Spring 2022

Department of Scientific Computing

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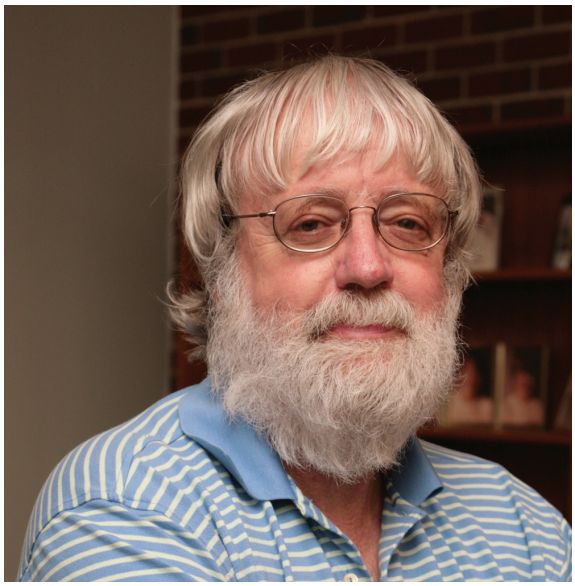
Distinguished professor offers data lectures

Professor Max Gunzburger, founding Chair of the Department of Scientific Computing, Robert O. Lawton Distinguished Professor and Marie Krafft Eminent Professor at Florida State University will give a short course on Saturday, April 16, 2022. The lecture series entitled, **Data Science before the machine learning bandwagon came to town**, will be held on campus and via Zoom.

In recent years, interest in "new" approaches in data science and machine learning such as the use of neural networks has exploded. However, some of those interested in jumping onto that bandwagon may not have a good background in ancient or recent developments in more traditional data science algorithms such as, among others and some in greater detail than others (Monte Carlo methods, compressed sensing, reduced-order modeling, multilevel and multifidelity methods, polynomial chaos, sparse grids, support vector machines, etc.) each of which have proved to be useful in at least some and, in some cases, many application settings. As a result, researchers in and users of the new approaches alluded to above may find it difficult to compare the results of their research with what can be done using other approaches. They also may find it difficult to combine the new approaches with the older ones to construct, as is currently being done by numerous researchers, even better machine learning algorithms.

The lectures are meant to give participants, including those not necessarily interested in the "new" approaches, a quick and dirty introduction to alternate approaches to data science such as, among others, Monte Carlo methods, compressed sensing, reduced-order modeling, multilevel and multifidelity methods, polynomial chaos, and sparse



Professor Max Gunzburger

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Grad student publishes research on enhanced model for studying problems in fundamental physics

Scientific Computing doctoral student Brandon Gusto has developed a new scheme for reactive flow simulations. The new method is the subject of a forthcoming paper, A hybrid adaptive multiresolution approach for the efficient simulation of reactive flows, authored by Gusto and his advisor Tomasz Plewa, which will be published in Computer Physics Communications in May.

Turbulent reactive flows play a critical role in many industrial, defense, and basic science applications. Typically, the physics acting in these types of flows span a wide range of spatial and temporal scales, leading computational modelers to utilize reduced accuracy models and methods for the sake of computational efficiency.

One of the most widely used approaches for reducing the computational expense of reactive flow simulations involves the use of an adaptive mesh which concentrates computing power in the regions of the flow with the most activity. These methods are classified as adaptive mesh refinement (AMR) methods. The new approach by Gusto & Plewa uses a multiresolution framework, previously developed from wavelet theory, not only to adapt the mesh but also to accelerate the flow solver in smooth regions by replacing direct calculations with interpolation from nearby grid points.

Gusto & Plewa demonstrated that the hybrid adaptive multiresolution approach (HAMR) achieves a modest reduction in computational time for several complex multiphysics benchmark problems. However, for problems characterized by highly localized structures, the overall computational cost can be reduced by a factor of several.

"One of the main issues with block-structured adaptive mesh refinement," said Gusto, "is that when refining a particular feature in the flow, the relatively smooth areas surrounding the feature can become over-resolved due to the graded nature of the mesh hierarchy. The new approach uses the multiresolution smoothness indicators to further accelerate computations in those regions, saving effort while maintaining the original level of accuracy.

"The approach is applicable not only to reactive flows but to any type of flow with spatially localized features; for example, it could be applied to aerodynamics as well."

Left: Doctoral student, researcher and author Brandon Gusto

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grids. Of course, a short course cannot hope to cover everything so that a particular foci of the course are settings in which obtaining lots of data have to be collected and in which obtaining that data is a very costly endeavor. Uncertainty quantification of complex systems is used to provide a specific context for the presentation.

The course requires little knowledge of the underlying subject areas such as probability, statistics, mathematics, and numerical methods so that the presentations should be, for the most part, understandable to even STEM-related advanced undergraduate students. Potential participants who are trying to decide whether or not to take the course are welcome to contact the lecturer at mgunzburger@fsu.edu for more information.

Coffee and refreshments will be served between lectures and lunch will be provided on site; registration is required for those attending in person.

Data Science before the machine learning bandwagon came to town

Saturday, April 16, 2022 at the Earth Ocean and Atmospheric Science Building, room 1050

On Campus attendance and via Zoom

Lecture 1: 9a-10:15a
Break (Refreshments)
Lecture 2: 10:45a-Noon

Lunch (Provided) Noon – 1:30p

Lecture 3: 1:30p – 2:45p
Break (Refreshments)
Lecture 4: 3:15p – 4:30p

This event is sponsored by the FSU Department of Scientific Computing, NewSciLabs and Knowli.

For more information or to register, go to https://www.sc.fsu.edu/news-and-events/short-courses/1648-2022-max-gunzburger

Lemmon named among highest cited researchers

Several Florida State University researchers are among the most cited academics worldwide, according to the annual Highly Cited Researchers 2021 list from Clarivate, a data and analytics company.

Three current university faculty members — Professor of Scientific Computing Alan Lemmon, Associate Professor of Biological Science Emily Moriarty Lemmon and Professor of Psychology Thomas Joiner — as well as the late Michael Davidson, the former head of the National High Magnetic Field Laboratory's optical microscopy program, are on this year's list.

"Florida State University's faculty are dedicated researchers who are prolific in their fields," said Interim Vice President for Research Laurel Fulkerson. "This list demonstrates how they are moving their respective fields forward and laying groundwork for other researchers looking to build upon that work."

The highly anticipated annual list identifies researchers who demonstrated significant influence in their chosen field or fields through the publication of multiple highly cited papers during the last decade. Their names are drawn from the publications that rank in the top 1% by citations for field and publication year in the Web of Science™ citation index.

The methodology that determines the "who's who" of influential researchers draws on the data and analysis performed by bibliometric experts and data scientists at the Institute for Scientific Information™ at Clarivate. It also uses the tallies to identify the countries and research institutions where these citation elite are based.

"It is increasingly important for nations and institutions to recognize and support the exceptional researchers who are driving the expansion of the world's knowledge," said David Pendlebury, senior citation analyst at the Institute for Scientific Information at Clarivate. "This list identifies and celebrates exceptional individual researchers at Florida State University who are having a significant impact on the research community as evidenced by the rate at which their work is being cited by their peers. The research they have contributed is fueling the innovation, sustainability, health and security that is key for our society's future."

The full 2021 Highly Cited Researchers list and executive summary can be found online at https://recognition.webofscience.com/awards/highly-cited/2021/ or webofsciencegroup.com.

This article first appeared on news.fsu.edu and was written by Kathleen Haughney.

Sagel takes second in 3 Minute Thesis

A Scientific Computing Ph.D. candidate in Computational Science and Fire Dynamics won second place in the Florida State University Three Minute Thesis (3MT™) annual competition. Daryn Sagel presented research entitled, Modern Methods of Analyzing Fire Spread, which discusses methods used to analyze and predict the spread of wildfires. 3MT™ is a research communication competition developed by The University of Queensland, Australia, that develops academic, research and presentation skills and supports the development of students' capacities to effectively explain their research (which can be quite complex) in language appropriate to an intelligent but non-specialist audience. Doctoral students have three minutes to present their dissertation topic and its significance in a compelling, clear and concise manner.

"Daryn combines computer vision techniques with atmospheric and fire science to characterize high-resolution fire and plume dynamics. Many models often simplify fire spread with a few numbers such as the burn time and the rate of spread," said Bryan Quaife, Sagel's professor. "Daryn demonstrated that this is an over-simplification, even for small controlled burns. Rather than using a few mean values, Daryn performed a statistical analysis of the burn time and rate of spread. She demonstrated that the downwind rate of spread can be well-approximated with an exponential distribution, implying that fire models can be interpreted as a Poisson process. Daryn is extending her methodology to investigate near-field plume dynamics which is supported by the Department of Defense Strategic Environmental Research and Development Program."

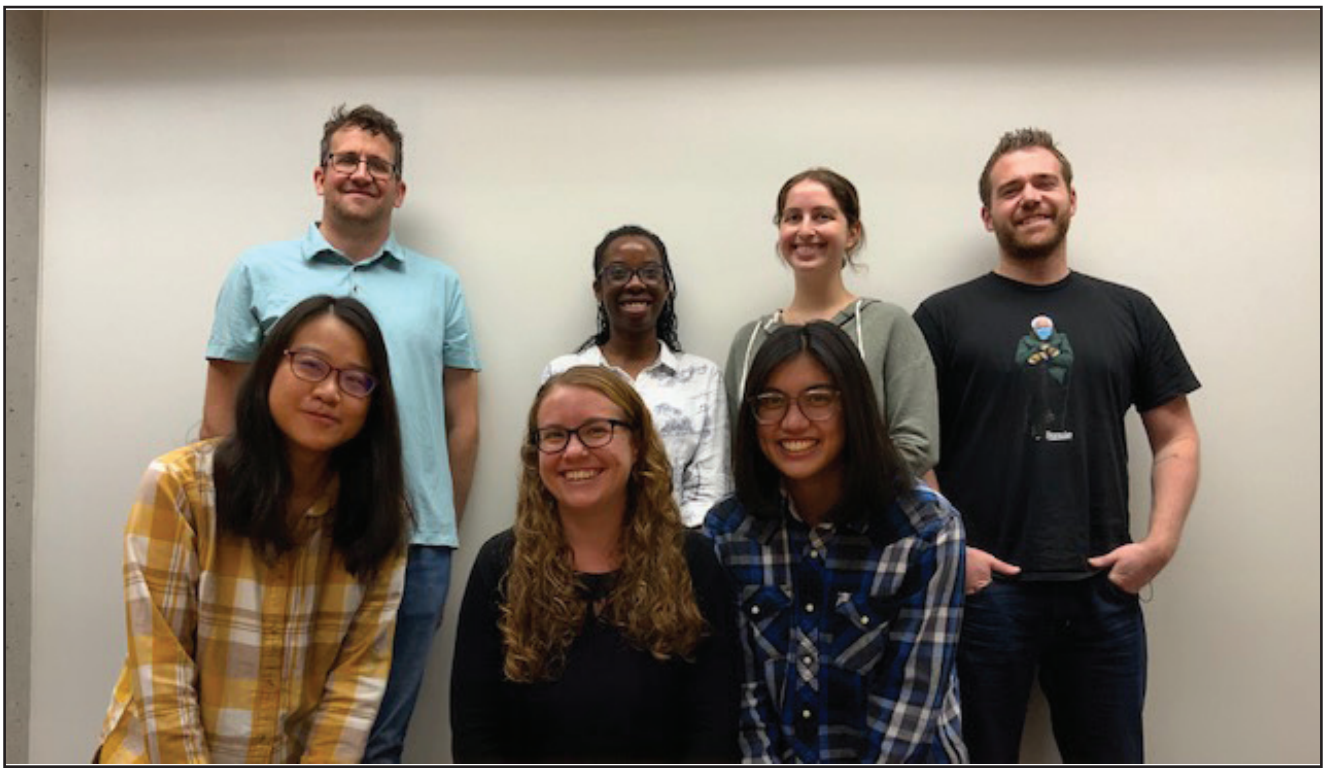
This is the ninth year of the competition at Florida State, and there were eight finalists. Sagel, who won $750, tied for second place with Nidha Walia, a student in Biological Science.

Daryn Sagel is a doctoral student in the Department of Scientific Computing..

To see her award winning presentation, go to https://vimeo.com/635894273.
For more on 3MT™, go to https://threeminutethesis.uq.edu.au/.
For more on Quaife and his group, go to https://people.sc.fsu.edu/~bquaife/.
For more on the department, go to sc.fsu.edu.

Right: Ph.D. student Daryn Sagel

Quaife Lab: Engaging students in research



Quaife Lab

The College of Arts and Sciences, Florida State University, and the FSU Board of Trustees recently awarded Dr. Bryan Quaife tenure and promotion to Associate Professor. Quaife joined the Department of Scientific Computing as an Assistant Professor in the Fall of 2016 after completing four years as a postdoctoral associate at the University of Texas at Austin. His research seeks to develop and implement numerical methods to efficiently and accurately describe both slow (groundwater flow, nanorod and biomembrane suspensions) and fast moving (fire and plumes) fluid flows.

Since arriving at the department, Quaife has expanded the scope of his research, applying his mathematical and computational knowledge base to a wide variety of problems. In slow moving fluid flows, he has studied transport properties in eroded materials, explored the statistical properties of a porous medium to flow and used adhesion to describe chains of biomembranes. He has made major contributions to the study of fast moving fluids, too, through his research on fire dynamics.

"The biggest change to my research is that I branched into a completely new field—fire dynamics. This research is much more interdisciplinary than my other projects, and it includes collaborators from Engineering, Statistics, Los Alamos National Lab, and Tall Timbers Research Station," said Quaife. "I am still active in projects that are more closely related to work I started before joining FSU. However, the biggest change to these projects is that I am now applying algorithms I developed before FSU to better understand physical processes such as erosion and cellular permeability."

Quaife's major accomplishments in fire dynamics and fast moving fluids include combining computations and experiments to characterize how atmospheric conditions affect low intensity prescribed fire; calculating burn times and probabilities of fire spread; and, along with then doctoral student David Robinson, implementing an augmented reality sandbox to visualize real-time fire spread in geometry with topography.

Historically, faculty concentrate on fundamental research during their early career and shift toward diversity and mentorship after receiving tenure. Assisting Quaife with these wide-ranging projects, however, is a bevy of enthusiastic students - students well in excess of the typical new assistant professor working to establish himself, his classes, and his research. Quaife embraces these experiences as positive, adding depth and dimensionality to his research.

"The way I see it, I have been fortunate to have many students show interest in working with me. These students are all doing great work, and through our collaborations we have been able to publish interesting papers and secure funding. The diversification of my research is also a direct consequence of the research interests of my students. As two examples, I co-advised Sid Bishnu with a scientist at Los Alamos National Laboratory to incorporate ocean dynamics into the Energy Exascale Earth System Model, I co-advised Lukas Bystricky with Sachin Shanbhag to simulated suspensions of rigid bodies with applications in polymer physics, and with Ashley Gannon I study suspensions of semipermeable and multicomponent membranes."

Since joining FSU, Quaife has received several grant awards, published fifteen papers in top tier journals, and taught undergraduate and graduate courses that combine algorithms, computer programming, theory, and applications. He is using Department of Defense funding for fire dynamics research to investigate the structure of near-field plumes, a collaboration between key performers from four institutions.

"I have been fortunate to teach classes and seminars that are related to different research projects. Through these courses several students have become interested in my research and are now working with me. I have two funded projects that are both in collaboration with faculty from other departments and institutions. By working with experts from different disciplines, my research has become much more interdisciplinary. Many of my other projects are also in collaboration with colleagues from different institutions."

To learn more about Quaife, his students, and his research, go to https://people.sc.fsu.edu/~bquaife/.

For more on the department, go to www.sc.fsu.edu.

The Department of Scientific Computing bids a fond farewell to our long time graphic designer, Bill Burgess, who worked for the department in all its incarnations for over 30 years. We wish Bill and his wife Maggie all good things at their new home in North Carolina.

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The department's mission is to be the focal point of science and computation at Florida State University. Gordon Erlebacher is Chair of the Department of Scientific Computing. He can be reached at 850.644.7024. Newsletters are issued three times each year. Subscriptions and single copies are available by calling 850.644.0196. This publication is available in an alternative format on request.

Gusto, continued from p. 2

Gusto is the recipient of the Science, Mathematics, and Research for Transformation (SMART) Scholarship Program.

For more on Gusto, go to https://people.sc.fsu.edu/~blg13/.
For more on the department, go to sc.fsu.edu.

This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility located at Lawrence Berkeley National Laboratory, operated under Contract No. DE-AC02-05CH11231 using NERSC award NP-ERCAP18509. The software used in this work was in part developed by the DOE Flash Center.
For more on Gusto, go to https://people.sc.fsu.edu/~blg13/.
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Right: Professor Tomasz Plewa, Gusto's advisor and co-author.

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