Texas Applied Mathematics and Engineering Symposium
Book of Abstracts

Max Bremer
Brendan Keith
Tom O'Leary-Roseberry
Timothy Smith
Gopal Yalla

September 21-23, 2017

Welcome Address

Dear Colleagues,

Hello and welcome to Austin, Texas! We are honored to be hosting graduate students, postdoctoral research scientists, and professors from the Lone Star State and beyond. We want to thank everyone for the widespread interest in this conference as we have talks in many areas of applied mathematics, ranging from computational biology to earth systems modeling. We hope that you find this meeting productive and invigorating.

Sincerely,

The TAMES Organization Committee

Max Bremer, Brendan Keith, Tom O'Leary-Roseberry, Timothy Smith, Gopal Yalla

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Plenary Speakers

Isogeometric Analysis of Solids, Structures, and Fluid-Structure Interaction: From Early Results to Recent Developments

Yuri Bazilevs

Professor and Vice Chair of Structural Engineering
Adjunct Professor of Mechanical and Aerospace Engineering
The University of California, San Diego

Friday, Sept. 22 @ 4:00pm, Room 2.302

This presentation is focused on Isogeometric Analysis (IGA) with applications to solids and structures, starting with early developments and results, and transitioning to more recent work. Novel IGA-based thin-shell formulations are discussed, and applications to progressive damage modeling in composite laminates due to low-velocity impact and their residual-strength prediction are shown. Fluid–structure interaction (FSI) employing IGA is also discussed, and a novel framework for air-blast-structure interaction (ABSI) based on an immersed approach coupling IGA and RKPM-based Meshfree methods is presented and verified on a set of challenging examples. The presentation is infused with examples that highlight effective uses of IGA in advanced engineering applications.

Bio:

Yuri Bazilevs is a Full Professor and Vice Chair in the Structural Engineering (SE) Department, and an Adjunct Full Professor in the Mechanical and Aerospace Engineering (MAE) Department, in the Jacobs School of Engineering at UCSD. Yuri completed his PhD and Postdoc training at UT Austin's Institute for Computational Engineering and Sciences (ICES) under the direction of Prof. Thomas J.R. Hughes. He joined UCSD as an Assistant Professor in July of 2008, was promoted to Associate Professor with tenure in July 2012, and, subsequently, to Full Professor in July 2014. Yuri develops sophisticated computational techniques and tools to build predictive models for a wide range of applications. His work addresses complex problems in the areas of medicine, such as blood flow in the heart and arteries, as well as in medical devices including blood pumps and artificial hearts; renewable energy, such as assessing damage to wind turbines due to extreme conditions in harsh offshore environments; and protecting infrastructure against man-made and natural disasters, such as assessing the response of structures to terrorist attacks. For his research contributions Yuri received several awards and honors. Most recently, he was included in the 2014, 2015, and 2016 Thomson-Reuters lists of Highly Cited Researchers and World's Most Influential Scientific Minds, both in the Engineering and Computer Science categories. More information about Yuri may be found at `http://ristretto.ucsd.edu/~bazily`.

Large-scale Bayesian inversion and the flow of the Antarctic ice sheet

Omar Ghattas

Jackson Chair in Computational Geosciences
Professor of Geological Sciences and Mechanical Engineering
Director, Center for Computational Geosciences & Optimization
Institute for Computational Engineering and Science
The University of Texas at Austin

Thursday, Sept. 21 @ 1:00pm, Room 2.302

Many geophysical systems are characterized by complex nonlinear behavior coupling multiple physical processes over a wide range of length and time scales. Mathematical and computational models of these systems often contain numerous uncertain parameters, making high-reliability predictive modeling a challenge. Rapidly expanding volumes of observational data–along with tremendous increases in HPC capability–present opportunities to reduce these uncertainties via solution of large-scale inverse problems. Bayesian inference provides a systematic framework for inferring model parameters with associated uncertainties from (possibly noisy) data and any prior information. However, solution of Bayesian inverse problems via conventional Markov chain Monte Carlo (MCMC) methods remains prohibitive for expensive models and high-dimensional parameters, as result from discretization of infinite dimensional problems with uncertain fields. Despite the large size of observational datasets, typically they can provide only sparse information on model parameters. Based on this property we design MCMC methods that adapt to the structure of the posterior probability and exploit an effectively-reduced parameter dimension, thereby making Bayesian inference tractable for some large-scale, high-dimensional inverse problems. We discuss inverse problems for the flow of the Antarctic ice sheet, which have been solved for as many as one million uncertain parameters at a cost (measured in forward problem solves) that is independent of the parameter dimension and the data dimension. This work is joint with Tobin Isaac, Noemi Petra, and Georg Stadler.

Bio:

Omar Ghattas is the John A. and Katherine G. Jackson Chair in Computational Geosciences, professor of geological sciences and of mechanical engineering, and director of the Center for Computational Geosciences in ICES. He also holds courtesy appointments in the Departments of Computer Science, Biomedical Engineering, and in the Texas Advanced Computing Center.

He earned his Ph.D. in computational mechanics from Duke University. He has general research interests in simulation and modeling of complex mechanical, geological, and biological systems on supercomputers, with specific interest in inverse problems and associated uncertainty quantification for large-scale systems. His centers current research is aimed at large-scale forward and inverse modeling of whole-earth, plate-boundary-resolving mantle convection; global seismic wave propagation;

dynamics of polar ice sheets and their land, atmosphere, and ocean interactions; and subsurface flows, as well as the underlying computational, mathematical, and statistical techniques for making tractable the solution and uncertainty quantification of such complex forward and inverse problems on parallel supercomputers.

He received the 2003 IEEE/ACM Gordon Bell Prize for Special Accomplishment in Supercomputing, was a finalist for the 2008 and 2010 Bell Prizes, and received the 2008 TeraGrid Capability Computing Challenge award.

Learning From Aggregated Data

Joydeep Ghosh
Schlumberger Centennial Chair Professor
Director, IDEAL (Intelligent Data Exploration and Analysis Lab)
Professor of Electrical & Computer Engineering
The University of Texas at Austin

Friday, Sept. 22 @ 11:20am, Room 2.302

Due to a variety of reasons including privacy, scalability, bandwidth restrictions and robustness, data is often aggregated or obfuscated in various ways before being released to the public. Is it possible to learn predictive models on aggregated data that can even come close in the predictive performance or parameter recovery possible if the full-resolution (non-aggregated) data were available? This is a challenging problem that requires significant algorithmic innovation since simple ways of imputing the missing data and then learning a model can fail dramatically. In this talk we present new approaches that are able to obtain reasonable results from aggregated data in four different scenarios: i) Certain sensitive features are reported only in terms of groupwise averages, while non-sensitive values are available at the individual level ii) When the dependent variable values are only available as histograms or order statistics iii) When both features and targets are in aggregated form as groupwise averages, and iv) When variables go through different types of spatio-temporal averaging.

For each setting we show that reasonable results are indeed possible, at least for specific model classes, using ideas from latent space representation, compressed sensing, monotonic retargeting and Fourier analysis.

Bio:

Joydeep Ghosh is currently the Schlumberger Centennial Chair Professor of Electrical and Computer Engineering at the University of Texas, Austin. He joined the UT-Austin faculty in 1988 after being educated at IIT Kanpur (B. Tech '83) and The University of Southern California (Ph.D '88). He is the founder-director of IDEAL (Intelligent Data Exploration and Analysis Lab), an IEEE Fellow (2004), and the 2015 recipient of IEEE CS Technical Achievement Award. Dr. Ghosh has taught graduate courses on data mining and web analytics to both UT students and to industry, for over two decades. He was voted as "Best Professor" in the Software Engineering Executive Education Program at UT. Dr. Ghosh's research interests lie primarily in data mining and web mining, predictive modeling / predictive analytics, machine learning approaches such as adaptive multi-learner systems, and their applications to a wide variety of complex real-world problems, including health informatics. He has published more than 400 refereed papers and 50 book chapters, and co-edited over 20 books. His research has been supported by the NSF, Yahoo!, Google, Paypal, ONR, ARO, AFOSR, Intel, IBM, etc. He has received 14 Best Paper Awards over the years, including the 2005 Best Research Paper Award across UT and the 1992 Darlington Award given by the IEEE Circuits and Systems Society for the

overall Best Paper in the areas of CAS/CAD. Dr. Ghosh has been a plenary/keynote speaker on several occasions such as ICHI'15, ICDM'13 and (Health Informatics workshops at) KDD'15, KDD14, ICML13 and ICHI13, and has widely lectured on intelligent analysis of large-scale data. Dr. Ghosh served as the Conference Co-Chair or Program Co-Chair for several top data mining oriented conferences, including SDM'13, SDM'12, KDD 2011, CIDM07, ICPR'08 (Pattern Recognition Track) and SDM'06. He was the Conf. Co-Chair for Artificial Neural Networks in Engineering (ANNIE)'93 to '96 and '99 to '03 and the founding chair of the Data Mining Tech. Committee of the IEEE Computational Intelligence Society. He has also co-organized workshops on health informatics, high dimensional clustering, Web Analytics, Web Mining and Parallel/ Distributed Knowledge Discovery. Dr. Ghosh has served as a co-founder, consultant or advisor to successful startups (including Accordion Health, CognitiveScale and Neonyoyo) and as a consultant to large corporations such as IBM, Motorola and Vinson & Elkins.

Personalized Blood Flow Simulation from an Image-Derived Model: Changing the Paradigm for Cardiovascular Diagnostics

Leo Grady
Senior Vice President of Engineering
HeartFlow

Saturday, Sept. 23 @ 9:00am, Room 2.302

Coronary heart disease is the leading cause of mortality worldwide, accounting for 1/3 of all global deaths. Treatment of stable coronary heart disease is typically performed by medication/lifestyle for a lower disease burden or PCI (stenting) for a greater disease burden. The choice between these treatments is best determined by an invasive diagnostic test that measures blood flow through a diseased area. Unfortunately, this invasive diagnostic test is expensive, dangerous and usually finds a lower disease burden. We are working to change the diagnostics paradigm with blood flow simulation in a personalized 3D heart model that is derived from cardiac CT angiography images. This simulation-based diagnostic is the first clinically available diagnostic that utilizes personalized blood flow simulation and is much safer and more comfortable for the patient as well as less expensive. Our diagnostic depends on a hyperaccurate image segmentation of the coronary arteries, physiological modeling and accurate computational fluid dynamics. In this talk I will discuss the algorithms that drive this technology, the machine learning that were doing with our database of segmented images and personalized hemodynamics, and the successful clinical trials that have proven the diagnostic accuracy and benefit to patients.

Bio:

Leo Grady is the Senior Vice President of Engineering at HeartFlow since 2012. Prior to joining HeartFlow, he worked at Siemens Corporate Research for nine years as a Principal Research Scientist following his PhD at Boston University. His work has focused on a range of computer vision and medical imaging applications in image segmentation and machine learning. He has written two books on computer vision and data analysis using graph theory, is an editor of several journals in computer vision and was recently inducted as a Fellow of the American Institute of Medical and Biomedical Engineers.

Multi-Resolution Geometric Modeling of the Mitral Heart Valve Leaflets

Michael Sacks
W. A. Moncrief, Jr. Simulation-Based Engineering Science Chair I
Institute for Computational Engineering Sciences
Professor of Biomedical Engineering
Director, Center for Cardiovascular Simulation
The University of Texas at Austin

Friday, Sept. 22 @ 8:30am, Room 2.302

An essential element of the heart function, the mitral valve (MV) ensures proper directional blood flow between the left heart chambers. Over the past two decades, computational simulations have made marked advancements towards providing powerful predictive tools to better understand valvular function and improve treatments for MV disease. However, challenges remain in the development of robust means for the quantification and representation of MV leaflet geometry. In this study, we present a novel modeling pipeline to quantitatively characterize and represent MV leaflet surface geometry. Our methodology utilized a two-part additive decomposition of the MV geometric features to decouple the macro-level general leaflet shape descriptors from the leaflet fine-scale features. First, the general shapes of five ovine MV leaflets were modeled using superquadric surfaces. Second, the finer-scale geometric details were captured, quantified, and reconstructed via a 2D Fourier analysis with an additional sparsity constraint. This spectral approach allowed us to easily control the level of geometric details in the reconstructed geometry. The results revealed that our methodology provided a robust and accurate approach to develop MV-specific models with an adjustable level of spatial resolution and geometric detail. Such fully customizable models provide the necessary means to perform computational simulations of the MV in a range of geometric detail, allowing identification of the complexity required to achieve predictive MV simulations to a desired accuracy level. This work is joint with Amir H. Khalighi and Andrew Drach.

Bio:

Michael Sacks is professor of biomedical engineering and holder of the W. A. "Tex" Moncrief, Jr. Endowment in Simulation-Based Engineering and Sciences Chair No. 1. He is also director of the ICES Center for Cardiovascular Simulation-based Engineering. Sacks formerly held the John A. Swanson Chair in the Department of Bioengineering at the University of Pittsburgh. He earned his B.S. and M.S. in engineering mechanics from Michigan State University, and his Ph.D. in biomedical engineering (biomechanics) from The University of Texas Southwestern Medical Center at Dallas.

In 2006, he was selected as one of the Scientific American top 50 scientists. In 2009, he won the Van C. Mow Medal from the American Society of Mechanical Engineers (ASME) Bioengineering Division and the Chancellors Distinguished Research Award at the University of Pittsburgh. He is a fellow of ASME and the

American Institute for Medical & Biological Engineering, and an inaugural fellow of the Biomedical Engineering Society. He is currently editor of the Journal of Biomechanical Engineering, and serves on the editorial board for 27 other journals.

He is a world authority on cardiovascular biomechanics, with a focus on the quantification and simulation of the structure-mechanical properties of native and engineered cardiovascular soft tissues. He is a leading authority on the mechanical behavior and function of heart valves, including the development of the first constitutive models for these tissues using a structural approach. He is also active in the biomechanics of engineered tissues, and in understanding the in-vitro and in-vivo remodeling processes from a functional biomechanical perspective. His research includes multiscale studies of cell/tissue/organ mechanical interactions in heart valves and he is particularly interested in determining the local stress environment for heart valve interstitial cells. His recent research has included developing novel constitutive models of right ventricular myocardium that allow for the individual contributions of the myocyte and connective tissue networks.

Volumetric Spline Parameterization for Isogeometric Analysis with Engineering Applications

Yongjie Jessica Zhang

Professor of Mechanical Engineering
Courtesy Appointment in Biomedical Engineering
Carnegie Mellon University

Thursday, Sept. 21 @ 12:10pm, Room 2.302

As a new advancement of traditional finite element method, isogeometric analysis (IGA) adopts the same set of basis functions to represent both the geometry and the solution space, integrating design with analysis seamlessly. In this talk, I will present our latest research on volumetric spline parameterization for IGA applications. For arbitrary objects, a new centroidal Voronoi tessellation (CVT) based surface segmentation method is developed to build polycubes whose topology is equivalent to the input geometry. First, eigenfunctions of the secondary Laplace operator (SLO) are coupled with the harmonic boundary- enhanced CVT (HBECVT) model to classify vertices of the surface into several components based on concave creases and convex ridges of an object. For each segmented component, we then apply the skeleton information to define local coordinates and include them into the HBECVT model to further segment it into several patches, with predefined geometric constraints applied for valid polycube construction. Based on the constructed polycube, we obtain volumetric control meshes via parametric mapping. After that, truncated hierarchical spline basis functions are derived to enable analysis- suitability, including partition of unity and linear independence. Furthermore, a blended B-spline- Bézier approach is recently developed to construct basis functions around extraordinary nodes, achieving an optimal convergence rate of IGA. The developed pipelines have been incorporated into commercial software such as Rhino, Abaqus and LS-DYNA for engineering applications.

Bio:

Yongjie Jessica Zhang is a Professor of Mechanical Engineering at Carnegie Mellon University with a courtesy appointment in Biomedical Engineering. She received her B.Eng. in Automotive Engineering, and M.Eng. in Engineering Mechanics from Tsinghua University, China; and M.Eng. in Aerospace Engineering and Engineering Mechanics and Ph.D. in Computational Engineering and Sciences from Institute for Computational Engineering and Sciences (ICES), The University of Texas at Austin. After staying two years at ICES as a postdoctoral fellow, she joined CMU in 2007 as an assistant professor, and then was promoted to an associate professor in 2012 and a full professor in 2016. Her research interests include computational geometry, mesh generation, computer graphics, visualization, finite element method, isogeometric analysis and their application in computational biomedicine, material sciences and engineering. She has co-authored over 150 publications in peer-reviewed journals and conference proceedings, and received the Autodesk Best Paper Award 1st Place

in SIAM Conference on Solid and Physical Modeling 2015, the Best Paper Award in CompIMAGE16 conference and one of the 5 Most Highly Cited Papers Published in Computer-Aided Design during 2014-2016. She recently published a book entitled "Geometric Modeling and Mesh Generation from Scanned Images" with CRC Press, Taylor & Francis Group. She is the recipient of ELATE Fellow at Drexel, Presidential Early Career Award for Scientists and Engineers, NSF CAREER Award, Office of Naval Research Young Investigator Award, USACM Gallagher Young Investigator Award, Clarence H. Adamson Career Faculty Fellow in Mechanical Engineering, George Tallman Ladd Research Award, and Donald L. & Rhonda Struminger Faculty Fellow.

Abstracts

Adaptive multiscale modeling of the flow and reactive transport using Numerical Homogenization and Enhanced Velocity Mixed FEM in porous media

Yerlan Amanbek, Gurpreet Singh, & Mary F. Wheeler
The University of Texas at Austin

Reservoir scale flow and reactive transport modeling is important in many subsurface applications such as enhanced oil recovery, CO2 sequestration, groundwater remediation as well as contaminant plume migration in heterogeneous porous media. Due to detailed characterization of the reservoir, the direct numerical simulation is computationally intensive. The main objective is to develop the multiscale approach to mitigate the usage of fine scale parameters as well as to achieve numerical solution within the accepted range of accuracy. We propose the adaptive numerical simulation using numerical homogenization and Enhanced Velocity Mixed Finite Element Method (EVMFEM). We focus on the permeability fields for upscaling in single phase, slightly compressible, flow and reactive transport model in heterogenous porous media. A lowest-order mixed finite element scheme is used for spatial discretization with rectangular parallelepiped, RT0 elements. Several criteria for refinement are discussed to capture the front of transport equation or the transient regions that benefits for sensitive concentration accuracy in upscaling. So the fine grids are used in the transient regions in detecting concentration values including in the high permeable regions in heterogenous porous media. Away from transient regions we employ the numerical homogenization locally to compute effective equations at coarse scale, so then we face nonmatching grids. We use the EVMFEM as a domain decomposition approach to couple the coarse and fine subdomains. We have a great agreement with the fine scale and the adaptive numerical homogenization solutions. Numerical experiments are also presented for extension to realistic SPE 10 data for evaluating scenarios of practical interest.

Adaptive Numerical Homogenization for Upscaling Single Phase Flow and Transport

Yerlan Amanbek, Gurpreet Singh, Mary F. Wheeler, & Hans van Duijn
The University of Texas at Austin

This poster presents an adaptive multiscale approach to improve the efficiency and the accuracy of numerical computations by combining upscaling and domain decomposition methods. The key objective of this research work is to develop upscaling approaches to minimize the use of fine scale information for time varying initial and boundary conditions. This includes changes in well parameter such as injection composition and specifications as well as in situ or initial conditions. A fine scale Darcys flow and transport problem is solved only in specific subdomains while solving a coarse scale problem in the rest of the domain. This involves special treatment of sharp interfaces associated with the transport equations. We define transient regions as subdomains where spatial changes in concentration are significant.

Away from the transient regions, upscaling is performed locally by using a numerical homogenization to obtain effective equations at the macroscopic scale. A fine grid is then used in the transient regions and a coarse grid everywhere else resulting in a non-matching multi-block problem. We use the Enhanced Velocity Mixed Finite Element Method (EVMFEM) as a domain decomposition approach to couple the coarse and fine subdomains. A number of numerical tests are also presented for verifying and demonstrating the capability of the adaptive numerical homogenization approach in upscaling flow and transport in porous medium. The numerical results on different layers of SPE10 also indicate that an upscaling based solely upon numerical homogenization is in good agreement with the fine scale solution for a Gaussian or periodic permeability distribution. An optimal tolerance for the adaptivity criteria is chosen to reduce computational cost without substantial loss in solution accuracy.

An in Silico Heart Model of Pulmonary Arterial Hypertension

Reza Avaz[1], Emilio Mendiola[1], Joao Soares[1], David Li[1], Richard Dixon[2], & Michael Sacks[1]

[1]University of Texas at Austin, Austin, TX
[2]Texas Heart Institute, Houston, TX

Pulmonary arterial hypertension (PAH) imposes a pressure overload on the right ventricular free wall (RVFW), leading to substantial growth of muscle cells and remodeling in fiber architecture. The effects of these alterations on the biomechanical behavior of the RVFW and the organ-level cardiac function remain largely unexplored. Recent experimental studies on the mechanical and morphological properties of normal and hypertensive RVFW myocardium suggest that myocardial wall stress is the primary mediator of RVFW growth and remodeling (G&R) responses. An accurate quantification of the wall stress evolution during the development of PAH is needed to determine the correlation between the wall stress and G&R mechanisms. To this end, there is a need to develop a detailed computational heart model that can accurately simulate the effect of PAH in the heart, and thus can be used to understand pathophysiology of RVFW remodeling, its connection to wall stress alterations, and its impact on organ-level cardiac function.

We have developed a high-fidelity finite-element (FE) heart model of PAH using extensive time-course datasets from a normal rat heart and from a hypertensive rat heart simulating the pressure overload in the right ventricle (RV). We have implemented a pipeline that integrates a meshed geometry from a high-resolution image of the rat heart, detailed imaging data on the fiber structure of the same heart, and a novel compressible hyperelastic material model accounting for both passive and active behaviors of myocardium. The developed heart model offers a high performance capability for inverse problems such as fine-tuning the active properties of myocardium or characterizing shape change patterns of the RV.

We used our model to investigate the correlations between the alterations in the wall stress, the remodeling of the RVFW microstructure, and the shape changes in the RV during the development of PAH. The detailed description of organ-level

remodeling patterns can replace the traditional measures of RV dimensions and volume that often lead to gross and limited information on cardiac performance. Ultimately, development and implementation of our model in patient-specific organ-level simulations will allow investigation of optimal diagnosis and new individualized stem-cell interventions for PAH.

Dynamic Fourier process applied to the study of geophysical time series

Md Al Masum Bhuiyan
The University of Texas at El Paso

This work is devoted to the study of modeling geophysical time series arising in earthquakes and mining explosions. We observe that the measurements of a sequence of geophysics are stochastically dependent on the time needed. In other words, there is a correlation among the numbers of data points at successive time intervals. Using the Fourier Transform, the time domain signal is transformed to the frequency domain where it is equivalent to an Amplitude Spectrum and a Phase. Fourier's theory states that a given signal can be synthesized as a summation of sinusoidal waves of various amplitudes, frequencies and phases. We therefore applied dynamic Fourier techniques to analyze the seismograms of a set of mining explosions, reported in catalogs as earthquakes, and compared them with natural earthquakes that occurred in the same region (within a radius of 10 km). The objective of the analysis is to summarize the spectral behavior of the signal as it evolves over time. We collect these continuous-time stationary sequences of mining explosions and earthquakes from three nearby seismic stations (IU.TUC, US.ANMO, IU.WUAZ) and observe that the seismograms generate different frequency spectra. The stationarity of the data is determined by testing some powerful tests in our study. Our results suggest that the Fourier representation of seismograms in the frequencytime domain is efficient in enforcing the characteristic parameters as a way to discriminate the signals of earthquake and explosions time series.

Higgs Boson Equation in the de Sitter Spacetime: Computational Results

Andras Balogh
The University of Texas Rio Grande Valley

We present the results of high performance computations about the Higgs Boson Equation in the de Sitter Spacetime. An explicit fourth order Runge-Kutta scheme is used on the temporal discretization along with fourth order finite difference discretization in space. We examine both the fully three space dimensional equation as well as its one space dimensional radial solutions. The numerical code for the three space dimensional equation was programmed in CUDA Fortran while the radial solution was programmed in MATLAB. Our numerical results demonstrate

the existing theoretical result that under certain conditions bubbles (isosurfaces of value zero inside the domain of support) form in the scalar field. Our numerical studies also suggest the previously unknown property that under some conditions no bubbles form. In addition to the numerical results some formal arguments are also presented about the long time behavior of the solutions, and their relation to the unforced, damped Duffing equations.

Reconstruction of a Compactly Supported Contrast function In The Presence of a Background Random Medium

Carlos Borges
The University of Texas at Austin

We address the problem of reconstructing an unknown compact contrast function embedded in a random noisy background medium given the scattered field and information regarding the background medium and the sound profile. We present different methods for the solution of this inverse problem using different amounts of scattered data, and information about the background medium and the sound profile, such as their probability distributions or the expected value of the background medium. We compare the accuracy and complexity of these methods. The fast Hierarcuical Poincaré-Steklov (HPS) solver is used to simulate the forward scattering operator and its Frechét derivative, while we use the recursive linearization algorithm (RLA) to recover a band-limited approximation of the sound-profile for the inverse problem. Numerical results are provided for the solution of diverse problems using the different methods presented.

Performance Comparison of HPX vs. MPI+X Threading Models for Discontinuous Galerkin Finite Element Methods

Max Bremer, Craig Michoski, Zach Byerly, Hartmut Kaiser, Clint Dawson
The University of Texas at Austin

Increasing vector widths and many-core architectures introduce significant challenges to achieving efficient compute resource utilization. High performance parallelX (HPX) is an asynchronous run-time specifically designed to address the bottlenecks associated with the massive concurrency on next generation supercomputers. We present a comparison of a traditional MPI+X threading model vs. an HPX implementation of standard and blended isogeometric discontinuous Galerkin wave kernels. We will present detailed performance profiling and discuss code optimization strategies for each parallelization paradigm. Scaling results will be presented on the Intel Knights Landing chips.

Magnetic drug targeting: a comparison between CFD and FSI simulations

Sara Calandrini, Eugenio Aulisa, & Giacomo Capodaglio
Texas Tech University

In magnetic drug targeting (MDT), magnetic particles are attached to a drug injected in blood vessels. By the use of an external magnet, the particles are directed to a specific target, like a tumor surrounding an artery or a thrombus that could be occluding an artery lumen. One of the goals of this procedure is to maximize the number of particles that reach the target. This is quantified by the capture efficiency, the ratio between the number of particles that dont leave the domain and the number of particles injected. In recent years, computational fluid dynamics (CFD) simulations of MDT in blood flows have been carried out to obtain further insight on the combination of param- eters that may provide the best capture efficiency. We want to further contribute to the research of MDT by considering a computational study that takes into account the mutual interaction between the blood flow and the vessel that contains it, framework known as fluid-structure interaction (FSI). I will present both CFD and FSI simulations and analyze how the capture efficiency predictions change from a CFD to an FSI framework. For the numerical simulations, we used the in-house finite element library FEMuS (`https://github.com/FeMTTU/femus`) where the FSI solver and the particle tracking algorithm are implemented.

Construction of h-refined finite element spaces with applications to multigrid algorithms

Giacomo Capodaglio, Eugenio Aulisa, & Guoyi Ke
Department of Mathematics and Statistics
Texas Tech University

I will present an algorithm for the construction of basis functions to be employed in h-refined finite element applications with local refinement and arbitrary hanging nodes configurations. This means that we do not impose the 1-irregularity condition on the mesh. Moreover, the algorithm is simple to implement and does not require the solution of a linear system to obtain the constraint coefficients necessary to enforce continuity of the basis functions. I will illustrate analytic results to prove that such functions are actually linearly independent and continuous. Finite element spaces are then defined as the spanning sets of these basis functions. These spaces are suitable for multigrid applications and convenient to use from an implementational point of view. Numerical results will be presented to study the convergence properties of a multigrid algorithm built on the finite element spaces here defined.

Effective Boundary Conditions for Viscous Incompressible Flow Over Rough Boundaries

Sean Carney & Björn Engquist
The University of Texas at Austin

The direct numerical simulation of viscous flow over a rough boundary is challenging due to the large number of degrees of freedom required to adequately resolve the flow struc- tures near the boundary. Previous mathematical analysis of the problem in the laminar regime has shown that replacing the no-slip condition on the rough boundary with a Navier-slip condition on a smooth boundary captures the average effect of roughness on the flow near the boundary, where the slip length is given by the average to a solution of an auxiliary cell problem. We describe a numerical multiscale method designed to estimate the slip length by coupling a coarse scale computation in the full domain with a high resolution computation localized to patches along the rough boundary. The method reproduces the proper slip length from the mathematical theory where it is applicable, and numerical results demonstrate the utility of the method even where the theory is no longer valid. We will briefly comment on the application of this coupling strategy as a wall model in a high Re Large Eddy Simulation. The physics is of course very different than the laminar regime considered here, but there are preliminary indications (Sandham et al, 2017) that this approach can successfully produce accurate turbulent flow statistics.

Discretely entropy stable discontinuous Galerkin methods

Jesse Chan
Rice University

High order methods offer several advantages in the approximation of solutions to hyperbolic equations, such as improved accuracy and low numerical dispersion and dissipation. However, high order methods also tend to suffer instabilities when applied to nonlinear hyperbolic equations, requiring filtering, limiting, or artificial dissipation to ensure that the solution does not grow unboundedly. At the root of these problems is the fact that the stability of the continuous problem does not imply stability at the discrete level. This talk will review the development of high order collocation schemes based on summation-by-parts operators which recover a discrete statement of entropy stability, and will discuss the extension of such methods to a more general class of discontinuous Galerkin methods. Numerical results for the one-dimensional shallow water and Euler's equations support the presented theoretical results.

Hessian-based sampling for goal-oriented model reduction with high-dimensional parameters

Peng Chen & Omar Ghattas
Institute for Computational Engineering & Sciences
The University of Texas at Austin

Model reduction techniques for parametric partial differential equations have been well developed to reduce the computational cost in many-query or real- time applications, such as optimal design/control, parameter calibration, and uncertainty quantification. However, it remains a great challenge to construct an efficient and accurate reduced order model (ROM) for high-dimensional para- metric problems. One reason is that sampling in the high-dimensional parameter space for the construction of the ROM often faces curse of dimensionality, i.e., the computational complexity grows exponentially with respect to the number of parameter dimensions. The other is that the parametric solution manifold may be essentially high-dimensional such that a very large number of reduced basis functions have to be used in order to achieve certain required accuracy, which limits the efficacy of the computational reduction. In this talk, we present a Hessian-based sampling method for goal-oriented model reduction to effectively construct a ROM that has good approximation property for some given quan- tity of interest (QoI) as a function of the parametric solution [1]. The rationale is that even the dimension of the solution manifold is high, the dimension of the quantity of interest, such as an average of the solution in a particular physical domain, is relatively low. To capture this low-dimensionality, we explore the curvature of the QoI in the parameter space informed by its Hessian [2, 3] as exploited for sparse quadrature and optimal control problems.

[1] P. Chen and O. Ghattas. Hessian-based sampling for goal-oriented model reduction with high-dimensional parameters. preprint, 2017.

[2] P. Chen, U. Villa, and O. Ghattas. Hessian-based adaptive sparse quadrature for infinite-dimensional Bayesian inverse problems. preprint, 2017.

[3] P. Chen, U. Villa, and O. Ghattas. Taylor approximation and variance reduction for PDE-constrained optimal control under uncertainty. preprint, 2017.

Uncertain Estimation of Mechanical Properties of Myocardium Tissue: A Variational Inverse Problem with Uncertainty Quantification

Joshua W. Chen[1], Umberto Villa[1], David Li[2], Omar Ghattas[1], & Michael Sacks[1]
[1]Institute for Computational Engineering & Sciences, The University of Texas at Austin
[2]Department of Biomedical Engineering, The University of Texas at Austin

In this work, we present novel computational tools for bayesian parameter inversion and optimal experimental design for determining the 3D strain energy function parameters for myocardial tissue. In previous work[1], we presented a framework for parameter inversion and optimal design based on an experimental setup for 1 cm^3 myocardial tissue samples that applies tri-axial Dirichlet boundary conditions incrementally in quasi-static equilibrium and measures resultant surface traction

forces (Figure 1 a). In the current work, we extend the framework to a Bayesian inversion context for parameter estimation and we consider more advanced techniques for optimal experimental design. We use the inverse problems Python library hIPPYlib[2] a toolbox for FEniCS that enables easy development of scalable algorithms for PDE-based deterministic and Bayesian inverse problems. In what follows, we introduce further the functionality of hIPPYlib, we then present the forward problem, the Bayesian inverse problem, and some thoughts on the optimal design of experiments.

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Using mathematical models to estimate the ratio of infectious to non-infectious viral production of RSV

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Respiratory syncytial virus (RSV) can cause severe, even fatal respiratory infections in infants and the elderly. There are currently no approved antivirals or vaccines for the disease and our understanding of some of the biological processes underlying the infection is limited. We use a mathematical model of within host viral infection to help improve our understanding of the infection. Through fitting of the mathematical model to patient data, we estimate several infection parameters including the ratio of production of infectious to non-infectious virions. We find that non-infectious virions are produced at a higher rate than infectious virions suggesting that RSV has a high mutation rate.

Numerical Simulation of Carbonate Matrix Acidization Using Adaptive Enriched Galerkin Method with Entropy Residual Stabilization

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[2] Florida State University

Carbonate matrix acidization is a reservoir stimulation technique to remove formation damage. Acid is injected into reservoir to dissolve mineral and create long highly conductive channels known as wormholes. Accurate modeling of wormhole requires very fine mesh to capture the physics at the vicinity of wormhole interface. However high resolution grids result in longer simulation runtime. We present an enriched Galerkin finite element method (EG) coupled with entropy residual stabilization to simulate matrix acidization. This method provides efficient solver, less grid dependency and sharp front for transport. The simulator can track the location of wormhole interface, refine mesh dynamically and coarsen mesh after displacement front passes. The EG is formulated by enriching the conforming continuous Galerkin finite element method (CG) with piecewise constant functions. EG is a higher-order method which has less numerical dispersion than standard finite difference or finite volume method. We use a two-continuum model proposed by (Panga et al. 2005) for matrix acidization problem. The flow and transport equations are solved sequentially and implicitly using EG. Entropy viscosity stabilization method is used to prevent any spurious oscillation of transport. Entropy residual can be also used as a posteriori error indicator to dynamically refine the mesh near moving wormhole interface. Our simulation results can reproduce different dissolution patterns under different injection rates from previous experiments. Entropy residual stabilization is very efficient to avoid spurious oscillation of higher-order EG method and capture sharp displacement fronts for reactive transport problem. The advantage of our simulator is to reduce gridblocks in non-computationally-intensive area, and therefore reduce simulation runtime, while capturing wormhole formation when compared with globally refined mesh on the whole domain. Practical matrix acidization design requires many runs of numerical simulator to optimize the design parameters. Our proposed method can shorten the optimization process and save design time.

The Double Membrane Problem

Luis Duque
The University of Texas at Austin

This double membrane problem consists on studying the position of equilibrium of two elastic membranes in contact to each other and was initially explored by Vergara-Caffarelli in 1971. After this, more general scenarios involving multiple elastic membranes (Chipot, Vergara Caffarelli, 1983) and non linear operators (Silvestre, 2005) have been considered. In this talk we will explain a probabilistic version of this problem and sketch the existence and optimal regularity of solutions in this new scenario. Joint work with Luis Caffarelli and Hernan Vivas.

Measuring the mechanical forces during cancer cell invasion using inverse-method traction microscopy

Xinzeng Feng[1], Manasa Gadde[2], Jongwan Park[2], M. Nichole Rylander[2,4], & Thomas E. Yankeelov[1,2,3,5]

[1] Institute for Computational Engineering and Sciences Department of [2] Biomedical Engineering, [3] Diagnostic Medicine, [4] Mechanical Engineering, & [5] Livestrong Cancer Institutes, The University of Texas at Austin

Introduction. Rapid volumetric growth and extensive invasion into normal tissues are hallmarks of many types of cancer. It is widely accepted that these processes involve mechanical forces that can lead to large deformation of the tissue (the so-called mass effect). However, it is less understood how to model the mechanical forces with respect to other measureable quantities, such as cell density, tissue stiffness, etc. This is especially critical in developing predictive biophysical models with mass effect. In the literature, one often assumes a linear relation between the cellular force and the gradient of cell density. This relation is yet not supported quantitatively by experiments. We are developing a combined experimental-computational approach to measure the forces exerted by a cell population on the surrounding tissue during invasion, and to study the relation between the force field and cell density.

Methods. We culture MDA-MB-231 breast cancer cells in a two-layer collagen gel. Initially, cells are seeded in the bottom layer of the gel. By introducing a nutrient gradient, we motivate the cells to invade the top layer in which fluorescent micro-beads are embedded. We use confocal microscopy to image the volume of interest. From the confocal images, we locate bead positions before and after cell invasion with image processing techniques and then use the relaxation method to track the displacement for each individual bead. The measured bead displacements are input into an adjoint-based, inverse-method algorithm to compute the cellular force. In particular, we minimize the sum of squared norm difference between the measured bead displacement and the displacement calculated by the forward problem. In the forward problem, we model the forces exerted by the cell population as a distributed body force on the collagen and assume that collagen behaves like a linear elastic material. The inverse problem is solved using the steepest gradient method in which the gradient of the objective function is calculated efficiently via the adjoint method. After solving the inverse problem, we will compare the computed cellular force with the gradient of the cell density using statistical methods to test the assumption of linearity.

Discussion. Our poster will present experimental data and use inverse method traction microscopy to study the relation between cellular forces during cancer cell invasion and cell density. Preliminary calculation on artificial displacement data indicates that our inverse method algorithm is capable of reconstructing the true force field used to generate the measurement.

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Inexact hierarchical scale separation: A two-scale approach for linear systems from discontinuous Galerkin discretizations

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Hierarchical scale separation (HSS) is an iterative two-scale approximation method for large sparse systems of linear equations arising from discontinuous Galerkin (DG) discretizations. HSS splits the linear system into a coarse-scale system of reduced size corresponding to the local mean values of the solution and a set of decoupled local fine-scale systems corresponding to the higher or- der solution components. This scheme then alternates between coarse-scale and fine-scale system solves until both components converge. The motivation of HSS is to promote parallelism by decoupling the fine-scale systems, and to reduce the communication overhead from classical linear solvers by only applying them to the coarse-scale system.

We propose a modified HSS scheme (inexact HSS, IHSS) that exploits the highly parallel fine-scale solver more extensively and only approximates the coarse-scale solution in every iteration thus resulting in a significant speedup. The tolerance of the coarse-scale solver is adapted in every IHSS cycle, con- trolled by the residual norm of the fine-scale system. Anderson acceleration is employed in the repeated solving of the fine-scale system to stabilize the scheme. We investigate the applicability of IHSS to systems stemming from the nonsymmetric interior penalty DG discretization of the CahnHilliard equa- tion, discuss its hybrid parallel implementation for large-scale simulations, and compare the performance of a widely used iterative solver with and without IHSS.

FESTUNG: Finite Element Simulation Toolbox for UNstructured Grids

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[3]Alfred Wegener Institut

FESTUNG (Finite Element Simulation Toolbox for Unstructured Grids) is a Matlab / GNU Octave toolbox for the discontinuous Galerkin method on un- structured grids. It is primarily intended as a fast and flexible prototyping platform and testbed for students and developers. FESTUNG relies on fully vectorized matrix/vector operations to deliver optimized computational perfor- mance combined with a compact, user-friendly interface and a comprehensive documentation.

Global stability of 2D plane Couette flow beyond the energy stability limit

Federico Fuentes

The University of Texas at Austin

A basic question in fluid stability is whether a laminar flow is nonlinearly stable to all perturbations. The typical way to verify stability, called the energy method, is to show that the energy of a perturbation must decay monotonically under a certain Reynolds number called the energy stability limit. The energy method is known to be overly conservative in many systems, such as in plane Couette flow. Here, we present a methodology to computationally construct Lyapunov functions more general than the energy through the use of sums-of-squares polynomials and semidefinite programming. We then apply this methodology to 2D plane Couette flow and under certain conditions we find a global stability limit higher than the energy stability limit. For this specific flow, this is the first improvement in over 110 years.

Impact of model-form-uncertainty of the simple susceptible-infectious-recovery epidemic models

Li Guan

Tulane University

This project explores the qualitative and quantitative impact on susceptible-infectious-recovery (SIR) epidemic models when the recovery time from infection is not exponentially distributed. It is motivated by the fact that in realistic situations, the recovery rate of an infectious population varies over time instead of being constant. Numerical experimentation reveals a wide range of behavior, suggesting that model misspecification can introduce biases into estimates of important epidemiological parameters, such as the force of infection and the basic reproductive number. We explore the magnitude of these biases in both simulated and real epidemic datasets.

Modelling and stabilization of quasistatic evolution of elastoplastic systems subject to periodic loading

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We develop an analytic framework to design both stress and stretching/compressing T-periodic loadings which make stresses in a one-dimensional arrangement of elastoplastic springs converging to a unique periodic regime. The solution of such an evolution problem is a function $t \mapsto (e(t), p(t))$, where $e_i(t)$ and $p_i(t)$ are the elastic and plastic deformations of spring i, defined on $[t_0, \infty)$ and corresponding to an initial condition $(e(t_0), p(t_0))$. We rigorously convert the problem into a Moreau sweeping process with a moving polyhedron using the general method for elastoplastic systems, proposed by Moreau[2]. Therefore it is natural to expect (based on a result by Krejci[3]) that the solution $t \mapsto (e(t), p(t))$ always converges to a T-periodic function. We spot a class of sweeping processes and closed-form estimates on eligible loadings where the Krejci's limit doesn't depend on the initial condition $(e(t_0), p(t_0))$ and so all the trajectories approach the same T-periodic solution. The proposed class of sweeping precesses can be described by a geometric condition. We further link this geometric condition to mechanical properties of the given network of springs. We discover that the geometric condition holds if the number of stretching/compressing constraints is 2 less the number of nodes of the given arrangement of springs and the magnitude of the stress loading is sufficiently large (but admissible). In other words, we offer an analogue of the highgain control method for elastoplastic systems, which can be used e.g. to design the properties of smart materials. We offer specific examples for the presented theoretical results. In particular, we convert elastoplastic systems into sweeping processes which have never been closely looked on so far. From the comptational perspective, numerical modelling of elastoplastic systems under consideration and the corresponding sweeping processes rely on constrained qudratic oprimization methods and is implemented in MATLAB.

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An Extended DEIM Algorithm for Subset Selection

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With large data sets becoming more prevalent, there is an increased demand for dimension reduction techniques. One approach to this problem is to select a subset of original samples using the discrete empirical interpolation method (DEIM), preserving the interpretability of the dimension-reduced data set. However, the number of DEIM-selected samples is limited to be no more than the rank of the original data matrix. While this is not an issue for many data sets, there are a number of settings in which this can limit the algorithms potential for selecting a subset that contains representatives from each class present in the data. In the presented work, we address this issue through an extension of the DEIM algorithm that allows for the selection of a subset with size greater than the matrix rank.

Uncertainty Quantification for a Predictive Model of Chemotherapy Efficacy

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In this work we consider the problem of predicting patient-specific treatment efficacy in cancer therapy using a PDE model for chemotherapy drug uptake and response. The model is calibrated to an individual patient using emission imaging data and statistical inversion methods for the radiative transport equation. The quantity of interest is the spatially averaged patient-specific *log cell kill* K_j, from which we can compute the clinically relevant probability of tumor control, as defined by $P_c = \mathbb{P}(K_j < k_0)$. We discuss a model for K_j and Monte Carlo methods for computing P_c.

A biophysical model for tumor induced angiogenesis calibrated and validated with a murine model of glioma

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Introduction: Angiogenesis is a critical part of early tumor growth that enables tumors to grow past the diffusion limit of nutrients. As the tumor continues to grow, more vasculature is recruited at the periphery while older vasculature is occluded or collapsed in the interior resulting in cell death. Accurate characterization of both tumor cellularity and vascularity would assist in the optimization of chemo- and radiotherapies for an individual patient. To this end, we have developed a predictive biophysical model of tumor growth and angiogenesis that is calibrated on an individual basis using diffusion-weighted MRI (DW-MRI) and dynamic contrast enhanced MRI (DCE-MRI).

Methods: The spatial-temporal evolution of tumor cells and blood volume were described using two coupled, partial differential equations consisting of proliferation, diffusion, and death terms. The model was implemented using a fully explicit 3D finite difference approach in MATLAB. To evaluate this model, rats (n = 4) with C6 gliomas were imaged seven times over 10 days with DW-MRI and DCE-MRI. DCE-MRI was used to identify tumor boundaries and quantify blood volume, while DW-MRI was used to estimate cellularity within the tumor. Model parameters were calibrated from the first three imaging time points. The calibrated parameters were then used in a forward evaluation of the model system to predict tumor growth and blood volume at the remaining four imaging time points. Prediction error was assessed by calculating the percent error in tumor volume, the concordance correlation coefficient (CCC), and the Pearson correlation coefficient (PCC).

Results: The predicted tumor growth had less than 12.1% error in tumor volume at all prediction time points compared to the measured tumor volume. At the voxel-level, a strong level of agreement and correlation was observed for both tumor cell number (CCC = 0.49, PCC = 0.62) and blood volume (CCC = 0.65, PCC = 0.60).

Conclusions: These preliminary results indicate the potential predictive accuracy of calibrating subject-specific biophysical models with clinically relevant imaging measurements.

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Dynamics of the Emerging Fungal Pathogen Batrachochytrium salamandrivorans on the Eastern Newt

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We developed and analyzed a stage-structured Susceptible-Infection (SI) type disease models for emerging fungal pathogen Batrachochytrium salamandrivorans (Bsal). Our models included two routes of pathogen transmission: direct transmission via contact between infected and susceptible individuals and environmental transmission via shed zoospores in the water. Unlike previous models, we categorized individuals into multiple stages of infection (susceptible, latency, and infectious). We found the invasion probability for Bsal (i.e., the basic reproductive number, $\mathcal{R}_0$) into a population of the Eastern Newt. We performed numerical sumulatons and paramerter sensitivity analysis using Latin hypercube sampling and partial rank coefficient correlation.

Improving the predictive ability of a mechanically coupled spatiotemporal model of breast cancer using patient specific MRI data

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Introduction: Clinical methods for assessing tumor response to neoadjuvant therapy are largely rudimentary, monitoring only temporal changes in tumor size. Our goal is to predict tumor response to neoadjuvant chemotherapy in breast cancer using a mathematical model that uses non-invasive imaging data obtained from individual patients. Previously, a reaction-diffusion model was developed that mechanically coupled tumor cell diffusion and surrounding tissues. The model was shown to outperform clinically used measures for predicting tumor response to therapy when initialized with patient specific magnetic resonance imaging (MRI) data. Here we extend the model to include the effects of vascularization on tumor cell proliferation and drug delivery.

Methods: The model is 2D, initialized using patient specific diffusion weighted (DW-) MRI and dynamic contrast-enhanced (DCE-) MRI data–where size, shape, and cellularity were calculated for the entire tumor. The parameters of the model, such as tumor cell diffusion and proliferation values, were calibrated using the first two of four MRI scans (pre-treatment, after first treatment cycle, at midpoint of treatment, and after treatment completion) during the course of neoadjuvant chemotherapy. The DCE-MRI data was used to identify spatiotemporal variations in tumor perfusion with the extended Tofts-Kety model. The derived MRI-based physiologic parameters

were then used to model changes in tumor cell proliferation and delivery of therapy within the tumor. An additional calibration for the tumor cell carrying capacity was also calculated on a patient-specific basis. All model simulations were evaluated using the Crank-Nicolson finite difference scheme.

Results and Discussion: With the above modifications, preliminary results from a cohort of five patients with varying subtypes of breast cancer and associated therapeutic regimens show substantial reductions in the percent error in cellularity and size between the model's prediction and the experimentallymeasured results from the MRI third scan. Next steps will include incorporation of drug-specific mechanisms for inducing cell death, temporally evolving the vasculature, and implementation of a fully three-dimensional model.

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Block-wise Implementation of the Kalman Filter Based Iterative Learning Control for MIMO Systems

Rangana Jayawardhana & Bijoy K. Ghosh
Texas Tech University

Iterative Learning Control (ILC) is based on the notion that a system that executes the same task repeatedly can learn from the previous executions to improve it's performance. ILC algorithm is particularly useful for systems with model uncertainties and repeated disturbances as only a minimal knowledge about the system parameters is necessary for convergence. Here we consider linear, time invariant, MIMO, causal, dynamical systems in discrete time. We propose a learning control scheme, based on the well known Kalman filter, wherein the learning control gain is generated by a Riccati equation. The algorithm only requires the knowledge of the first Markov parameter of the system and is implemented block-wise. Exponential convergence of the algorithm is guaranteed and we provide a design strategy to minimize the transient error growth.

Cooperative Learning with Iterative Learning Control

Rangana Jayawardhana & Bijoy K. Ghosh
Texas Tech University

Iterative Learning Control (ILC) is based on the notion that a system that executes the same task repeatedly can learn from the previous executions to improve it's performance. ILC algorithm is particularly useful for systems with model uncertainties and repeated disturbances as only a minimal knowledge about the system parameters is necessary for convergence. Recently an ILC based controller has been used in the upper limb rehabilitation of stroke patients with successful clinical trials. The goal of rehabilitation is to force the brain to re-learn the lost skill of upper limb control using the assistance given by the ILC device. By taking

insight from this cooperation between the brain and the ILC device, we introduce how multiple iterative learning controllers can be used to learn a desired output using novel algorithms based on the Luenberger Observer and the Kalman Filter.

Numerical simulation of deformability-based red blood cell separation in a microfluidic device

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Microfluidic cell separation techniques are of great interest since they help rapid medical diagnoses and tests. Deterministic lateral displacement (DLD) is one of them. A DLD device consists of arrays of pillars. Main flow and alignment of the pillars define two different directions. Size-based separation of rigid spherical particles is possible as they follow one of these directions depending on their sizes. However, the separation of nonspherical deformable particles such as red blood cells (RBCs) is more complicated than that due to their intricate dynamics. We study the separation of RBCs in DLD using an in-house integral equation solver. We systematically investigate the effects of the interior fluid viscosity and the membrane elasticity of an RBC on its behavior. These mechanical properties of a cell determine its deformability, which can be altered by several diseases. We particularly consider deep devices in which an RBC can show rich dynamics such as tank-treading and tumbling. It turns out that strong hydrodynamic lift force moves the tank-treading cells along the pillars and downward force leads the tumbling ones to move with the flow. Thereby, deformability-based separation of RBCs is possible. We also assess the efficiency of the technique for dense suspensions.

IMEX HDG-DG: A coupled implicit hybridized discontinuous Galerkin and explicit discontinuous Galerkin approach for Euler systems

Shinhoo Kang, Sriramkrishnan Muralikrishnan, & Tan Bui-Thanh
The University of Texas at Austin

We propose IMEX HDG-DG schemes for Euler systems. Of interest is subsonic flow, where the speed of the acoustic wave is faster than that of the nonlinear advection. In order to simulate these flows efficiently, we split the governing system into stiff part describing the fast waves and non-stiff part associated with nonlinear advection. The former is discretized implicitly with HDG method while explicit Runge-Kutta DG discretization is employed for the latter. The proposed IMEX HDG-DG framework: 1) facilitates high-order solution both in time and space; 2) avoids overly small time stepsizes; 3) requires only one linear system solve per time step; and 4) relatively to DG generates smaller and sparser linear system while promoting further parallelism owing to HDG discretization. Numerical results for various test cases demonstrate that our methods are comparable to explicit Runge-Kutta DG schemes in terms of accuracy, while allowing for much larger time stepsizes.

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dgswemv2: a modern c++ discontinuous Galerkin finite element solver

Kazbek Kazhyken, Max Bremer, Clint Dawson
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Due to the lack of theory surrounding hyperbolic systems of conservation laws, algorithm development for these problems typically relies on heuristic approaches. Due to the large effort required in porting new methods to feature-complete code bases, evaluations of these new algorithms are typically centered around simplified test problems. The application to highly non-linear real world problems often remains unexplored leaving the algorithm's viability unanswered. dgswemv2 is a discontinuous Galerkin finite element solver written in c++14 designed to minimize the amount of time to take an algorithm from paper to a massively parallel simulation. Presently, dgswemv2 is designed to solve 2D shallow water equations. However, the code is designed to easily interchange the PDEs being modeled. We will present the basic outline of the data structures, software engineering support set-up around the code base, and preliminary results.

Goal-oriented adaptive mesh refinement with discontinuous Petrov–Galerkin methods

Brendan Keith, Ali Vaziri Astaneh, Leszek Demkowicz
The University of Texas at Austin

In this talk, a new duality theory is used to motivate goal-oriented adaptive mesh refinement algorithms for use with Discontinuous Petrov–Galerkin (DPG) methods. The focus here is mainly on broken ultraweak variational formulations for steady boundary value problems, however, many of the ideas are general enough that they be extended to any corresponding well-posed variational formulation. The proposed goal-oriented adaptive mesh refinement procedures require the construction of refinement indicators for both a primal problem and a dual problem. The primal problem is simply the system of linear equations coming from a standard DPG method. The dual problem is a similar system of equations, coming from a new method which is dual to DPG; having the same coefficients as the DPG method but different constant terms. We refer to this new finite element method as a DPG* method. Results of numerical experiments are provided for Poisson's boundary value problem in a three-dimensional domain. These results clearly demonstrate the utility of goal-oriented adaptive mesh refinement for DPG methods with quantities of interest with either interior or boundary terms.

Stochastic Simulation Method for Reactive Microfluids under Thermal Fluctuations

Changho Kim

Lawrence Berkeley National Laboratory

One of the essential components needed for realistic simulation of microfluids is the inclusion of thermal fluctuations. Our approach, fluctuating hydrodynamics, adds fluctuations by incorporating random fluxes into diffusion processes. While this description dates back to Landau and Lifshitz, developing general formulations and corresponding numerical schemes beyond the linear approximation of weak fluctuations has been attempted only recently. Accurately modeling fluctuations is even more crucial for simulating a reactive microfluid due to the relatively small population of reactant chemical species and the Poisson character of reactions. We present a robust and efficient numerical method, that is constructed systematically by stochastic analysis. We focus on the simulation of aqueous solutions under the Boussinesq approximation. Our method is designed to have good performance in the large Schmidt number regime. To demonstrate capabilities of our method, we present several numerical examples, where fluctuations in chemistry and hydrodynamics play an essential role.

Simulating Bacterial Motility in Confined Environments

John LaGrone, Lisa Fauci, & Ricard Cortez

Department of Mathematics
Tulane University

We are interested in the propulsion dynamics of bacteria in porous materials such as soil, specifically with applications related to environmental remediation. In order to characterize bacterial swimming in confined environments, we present a computational model of flagellar driven bacteria and their hydrodynamic interactions. We construct an elastic body and flagella using networks of springs and drive the motion using a flagellar motor modeled by placing torques and the base of each flagella. The interaction with the surrounding fluid is modeled using the method of regularized Stokeslets. By placing the modeled bacteria in narrow tubes, we investigate how confinement influences the swimming properties. We observe self centering behavior in some cases and a propensity to swim toward and into the wall in other cases. Additionally, we observe increased swimming speed in tubes of smaller radii and are investigating how the confinement influences the tumbling dynamics of the swimming bacteria.

Model Reduction via Domain Decomposition-based Methods for Large-Scale Inverse Problems

Ellen Le, Vishwas Rao, & Tan Bui-Thanh
The University of Texas at Austin

We present three computationally-efficient domain decomposition-based methods for solving inverse problems in high-dimensional parameter spaces. The methods are particularly relevant for problems with spatially concentrated observations and/or dynamics. For a synthetic PDE-constrained inverse problem we show the methods result in 1) an improved reconstruction over the full domain reconstruction and 2) in a reduced number of PDE solves over existing truncated domain methods and the full domain inversion. The key to the most accurate methods is a careful construction of the low-rank basis for the approximated Dirichlet-to-Neumann operator via a goal-oriented, model-constrained approach.

Multiscale methods for filtering turbulent systems

Yoonsang Lee
Lawrence Berkeley National Laboratories

Data assimilation or filtering of nonlinear dynamical systems combines numerical models and observational data to provide the best statistical estimates of the systems. Ensemble-based methods have proved to be indispensable filtering tools in atmosphere and ocean systems that are typically high dimensional turbulent systems. In operational applications, due to the limited computing power in solving the high dimensional systems, it is desirable to use cheap and robust reduced-order forecast models to increase the number of ensemble for accuracy and reliability. This talk describes a multiscale data assimilation framework to incorporate reduced-order multiscale forecast methods for filtering high dimensional complex systems. A reduced-order model for two-layer quasi-geostrophic equations, which uses stochastic modeling for unresolved scales, will be discussed and applied for filtering to capture important features of geophysical flows such as zonal jets. If time permits, a generalization of the ensemble-based methods, multiscale clustered particle filters, will be discussed, which can capture strongly non-Gaussian statistics using relatively few particles.

Fractional-Parabolic Deformations With Sinh-Acceleration

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We develop a general simple methodology for very fast and accurate evaluation of integrals of functions that admit analytic continuation into wide regions of the complex plane or into appropriate Riemann surfaces. We use a family of fractionalparabolic deformations of the contours of integration to appropriate Riemann surfaces, make the corresponding conformal changes of variables and use the simplified trapezoid rule. An additional change variables leads to numerical schemes of complexity of the order of $A\pi^{-2}E^2$, where $E = \ln(1/\epsilon)$, ϵ is the error tolerance, and A is, typically, in the range [0.5, 3], or even $A\pi^{-2}E\ln E$ (the Laplace and Fourier inversion, the Laplace transform and other integrals with exponentially decreasing or oscillating factors). Simple efficient error bounds make adaptive procedures unnecessary. As applications, we consider special functions of several classes, and outline applications to the Wiener-Hopf factorization, calculation of various probability distributions and pricing vanillas and exotics in the Lévy models, Heston model, and more general stochastic volatility models and affine models. The method can be applied to various boundary problems for partial differential and pseudo-differential equations, and in essentially all situations when the saddle point method or reduction to a cut are applied.

Simple approximate recommendations for the choice of parameters of the scheme lead to programs that are accurate and competitive with Mathematica and Python, even without parallelization. In a number of situations, for the error tolerance 10^{-15} , the resulting programs are dozens, hundreds and even thousands times faster than functions implemented in MATLAB, 8-15 times faster than SymPy. For ${}_1F_1$ and ${}_2F_1$, in some regions in the parameter space, the new programs are faster than functions implemented in Mathematica. Pricing of vanillas in the Heston model requires the summation of 6-15 terms for options of maturities $T \geq 0.004$, in a wide region of strikes; the number of terms is a decreasing function of T.

A DG method for the coupled Navier-Stokes and Cahn-Hilliard equations

Chen Liu
Rice University

Advances in pore-scale imaging, increasing availability of computational resources, and developments in numerical algorithms have started rendering direct pore-scale numerical simulations of multiphase flow on pore structures feasible. This talk presents a discontinuous Galerkin (DG) method for a system consisting of Navier-Stokes equation and Cahn-Hilliard equation. This system describes phase separation of an incompressible immiscible binary mixture transport through porous media. The computational domain, which stems from micro-CT scan, is defined on voxel

sets representing the pore space of rock samples at micrometer scale. The numerical validation tests show optimal convergence rates for the DG discretization. Porous media simulations for two-component flow demonstrate the consistency of the velocity field and mass distribution obtained within the computational framework and exhibit the potential for tackling realistic problems.

Perturbation Theory Applied to a Multiscale Mixed Method: A Parallel Algorithm

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In the formulation of multiscale methods for second order elliptic equations that are based on domain decomposition procedures, (see e.g. the Multiscale Mortar Mixed Finite Element Method (MMMFEM) [1], the Multiscale Mixed Method (MuMM) [2], Multiscale Robin Coupled (MRC) [3], the Multiscale Hybrid - Mixed Finite Element Method (MHM) [4]) typically the computational domain is decomposed into subdomains, and for each subdomain a set of multiscale basis functions is numerically constructed. Consider the application of such a method to solve a multiphase flow problem or in a Markov chain Monte Carlo (McMC) uncertainty quantification study with a random walk sampler. In these problems (from a time step to the next, for the flow problem and from one sample to the next, for the McMC study) in principle the multiscale basis functions should be recomputed, because the coefficients of the underlying PDE will change. However, these changes are typically small. Thus, instead of calculating again all the multiscale basis function, we invesgate the possibility of finding an approximate solution for the equation with modified coefficients using simple perturbation theory. In this presentation we focus on the MuMM [2], and show that, in fact, the perturbation theory may produce accurate solutions, while taking advantage of multiscale basis function associated with the elliptic equation with distinct coefficients. An efficient parallel algorithm is implemented in multi-core machines. Numerical experiments, where the perturbation theory results are compared with direct fine grid solutions, are presented and discussed.

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[2] A. Francisco, V. Ginng, F. Pereira, J. Rigelo. Design and implementation of a multiscale mixed method based on a nonoverlapping domain decomposition procedure. Math. Compute. Simul. 99:125 138, 2014.

[3] R. Guiraldello, R. Ausas, F. Sousa, F. Pereira, G. Buscaglia. A generalised multiscale method with Robin boundary conditions. (Submitted)

[4] R. Araya, C. Harder, D. Paredes, and F. Valenn. Multiscale Hybrid-Mixed Method. SIAM Journal on Numerical Analysis, 51(6):305053531, 2013.

A Bayesian Approach to Model Inadequacy

Brad Marvin, Aaron Myers, & Tan Bui-Thanh
The University of Texas at Austin

In this poster we cast the model inadequacy problem into a Bayesian inverse problem. We postulate that the discrepancy between the PDE and true (physical) solutions can be described by a Gaussian process. Following a Bayesian approach, we assume a Gaussian prior measure on the discrepancy and incorporate observation data to form a posterior measure. The posterior mean can be used to make predictions about the true state and quantities of interest while the posterior covariance allows us to quantify the uncertainty in those predictions. We provide a rigorous construction and analysis of the proposed approach in the infinite dimensional setting for linear PDEs. The method is tested on an elliptic problem in one, two, and three spatial dimensions solved using the finite element method. Ongoing work will extend the approach to hyperbolic PDEs and nonlinear PDEs.

A generalized wavelet based grid-adaptive and scale-selective implementation of WENO schemes for conservation laws

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We devise a framework for the scale-selective application of a fifth-order WENO scheme for the simulation of hyperbolic conservation laws exhibiting strong discontinuities. A generalized wavelet based multiresolution (MR) procedure, embedded in a conservative finite volume formulation, is used for a dynamic grid adaptation of the solution field. Taking advantage of the structure detection properties of this MR algorithm, the nonlinear weights of the conventional WENO implementation are 'adapted' to ensure linear dissipation in smoother areas. This adaptation is implemented through a linear transition from the linear fifth-order upwind stencil at the smoothest areas of the adapted grid to fully nonlinear WENO-5 at the areas of high irregularity. Our computing algorithm consisting of a dynamic grid adaptation strategy, a conservative flux calculation and a total variation diminishing time advancement which are implemented in an object oriented dynamic memory framework for a general system of one-dimensional hyperbolic equations. Results are presented for the inviscid Burgers, shallow water, Euler and the magnetohydrodynamic equations. Our findings are promising in that they represent a novel direction for the addition of scale selective dissipation without a compromise on shock capturing behavior for conservation laws with implications for implicit large eddy simulation based turbulence modeling.

Scaling of Lyapunov Exponents in Homogeneous Isotropic Turbulence

Prakash Mohan, Nicholas Fitzsimmons, & Robert D. Moser
The University of Texas at Austin

Lyapunov exponents measure the average exponential growth rate of typical linear perturbations in a chaotic system, and the inverse of the largest exponent is a measure of the time horizon over which the evolution of the system can be predicted. Here, Lyapunov exponents are determined in forced homogeneous isotropic turbulence for a range of Reynolds numbers. Results show that the maximum exponent increases with Reynolds number faster than the inverse Kolmogorov time scale, suggesting that the instability processes may be acting on length and time scales smaller than Kolmogorov scales. Analysis of the linear disturbance used to compute the Lyapunov exponent, and its instantaneous growth, show that the instabilities do, as expected, act on the smallest eddies, and that at any time, there are many sites of local instabilities.

High-order polygonal discontinuous Petrov-Galerkin (PolyDPG) methods using ultraweak formulations

Ali Vaziri Astaneh, Federico Fuentes, Jaime Mora, Leszek Demkowicz
The University of Texas at Austin

Developing finite elements with unconventional shapes has gained a significant interest over the past decade. In this work we present the first endeavor in using ultraweak formulations to implement high-order polygonal finite element methods via the discontinuous Petrov-Galerkin (DPG) methodology. Ultraweak variational formulations are nonstandard in that all the weight of the derivatives lies in the test space, while most of the trial space can be chosen as copies of L^2-discretizations that have no need to be continuous across adjacent elements. Additionally, the test spaces are broken along the mesh. This allows constructing conforming polygonal finite element methods, termed as PolyDPG methods, by defining most spaces by restriction of a bounding triangle or box to the polygonal element. The only variables that require nontrivial compatibility across elements are the so-called interface or skeleton variables, which can be defined directly on the element boundaries. Unlike other high-order polygonal methods, PolyDPG methods do not require ad hoc stabilization terms thanks to the crafted stability of the DPG methodology. We present various numerical examples to demonstrate the delivery of optimal convergence rates (for the field variables) in the L^2 norm. These include polygonal meshes with n-sided convex elements and with highly distorted concave elements, as well as the modeling of discontinuous material properties along an arbitrary interface that cuts a uniform grid. Since PolyDPG methods have a natural a posteriori error estimator a polygonal adaptive strategy is developed and compared to standard adaptivity schemes based on hanging nodes. Extension of the presented technique to arbitrary three-dimensional polyhedral elements is in progress.

Multilevel and Multigrid solvers for hybridized discontinuous Galerkin (HDG) methods

Sriramkrishnan Muralikrishnan, Tim Wildey, & Tan Bui-Thanh
The University of Texas at Austin

In this talk we present nested dissection based geometric multilevel and multigrid strategies for HDG methods. These solvers are proposed entirely on the skeletal system and utilize the underlying structure of HDG methods. Multigrid solvers on the skeletal system represent difficulty because of the non-nested nature of the grids i.e. new edges appear on refinement which does not have parents from the previous level. With the help of various examples, we show how different multilevel and multigrid solvers can be constructed efficiently for HDG methods.

Characterizing Efficiency of Doxorubicin in Breast Cancer Treatment

Hope Murphy, Elizabeth Sizemore, Anton Naumov, & Hana Dobrovolny
Texas Christian University

Three million women have breast cancer in US, causing breast cancer to be the second most common cause of death from cancer for women. Doxorubicin is a commonly used drug for cancer treatment. The focus of my research is characterizing the drug efficacy for doxorubicin in the human breast cancer cell line MCF-7. There are two quantities that characterize the effect of a drug: E_max is the maximum possible effect from a drug and IC_50 is the drug concentration where the effect diminishes by half. We are using mathematical modeling to extract E_max and IC_50 for Doxorubicin in MCF-7 cells. This work is intended to characterize the efficacy of anticancer drug treatments and determine the correct doses before trying those in patients to get the most effective therapeutic treatment for patients.

A DPG Approach to the Full Vectorial Transverse Mode Instability Model of Optical Laser Amplifiers

Leszek Demkowicz[1], Sriram Nagaraj[1], Jacob Grosek[2]
[1]Institute for Computational Engineering & Science, The University of Texas at Austin
[2] Kirtland Air Force Base

In this work, we study the DPG methodology with its attractive properties of mesh independent stability, automatic adaptivity and parallelizability applied to a weakly coupled Maxwell-heat equation equation system arising in the context of laser amplification in optical fibers. The interaction of heating effects with the Maxwell system gives rise to the phenomenon of transverse mode instability (TMI). We consider the usual set of Maxwell equations with no free charges with the polarization vector including background, gain and thermal contributions. The primal DPG method is used with an implicit Euler time-stepping approach for the

heat equation with radial Dirichlet conditions along the fiber. The Maxwell system is then solved with the ultraweak DPG formulation (which is known to be effective in high-frequency wave propagation problems) with polarization values obtained from the heat equation. We then iterate between the heat and Maxwell system updating the relevant quantities until convergence. The use of DPG adaptivity for the Maxwell system along with the guaranteed discrete stability of the ultraweak/primal formulations is critical for a numerically stable and tractable method which allows us to effectively simulate the TMI phenomenon.

A PDE Constrained Optimization Approach to the Solution of the Stefan Problem

Tom O'Leary-Roseberry, Umberto Villa, Patrick Heimbach, Omar Ghattas
The University of Texas at Austin

The dynamics of ice ocean interaction (including melting at the interface and implied geometry changes) can be modeled as an implicit surface moving in accordance with conservation laws; this is known as the Stefan problem. In practice there are numerous sources of uncertainty in the problem (initial conditions, boundary conditions and material properties etc.); a Bayesian framework provides a way to estimate these parameters and indeed quantify their uncertainty. In order to solve the Bayesian inverse problem described here an adjoint capable formulation must be constructed. While many robust methods are available for solving the forward Stefan problem (finite difference based level set methods, fast marching methods etc.), these methods are not well equipped to handle the inverse problem. In this work a PDE constrained variational optimization formulation is proposed. This formulation is well suited to a Bayesian inverse problem framework, as well as extension to more general conservation laws such as those formulated in ocean circulation models etc. Preliminary results will be shown for a known analytic solution of the Stefan problem as well as for test cases with simple geometries.

A second-order partitioned scheme for fluid-structure interaction problems

Oyekola Oyekole
Notre Dame University

We propose and analyze a novel, second order in time, partitioned method for the interaction between an incompressible, viscous fluid and a thin, elastic structure. The proposed numerical method is based on the Crank-Nicolson discretization scheme, which is used to decouple the system into a fluid sub-problem and a structure sub-problem. The scheme is loosely coupled, and therefore at every time step, each sub-problem is solved only once. Energy and error estimates for fully discretized scheme using finite element spatial discretization are derived. We prove that the scheme is stable under a CFL condition and second-order convergent in time. We

also prove optimal spatial convergence. Numerical examples support the theoretically obtained results and demonstrate long time stability on a realistic example of blood flow.

Hypersurface model of the fracture for nonlinear fluid flows

Pushpi Paranamana, Eugenio Aulisa, Magdalena Toda, & Akif Ibragimov
Department of Mathematics & Statistics
Texas Tech University

In this work, we analyze the flow filtration process of slightly compressible fluids in porous media containing fractures with complex geometries. We model the coupled fracture-porous media system where the linear Darcy flow is considered in porous media and the nonlinear Forchheimer equation is used inside the fracture. Also, we devise a model to address the complexity of the fracture geometry which examines the flow inside fractures with variable thickness on a general manifold. The fracture is represented as the normal variation of a surface immersed in $\mathbb{R}^3$ and using Laplace Beltrami operator, we formulate an equation that describes the flow and then further simplifications were done. Using the model, pressure distribution of a nonlinear flow is analyzed and compared with the actual pressure distribution obtained numerically in order to validate the model.

The DPG Method for High Frequency Time-harmonic Wave Propagation Problems

Socratis Petrides
The University of Texas at Austin

In this talk, we outline the most important properties of the Discontinuous Petrov Galerkin (DPG) method, for the solution of high-frequency wave propagation problems. The DPG method guarantees discrete stability, even in the pre-asymptotic region, and it comes with a built-in local error indicator. This allows for automatic hp-adaptivity, starting from very coarse meshes. In the first part of the talk, we demonstrate these attractive features of the DPG method, by simulating a high frequency Gaussian beam in two space dimension, scattering by a resonating cavity. We start the simulation with a very coarse mesh that captures the geometry, and perform successive hp-adaptive refinements. Our results show that the method avoids unnecessary computations in areas of the domain where the wave doesnt exist, i.e, the mesh is built along with the solution. In the second part of the talk, we present a new iterative solution scheme, for the solution of the DPG system. The need for iterative solvers, comes from the fact that the problem has to be solve several times throughout the adaptive procedure. Employing a direct solver, at every adaptive step is far from optimal and unnecessary. The adaptive refinements can be driven by a partially converged solution, by employing an iterative solver. Being a minimum residual method, DPG always delivers a Hermitian positive definite stiffness matrix.

Thus, the Conjugate Gradient (CG) method is the best candidate, provided that it is combined with an effective preconditioner. We introduce such a preconditioner, which exploits information form previous meshes. This new solver is integrated with in the DPG adaptive procedure, by borrowing ideas of the two grid solver technology. We apply our solver for the solution of the acoustics problem in two space dimension. Our results show convergence in terms of iterations at a rate independent of the mesh and the wavenumber.

Two Possible Mechanisms of Chronic Viral Coinfections: Cellular Regeneration and Superinfection

Lubna Pinky[1], Gilberto González-Parra[2], & Hana M. Dobrovolny[1]

[1]Department of Physics and Astronomy, Texas Christian University
[2]Grupo de Matemática Multidisciplinar, Universidad de los Andes Mérida

A significant number of patients hospitalized with influenza-like illness are reported to have coinfections simultaneous infection with more than one type of respiratory virus. The impact of coinfections on disease severity compared to single viral infection is unclear, since there is evidence for more severe illness as well as less severe illness in clinical studies. To determine the effect of coinfections on disease severity, a mathematical model is developed based on ordinary differential equations which allows single cells to be infected simultaneously with two different respiratory viruses (superinfection). To assess the full behavioral dynamics of coinfection, mathematical analysis along with computer simulation are performed using the superinfection model with and without the mechanism of cellular regeneration in respiratory tract. Coinfection with respiratory syncytial virus and influenza A virus is considered as an example to explore possible model outcomes. Model study shows that superinfection alone can not produce chronic coinfection while superinfection with cellular regeneration gives chronic coinfection.

Modeling of Viral Coinfection in Human Respiratory Tract Using Stochastic Method

Lubna Pinky[1], Gilberto González-Parra[2], & Hana M. Dobrovolny[1]

[1]Department of Physics and Astronomy, Texas Christian University
[2]Grupo de Matemática Multidisciplinar, Universidad de los Andes Mérida

Respiratory viral infections are a leading cause of mortality worldwide. As many as 40% of patients hospitalized with influenza-like illness are reported to be infected with more than one type of viruses. Mathematical models can be used to help us understand the dynamics of respiratory viral coinfections and their impact on the severity of the illness. Most models of viral infections use ordinary differential equations (ODEs) which reproduce the average behavior of the infection. In reality, viral infections are discrete and stochastic. Stochastic simulations of single virus infections have shown that there is an extinction probability that depends on the

size of the initial viral inoculum and parameters that describe virus-cell interactions. Thus the chronic coinfections predicted by the ODEs might be difficult to observe in reality. Using the Gillespie method for stochastic simulation, we examine whether stochastic effects early in the infection can determine which virus dominates the infection. We found that even if the two viruses are given the same initial viral inoculum, one virus can have higher extinction probability than the other, making it possible for one virus to go extinct while the other viral infection grows.

A Stochastic Operator Approach to Model Inadequacy with Applications to Contaminant Transport

Teresa Portone, Damon McDougall, Robert D. Moser, & Todd A. Oliver

The University of Texas at Austin

We present recent developments on the uncertainty quantification of models. Models are imperfect representations of complex physical processes, hence exploring representations of the model inadequacies is crucial. We introduce an inadequacy model in the form of a linear operator acting on the model solution and explore methods for incorporating knowledge of model shortcomings and relevant physics. This representation is developed in the context of scalar dispersion in porous media, but the methods presented are applicable for other models. Authors:

Respiratory Control System Model During Exercise With Two Delays

Saroj Pradhan

Lecturer at Prairie View A&M University

We study the effects of changes of cardiac output during exercise on transport delays (peripheral and central), control gains (peripheral and central), and the instability/stability of the human respiratory control system with two delays and two control loops. Our conclusion is that the sudden increase of exercise creates more unstable respiration than a gradual increase of exercise.

Multiscale Optimization Using Generalized Mortar Methods

Tom Seidl, Tim Wildey, & Bart van Bloemen Waanders
Sandia National Laboratories

A long-standing challenge in computational science and engineering is the accurate and efficient modeling of physical systems with interactions that occur over multiple length and/or time scales. When such systems represent constraints in inverse and optimal control problems their solution may be required hundreds to thousands of times over the course of the optimization algorithm. In such problems, direct numerical simulation is often prohibitive and thus a multitude of numerical methods that utilize a coarse scale approximation of the underlying fine scale physics have been developed. In this talk we present a variant of the multiscale mortar method where the macroscale discretization is defined in terms of the trace of the basis functions on the interior skeleton of a macro-scale finite element mesh. Each macro-element contains a localized and independent representation of the fine scale problem physics, i.e. mesh, model fidelity, time integration scheme, etc can vary within each macro-element. Given the coarse-scale solution as Dirichlet data, these local fine-scale problems are solved independently leading to an efficient parallel implementation that can leverage emerging heterogeneous computational architectures. The coarse scale residual and Jacobian are defined in terms of the local Dirichlet-to-Neumann map projected into the mortar space. We show that this approach has a consistent space-time variational formulation and is thus amenable to adjoint-based sensitivity calculations. Given an objective function, we formulate and solve a multi-scale adjoint problem leading to an efficient and accurate calculation of its gradient. We demonstrate our approach on an inverse problem with a variable density of sensor measurements and compare our results to those obtained single-scale models.

High-order Relaxed Multirate Infinitesimal Step Methods for Multiphysics Applications

Jean Sexton, Daniel R. Reynolds
Southern Methodist University

In this work, we consider numerical methods for integrating multirate ordinary differential equations. We are interested in the development of new multirate methods with good stability properties and improved efficiency over existing methods. We give context on the development of multirate methods, particularly focusing on those that are based on Runge-Kutta theory. We introduce the theory of Generalized Additive Runge-Kutta methods proposed by Sandu and Guenther. We also introduce the theory of Recursive Flux Splitting Multirate Methods with Subcycling described by Schlegel, as well as the Multirate Infinitesimal Step methods this work is based on. We propose a generic structure called Flexible Multirate Generalized-Structure Additively-Partitioned Runge-Kutta methods which allows for optimization and more rigorous analysis. We also propose a specific class of higher-order methods, called Relaxed Multirate Infinitesimal Step Methods. We will leverage GARK theories to develop new theory about the stability and accuracy of these new methods.

Dynamical Reconstruction of AMOC Variability at 34°S

Timothy Smith[1] & Patrick Heimbach[1,2]

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[2] Jackson School of Geosciences, The University of Texas at Austin

In the global ocean, the Atlantic Meridional Overturning Circulation (AMOC) is a metric for the northward volumetric transport of water in the upper ∼1000m of depth, computed as a function of latitude and time. This quantity provides a convenient proxy for global ocean circulation, as it represents the mechanism for carrying warm and salty water to the North Atlantic where oxygen-rich deep water is formed. Here, we show the sensitivity of the AMOC at 34° S to global atmospheric forcing (e.g. wind stress, air temperature), where these gradients are computed with the model adjoint as the lagrange multipliers associated with the AMOC objective function. Evolving backward in time, these sensitivity patterns highlight the important dynamical pathways for communicating perturbations in the atmospheric state, i.e. our boundary conditions, to 34° S. Using these sensitivities and historical atmospheric forcing, we reconstruct the monthly AMOC anomaly from 1992-2011 and attribute variability to its origination as atmospheric anomalies. Importantly, we find that zonal wind stress dominates seasonal to interannual variability, corroborating past forward sensitivity experiments. In contrast to past studies in the North Atlantic, however, the AMOC at this latitude is shown to have a wide domain of influence, spanning neighboring ocean basins on short time scales. The El Niño Southern Oscillation, for instance, is shown to have an important influence on the interannual AMOC behavior. This result emphasizes the importance of continuous widespread observations of the global atmospheric state for attributing and (eventually) forecasting AMOC variability.

Identification of Minimum Power Dominating Sets in Re-Configurable Graph Networks

Logan Smith

Computational and Applied Mathematics Department
Rice University

Phase Monitoring Units (PMUs) can be used to monitor electrical grid activity in real-time, allowing for immediate responses to changes in energy consumption. Due to both the prohibitively high cost of PMUs, the optimal placement of a minimal number of PMUs able to fully observe an electrical network is a problem of interest amongst electrical engineers. The PMU Placement problem can be equivalently considered as identifying minimum power dominating sets in a graph network, which is an active problem in graph theory. In addition to the incorporation of PMUs, several innovations in smart grid designs include on the fly grid topology reconfiguration, introducing new challenges to the observation problem. Motivated by recent advances in the closely related minimal zero forcing set problem, novel techniques for identifying power dominating sets in graphs and families of graphs are presented and computational results are compared.

New families of $H(div)$ mixed finite elements on cuboidal hexahedra

Todd Arbogast & Zhen Tao
The University of Texas at Austin

We generalize the two dimensional mixed finite elements of Arbogast and Correa [1] defined on quadrilaterals to three dimensional cuboidal hexahedra. The construction is similar in that polynomials are used directly over the element and supplemented with functions defined on a reference element and mapped to the hexahedron using the Piola transform. The main contribution is providing a systematic procedure for defining supplemental functions that are divergence-free and have any prescribed polynomial normal flux. Both full and reduced $H(div)$-approximation spaces may be defined, so the scalar variable, vector variable, and vector divergence are approximated optimally.

[1] T. Arbogast and M. R. Correa, SIAM J. Numer. Anal., 54 (2016), pp. 3332–3356

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hIPPYlib: An Extensible Software Framework for Large-Scale Deterministic and Linearized Bayesian Inverse Problems

Umberto Villa, Noemi Petra, Omar Ghattas
Institute for Computational Engineering and Sciences
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In this talk, we present hIPPYlib (hippylib.github.io), an extensible software framework for the solution of large-scale deterministic and linearized Bayesian inverse problems governed by partial differential equations (PDEs) with possibly infinite-dimensional parameter fields (which are high-dimensional after discretization). hIPPYlib overcomes the prohibitive nature of Bayesian inversion for this class of problems by implementing state-of- the-art scalable algorithms for PDE- based inverse problems that exploit the structure of the underlying operators, notably the Hessian of the log posterior.

hIPPYlib relies on FEniCS (fenicsproject.org), a powerful finite element toolkit, for the discretization of the PDE, and on PETSc (`https://www.mcs.anl.gov/petsc/`) for scalable and efficient linear algebra operations and solvers. It also relies on FEniCS for its symbolic differentiation capability to automatically and efficiently generate the variational forms for the adjoint and incremental PDE problems needed to facilitate efficient gradient and Hessian evaluations.

To demonstrate hIPPYlib's algorithmic features, I will discuss the solution of two representative inverse problems: inversion for the coefficient field of an elliptic PDE and inversion for the initial condition field of a parabolic PDE. I will derive the optimality conditions using the Lagrangian formalism and I will present efficient solution algorithms in each case. I will state the Bayesian inversion framework for the case of Gaussian noise and prior probability densities, and construct a quadratic approximation of the negative log likelihood at the maximum a posteriori

(MAP) point to produce a Gaussian approximation of the posterior. The mean of the posterior is approximated by the MAP point, which is found by minimizing the negative log posterior. This deterministic nonlinear least squares optimization problem is solved with an inexact matrix-free Newton-CG method. The posterior covariance is approximated by the inverse of the Hessian of the negative log posterior evaluated at the MAP point. The construction of the posterior covariance is made tractable by invoking a low-rank approximation of the Hessian of the log likelihood (the data misfit component) via a randomized SVD algorithm.

The key property of hIPPYlib is that solution of the inverse problem is computed at a cost, measured in forward PDE solves, that is independent of the parameter dimension. The goal of hIPPYlib is to make these advanced deterministic and Bayesian inversion algorithms accessible to domain scientists and provides an environment that expedites the development of new algorithms.

Isogeometric shape optimization on triangulations

Cunfu Wang & Xiaoping Qian
Department of Mechanical Engineering
University of Wisconsin-Madison

This research presents a Bézier triangle based isogeometric shape optimization method. Bézier triangles are used to represent both the geometry and physical fields. For a given physical domain defined by B-spline boundary, a coarse Bézier triangular parameterization is automatically generated. This coarse mesh is used to maintain parameterization quality through positivity of Jacobian ordinates of the Bézier triangles and move mesh by solving a pseudo linear elasticity problem. Then a fine mesh for isogeometric analysis is generated from the coarse mesh through degree elevation and refinement. As the fine mesh retains the same geometric map as the coarse mesh, we can guarantee mesh validity with the coarse mesh only. This bi-level mesh allows us to achieve high numerical accuracy of isogeometric analysis and lower computational cost on mesh validity control and mesh movement. Due to the use of B-spline boundary, the optimized shape can be compactly represented with a relatively small number of optimization variables. Due to the use Bézier triangles, this shape optimization method is applicable to structures of complex topology and allows for local refinement for analysis. By representing the squared distance between two Bézier curves as a Bézier form, a distance check scheme is also introduced to prevent intersections of design boundaries and control the thickness of structural connections. Numerical examples on minimal compliance design and design of negative Poisson ratios are presented to demonstrate the efficacy of the proposed method.

Fluidstructure interaction modeling of bioprosthetic heart valves

Rana Zakerzadeh, Michael C. H. Wu, Ming-Chen Hsu, & Michael S. Sacks
The University of Texas at Austin

A computational framework is developed to study the coupling of blood flow interacting with a bioprosthetic heart valve incorporating anisotropic material model. Blood is modeled as an incompressible, viscous, Newtonian fluid using the Navier-Stokes equations and the elastodynamics of the leaflets is modeled by the Kirchhoff-Love shell formulation. To approximate this problem, the fluid-structure interaction (FSI) simulations are carried out using our hybrid immersogeometric/arbitrary LagrangianEulerian approach. We simulated the coupling of deforming aortic root, heart valves, and the surrounding blood flow under physiological conditions through several cardiac cycles. A parametric study is performed to identify the role of leaflet's shape and anisotropic material model on valve performance. The functionality of valve is evaluated by its effective orifice area and leaflet coaptation without regurgitation for different designs of the leaflets. We observed a noticeable influence of the leaflet design on the valve performance and the overall tissue deformation. Moreover, numerical results suggest that it is important to select a realistic tissue model that capture fiber recruitment behavior and inherent anisotropy.

A New Discontinuous Galerkin Method for the Wave Equation With Background Flow

Lu Zhang
Southern Methodist University

In this work, we investigate the wave equation with background flow by a new discontinuous Galerkin method. The method defines inter-element fluxes in a direct, mesh independent way. It can be either energy conserving or energy dissipating, depending on a simple choice of the numerical fluxes. We also carry out rigorous analysis to obtain a priori error estimates in the energy norm for certain fluxes and provide some numerical simulations to show the optimal convergence rate in L^2.

Accuracy of Adaptive Order WENO Schemes for Solving Conservation Laws

Xikai Zhao, Todd Arbogast, & Chieh-Sen Huang
The University of Texas at Austin

Recently, Balara, Garain and Shu [JCP, 2016] introduced a new class of WENO schemes with adaptive order (WENO-AO). They defined a recursive, multilevel process to define the WENO reconstructions. We present an analysis of the accuracy of WENO-AO and the conditions under which it achieves optimal order accuracy for both smooth solutions and solutions with shocks. We also give a new multilevel WENO-AO scheme which achieves optimal order accuracy for a wider choice of levels.

Fast algorithm in radiative transfer

Yimin Zhong, Kui Ren, & Rongting Zhang
The University of Texas at Austin

We propose in this work a fast numerical algorithm for solving the equation of radiative transfer (ERT) in isotropic media. The algorithm has two steps. In the first step, we derive an integral equation for the angularly averaged ERT solution by taking advantage of the isotropy of the scattering kernel, and solve the integral equation with a fast multipole method (FMM) or fast direct solvers. In the second step, we solve a scattering-free transport equation to recover the original ERT solution. Numerical simulations are presented to demonstrate the performance of the algorithms for both homogeneous and inhomogeneous media.

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