Georgia Scientific Computing Symposium
Emory University
February 29, 2020

9:30  Registration, Poster Setup, Coffee

9:50  Opening Remarks

10:00  Yingjie Liu, Georgia Institute of Technology
New finite difference methods on irregular grids for solving the Maxwell’s equations

10:45  Marta D’Elia, Sandia National Laboratories
Nonlocal models in computational science and engineering

11:30  Poster Blitz

12:00  Lunch, Posters, Group Photo

1:30  Vince Calhoun, Georgia State University
An extensible computational eco-system for capturing, managing, processing, and accessing brain imaging data

2:15  Xiuwei Zhang, Georgia Institute of Technology
Evaluating computational methods for single cell data analysis and next steps

3:00  Break and Posters

3:30  Lin Mu, University of Georgia
The Recent Development of Weak Galerkin Finite Element Methods

4:15  Lars Ruthotto, Emory University
Partial Differential Equations meet Deep Learning:
Old solutions for new problems and vice versa

5:00  Reception
Titles and Abstracts of Invited Talks

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New finite difference methods on irregular grids for solving the Maxwell’s equations

This talk is based on a recent joint work with Dr. Xin Wang. We have developed new, simple and efficient second order finite difference methods for solving Maxwell’s equations on non-staggered irregular grids with large CFL numbers (greater than or equal to 1 in one, two or three dimensions). The methods don’t need to compute the local characteristic information for the hyperbolic system and are easy to implement on unstructured meshes. The schemes can be naturally adapted to the perfectly matched layers (PML) for absorbing boundaries. BFECC had been applied to schemes for scalar advection equations to improve their stability and order of accuracy. In this talk similar theoretical results for systems will be introduced. These results are robust for irregular meshes and for nonlinear equations. We apply BFECC to the central difference scheme (unstable if used along), Lax-Friedrichs scheme or a combination of them for the Maxwell’s equations and obtain second order accurate schemes with large CFL numbers. The method is further applied to schemes based on the least-squares linear interpolation on non-orthogonal, non-staggered irregular grids to obtain second order stabilized versions. Numerical examples are given to demonstrate the robustness of the new schemes.

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Nonlocal models in computational science and engineering

Nonlocal models such as peridynamics and fractional equations can capture effects that classical partial differential equations fail to capture. These effect include multiscale behavior, discontinuities in the solutions such as cracks, and anomalous behavior such as super- and sub-diffusion. For this reason, they provide an improved predictive capability for a large class of engineering and scientific applications including fracture mechanics, subsurface flow, turbulence, plasma dynamics, and image processing, to mention a few. However, the improved accuracy of nonlocal formulations comes at the price of modeling and computational challenges that may hinder the usability of these models. Challenges include the prescription of nonlocal boundary conditions, the treatment of nonlocal interfaces, the identification of model parameters and the incredibly high computational cost. In this talk I will discuss these challenges and describe in detail how we are addressing some of them at Sandia National Labs. Specifically, I will describe a recently developed machine learning approach to the estimation of model parameters in nonlocal diffusion models based on physics informed neural networks. If time allows, I will also briefly present a recently developed theory of nonlocal interfaces that allows for a mathematically rigorous and physically consistent treatment of material heterogeneities.
Vince Calhoun  
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An extensible computational eco-system for capturing, managing, processing, and accessing brain imaging data

The brain imaging field has been dramatically changed by advances in computation and cloud computing as well as the availability data. And while there are a wealth of promising new tools and frameworks which have been developed, there are still many gaps in their ability to provide a comprehensive solution. In this talk I will discuss some of our attempts at TReNDS to develop solutions that can address some keys areas including: 1) the ability to perform data capture, management, and workflow while protecting sensitive information, 2) tools to provide both centralized and standardized analytic pipelines and also dashboarding and access, and finally 3) approaches to enable the analysis of data which cannot be shared for various reasons. I will also highlight some of the analysis approaches we have found useful, including both preprocessing, group level inference, and machine learning approaches. We are still only touching the surface of the potential to leverage the current technological landscape to help us uncover the secrets held within the most complex organ in the human body, however the advances within the past few years have given us a glimpse of the enormous untapped potential and the possibility of new tools to make an impact on psychiatric and neurological disorders.

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Evaluating computational methods for single cell data analysis and next steps

In the era of big data, the data in molecular biology grows not only in scale, but also in resolution and modality. Developments in single cell genomics are transforming our understanding of biological systems by capturing differences between single cells which allows researchers to identify new cell types, states, and transitions across cell states. Appropriate computational methods are crucial to making these discoveries. To evaluate new computational methods for processing and interpreting transcriptomes at a single cell resolution, we need in-silico platforms. Simulated datasets which resemble the properties of real datasets can aid in method development and prioritization as well as in questions in experimental design by providing an objective ground truth. We present SymSim, a simulator software that explicitly models the processes that give rise to data observed in single cell RNA-Seq experiments. We demonstrate how SymSim can be used for benchmarking methods for clustering, differential expression trajectory inference and regulatory network inference, and for examining the effects of various parameters on their performance. Moving ahead, although single cell RNA-Seq data has significantly advanced our knowledge of biological systems, to obtain a comprehensive picture of cellular mechanisms, we need to integrate other types of data at single cell level. We develop methods based on matrix factorization and deep learning for integrative analysis of multi-modality single cell data.
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The Recent Development of Weak Galerkin Finite Element Methods

In this talk, we shall introduce the weak Galerkin finite element method (FEM), which is a new polygonal FEM, for solving partial differential equations. The key concept of discrete weak derivatives will be introduced and discussed for the development of numerical schemes. Weak Galerkin (WG) Method is a natural extension of the classical Galerkin finite element method with advantages in many aspects. For example, due to its high structural flexibility, the weak Galerkin finite element method is well suited to most partial differential equations on the general meshing by providing the needed stability and accuracy in approximation. In this talk, the speaker shall discuss the basics of weak Galerkin finite element methods, including a priori error estimate and a posteriori error estimate. We start with second-order elliptic equations, for which WG shall be applied and explained in detail. Later, we shall extend our schemes to several CFD models, including Stokes equations, Brinkman equations, and Navier-Stokes equations. We shall discuss the new divergence preserving schemes and upwind stabilization techniques in designing the robust numerical schemes.

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One of the most promising areas in artificial intelligence is deep learning, a form of machine learning that uses neural networks containing many hidden layers. Recent success has led to breakthroughs in applications such as speech and image recognition. However, more theoretical insight is needed to create a rigorous scientific basis for designing and training deep neural networks, increasing their scalability, and providing insight into their reasoning.

In the first part of my talk, I will outline several recent advances made by interpreting some widely used deep learning techniques as discretizations of (partial) differential equations. This viewpoint has opened the door to applications of established mathematical theory and numerical algorithms to machine learning in novel ways. I will provide several examples to represent this promising direction toward more reliable and efficient deep learning.

In the second part of my talk, I will showcase how deep learning promises new ways to solve classical mathematical problems at an ever-larger scale. As a prototypical example, I will demonstrate how deep learning can enable the solution of the century-old optimal mass transport problem in high dimensions. Using this example, I will also discuss how the classical applied mathematics paradigm in research and teaching is reshaping in the era of machine learning.

The primary references for my talk are:

https://arxiv.org/abs/1705.03341
https://arxiv.org/abs/1804.04272
Posters

Each poster presenter will have one minute during the poster blitz to briefly describe an overview of their poster. This is a rapid fire event! Poster presenters should line up on the left side of the room, in the order given below. When one person finishes, the next person steps up.

1. Begovic, Erna
   University of Zagreb
   *On the convergence of complex Jacobi methods*

2. Cui, Jianbo
   Georgia Institute of Technology
   *TBA*

3. Erlandson, Lucas
   Georgia Institute of Technology
   *Accelerating Hierarchical Matrix-Vector Products*

4. Gharbi, Aroua
   Georgia Institute of Technology
   *Augmenting SysML with Analytics Capabilities*

5. He, Huan
   Emory University
   *FAST: A Fast Asynchronous Stochastic gradient descent algorithm for Sparse tensor decomposition*

6. Huang, Haoxiang
   Georgia Institute of Technology
   *Physics Constraint Neural Network for Engineering Problem*

7. Huang, Ru
   Emory University
   *Regularized Generalized Matrix Function*

8. Ji, Yuliang
   Emory University
   *Twin Graph*

9. Kan, Kelvin
   Emory University
   *A Projected Newton-Krylov Method for Large-Scale Bound-Constrained Optimization Problems*

10. Kim, Junghyun
    Georgia Institute of Technology
    *A Data-Driven Approach using Machine Learning for Real-Time Flight Path Optimization*

11. Liao, Wenjing
    Georgia Institute of Technology
    *Nonparametric regression on low-dimensional manifolds using deep ReLU networks*

12. Liu, Hao
    Georgia Institute of Technology
    *Learning functions varying along an active subspace*

13. Liu, Shu
    Georgia Institute of Technology
    *Parametric Fokker-Planck equation*
14. Ma, Shaojun  
Georgia Institute of Technology  
*Learning Stochastic Behaviour of Aggregate Data*

15. Meng, Chang  
Emory University  
*Krylov Methods for Low-Rank Regularization*

16. Morciglio, Anthony  
Georgia State University  
*Leader, Follower, and Intermediates: Modeling Collective Cancer Invasion*

17. Nagy, James  
Emory University  
*IRtools: MATLAB Package for Large-Scale Inverse Problems*

18. Onken, Derek  
Emory University  
*PDE-based Neural Networks for Lung Cancer Detection using 3-D LDCT Images*

19. Pandey, Arti  
Indian Institute of Technology Ropar  
*Multiple Intents Re-ranking*

20. Verner, Eric  
Georgia State University  
*Cloud-based Tools for Advanced Brain Imaging Analysis*

21. Viguerie, Alex  
Università di Pavia  
*Two-level methods for additive manufacturing and nonhomogenous material problems*

22. Zhang, Bin  
Georgia State University  
*Leader and follower: modeling collective invasion using a game theory model*

23. Zhang, Ziqi and Oh, Sooyoun  
Georgia Institute of Technology  
*Computational methods to study cell mechanisms from single cell data*