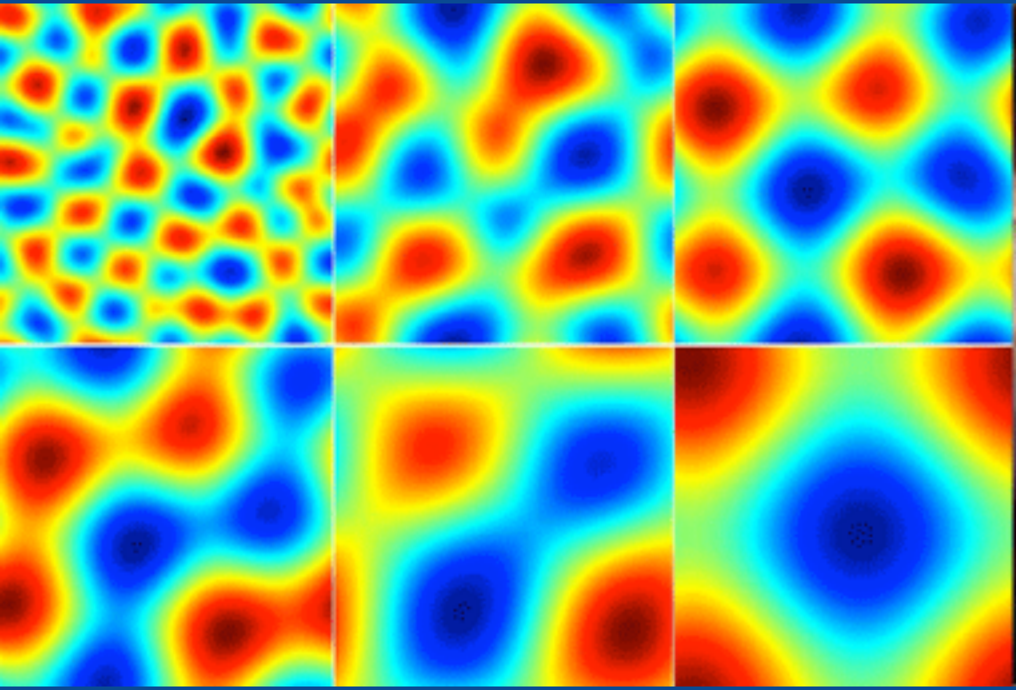
Design of solids and thin walled structures



Dr. Mazdak Tootkaboni (CE) is funded by the NSF for applying computational uncertainty quantification techniques and model validation for the design of thin-walled structures. This work was recently funded by the NSF with a grant of $215,255. He was also recently awarded an NSF CAREER grant.

Numerical methods for modeling tumor growth and crystal formation



Dr. Cheng Wang (Math) is developing and analyzing algorithms for numerical simulations of Cahn-Hilliard-Hele-Shaw model that model tumor growth and epitaxial thin film growth. His work is funded by the NSF for developing numerical methods for bistable gradient equations ($104,283).

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Statistical methodology and machine learning algorithms

Dr. Donghui Yan (Math) was a principal data scientist at Walmart Labs before he joined the math Department this September. His research interests are in statistical methodology and machine learning algorithms as well as applied statistics in various domains. The central goal is to enable reasoning under uncertainty, to understand natural and statistical phenomena, and to meet challenges from modern data.

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