Society for Industrial and Applied Mathematics

1st Annual Meeting of SIAM Central States Section

Meeting Program

MISSOURI UNIVERSITY OF SCIENCE AND TECHNOLOGY

Rolla, Missouri

Society for Industrial and Applied Mathematics

Organizing Committee

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Xiaoming He
Missouri University of Science and Technology (S&T)

Section Vice President
Erik Van Vleck
University of Kansas

Section Secretary
Xiu Ye
University of Arkansas at Little Rock

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Yanzhi Zhang (S&T)
Peizhen Zhu (S&T)

Conference Coordinator
Michelle Wiginton (S&T)

Conference Secretary
Tammy Mace (S&T)

Welcome to SIAM Central States Section First Annual Meeting

Welcome to Missouri University of Science and Technology and the first annual meeting of the SIAM Central States Section.

This first meeting promises to be an excellent start for the new SIAM section. The conference features presentations by four plenary speakers, over 160 invited and contributed presentations split between 40 parallel sessions, and a poster session. We are honored to have Mark Ablowitz, Susanne Brenner, Arnd Scheel, and Junping Wang as plenary speakers.

One of the primary goals of the new SIAM Central States Section is to promote communication and collaboration among SIAM members in the central region, consisting of Arkansas, Colorado, Iowa, Kansas, Mississippi, Missouri, Nebraska, and Oklahoma. We hope that you take advantage of the many opportunities to network with colleagues from the central region and many other locations.

We are very grateful to SIAM for the support in starting the SIAM Central States Section. We also thank all of the individuals who contributed to the organization of the conference, and Missouri S&T and SIAM for their support.

We hope everyone enjoys the conference and finds it valuable. Thanks to everyone for attending and participating, and for supporting our new SIAM Central States Section.

About SIAM Central States Section – http://siamcentral.mst.edu

The SIAM Central States Section was formed in 2014 to serve SIAM members in Arkansas, Colorado, Iowa, Kansas, Mississippi, Missouri, Nebraska, and Oklahoma. The purpose of this section is to enhance the communication among the section members, promote the collaboration for both basic research and applications of mathematics to industry and science, represent applied and computational mathematics, and support the SIAM mission in the central region of the USA.

The proposed activities for the SIAM Central Section include annual section meetings, seminars and workshops for advanced topics of common interests of the section members, encouraging new SIAM student chapters and facilitating the SIAM student chapters in the central region to connect together, promoting collaboration in applied mathematics and its applications to industry and science, and expanding the influence of SIAM in the central states.

Participation in SIAM Central States Section activities will be open to all institutions and industries in the region with an interest in applied and computational mathematics.

SIAM Central States Section Officers:

President
Xiaoming He
Missouri University of Science and Technology

Vice President
Erik S. Van Vleck
University of Kansas

Treasurer
Stephen D. Pankavich
Colorado School of Mines

Secretary
Xiu Ye
University of Arkansas at Little Rock

Schedule at a Glance

Friday, April 10, 2015

7:00 p.m. – 9:00 p.m.
Social Mixer & Cash Bar
The Public House

Saturday, April 11, 2015
MORNING SCHEDULE

7:30 a.m. – 6:00 p.m.
Registration Desk Open
Coffee Station
Butler Carlton Hall (BCH) Atrium

8:20 a.m.
Welcome Remarks
125 BCH

8:30 a.m.
Plenary Speaker
Mark J. Ablowitz
125 BCH

9:20 a.m.
Plenary Speaker
Susanne Brenner
125 BCH

10:10 a.m.
Refreshment Break
BCH Atrium

10:40 a.m. – 12:20 p.m.
Parallel Sessions
BCH (various locations)
See full schedule on pages 4-5 for details

Saturday, April 11, 2015
AFTERNOON SCHEDULE

12:20 p.m. – 1:45 p.m.
Lunch Break
(on your own)

2:00 p.m.
Plenary Speaker
Arnd Scheel
125 BCH

2:50 p.m.
Plenary Speaker
Junping Wang
125 BCH

3:40 p.m.
Group Photo & Refreshment Break
BCH Atrium

4:10 p.m. – 5:50 p.m.
Parallel Sessions
BCH (various locations)
See full schedule on pages 6-7 for details

6:00 p.m. – 8:00 p.m.
Banquet & Poster Session
St. Pat's Ballroom, Havener Center

Sunday, April 12, 2015

8:00 a.m.
Registration Desk Open
Coffee Station
BCH Atrium

8:30 a.m. – 10:10 a.m.
Parallel Sessions
BCH (various locations)
See full schedule on page 8 for details

10:10 a.m.
Refreshment Break
BCH Atrium

10:40 a.m. – 12:20 p.m.
Parallel Sessions
BCH (various locations)
See full schedule on page 9 for details

12:30 p.m.
Meeting Adjourns

Department of Mathematics and Statistics, Missouri S&T

http://math.mst.edu/

The Department of Mathematics and Statistics at Missouri S&T has approximately 80 undergraduate majors and 50 graduate students pursuing bachelor's and master's degrees in applied mathematics, master's for teachers, and doctorates in mathematics. The Ph.D. program, which has been active for 45 years, consists of emphasis areas in mathematics, statistics, and applied and computational mathematics. Research interests of the faculty cover a wide spectrum with major concentrations in algebra and discrete mathematics, analysis, differential and difference equations, scientific computing and numerical analysis, statistics, and topology. Several faculty members are actively involved in interdisciplinary work in collaboration with researchers in a wide variety of disciplines.

Missouri Institute For Computational and Applied Mathematical Sciences (MICAMS)

The institute promotes the development of multidisciplinary research communities engaging applied mathematicians, computational scientists and engineers in innovative research on important scientific and technological problems. In pursuit of its mission, the institute supports research, provides educational opportunities at all levels, and serves as a resource for the state in support of high-technology industrial development.

THANK YOU SPONSORS

The organizing committee of the 1st Annual SIAM-CSS 2015 Conference wishes to express our sincere thanks to SIAM and Missouri S&T for their generous support in making it possible for us to bring this premier conference to our region.

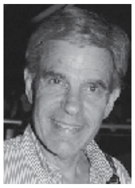
Conference Schedule
Saturday Morning – April 11, 2015

MORNING SCHEDULE

7:30 a.m. – 6 p.m.
Registration Desk Open
Coffee Station
Butler Carlton Hall Atrium (BCH)

8:20 a.m.
Welcome Remarks
125 BCH

8:30 a.m. – 9:20 a.m.
Plenary Session
125 BCH



The Nonlinear Waves — Always Intriguing
Mark J. Ablowitz
Speaker details on page 10

9:20 a.m. – 10:05 a.m.
Plenary Session
125 BCH

Finite Element Methods for Fourth Order Elliptic Variational Inequalities
Susanne Brenner
Speaker details on page 10

10:10 a.m. – 10:35 a.m.
Refreshment Break
BCH Atrium

10:40 a.m. – 12:20 p.m.
Parallel Sessions
Details on right

Parallel Sessions | 10:40 a.m. – 12:20 p.m.

101 BCH: Discontinuous Galerkin Methods for Partial Differential Equations: Theory and Applications

Organizer: Mahboub Baccouch

1001 - Recovery-Based Error Estimators for the DG Method for Scalar Conservation Laws
1002 - On a Class of Nonlocal Wave Equations from Applications
1008 - High Order Maximum Principle Preserving Discontinuous Galerkin Method for Convection-Diffusion Equations
1004 - HDG Methods For Diffusion: Superconvergence by M-decompositions

120 BCH: Advances in High-order Computational Methods

Organizer: Huiqing Zhu

1019 - A Balanced FEM for a System of Singularly Perturbed Reaction-Diffusion Two-Point Boundary Value Problems
1026 - A Hybridizable Discontinuous Galerkin Method for PDE Constrained Optimal Control Problems
1025 - Solving the Yang-Baxter-like Matrix Equation
1017 - Incorporating Local Boundary Conditions Into Nonlocal Theories

121 BCH: Algorithms and Analysis for Efficient Simulation of Wave Propagation Models

Organizer: Mahadevan Ganesh

1032 - Suitable Transmission Conditions for Domain Decomposition Algorithms in the Case of the Helmholtz Equation
1033 - A Class of Staggered-Grid Algorithms and Analysis for Simulation of Time-Domain Maxwell Systems
1034 - High-Order Discretizations for 2D Helmholtz Boundary Layers on Smooth Boundaries
1035 - Sign-Definite Preconditioned Systems for Wave Propagation In Heterogeneous Media: Formulation, Analysis and High-Order FEM

124 BCH: Mathematical and Computational Issues in Big Data

Organizers: Suely Oliveira and David Stewart

1048 - Parallel Algorithm for Community Detection Using Multicore Architecture
1050 - Matrix Completion Algorithms and Recommender Systems
1051 - Randomized Algorithms in Machine Learning
1049 - Matrix Optimization for Clustering

125 BCH: Recent Advances in Finite Element Methods

Organizer: Xianping Li

1077 - Finite Element Methods for a Fourth Order Curl Operator on Planar Domains
1072 - Analysis and Approximation of the Dynamic Ginzburg-Landau Equations In Nonconvex Polygons Based on Hodge Decomposition
1075 - An Efficient Numerical Method for Acoustic Wave Scattering in Random Media
1079 - BPX Preconditioner for Nonstandard Finite Element Methods for Diffusion Problems

Conference Schedule
Saturday Morning – April 11, 2015

Parallel Sessions | 10:40 a.m. – 12:20 p.m. *Session Abstracts on pages 11-32*

215 BCH: Contributed presentations in lecture format

1083 - Parallel Simulation of Nonlocal Sub-Diffusion Models
1085 - Numerical Solution of Dynamic Electrical Circuits With Diodes
1086 - A Modified Weighting Algorithm for Immersed Finite Element Particle-In-Cell(IFE-PIC) Method
1087 - Numerical Simulation of an Impact Problem
1088 - Simulation of Properties of Acoustic Wave Propagation Configurations

216 BCH: Interactions Among Analysis, Optimization and Network Science

Organizers: Nathan Albin and Pietro Poggi-Corradini

1111 - An Introduction to Modulus of Path Families from a Historical Point Of View
1106 - Three Notions of Parabolicity for Networks
1112 - Impact of Preventive Responses to Epidemics in Rural Regions
1103 - Modulus of Families of Walks on Graphs

314 BCH: Recent Advances in Numerical Methods for Fluid Flows

Organizer: Zhu Wang

1119 - Magnetohydrodynamic Flows: Boussinesq Conjecture
1117 - Mimetic and Convergent Discretization of Vector Fields on Unstructured Meshes
1122 - Predicting Orientation of Fibers in Injection Molded Plastics
1116 - Numerical Methods for Flow in Poroelastic Media

315 BCH: Analytical and Computational Methods in Nonlinear Problems of Solid Mechanics

Organizer: Zemlyanova Anna

1135 - Domain Formation in Membranes Near Onset of Instability
1136 - Qualitative Properties of the Solution of the Equations in Non-Divergent Form with Zaremba Type of Boundary Conditions in Non-Smooth Domain
1137 - Neutrality of Coated Ellipsoids with a Linear Shell and a Nonlinear Core
1134 - Approximation of DtN Map in a High Contrast Conductivity Problem

316 BCH: Current Trends in Ecology and Disease Modeling

Organizers: Naveen Vaidya and Majid Bani-Yaghoub

1141 - Ideal Treatments for HIV-TB Co-Infected Populations: Modeling and Optimal Control Theory Perspectives
1143 - Mathematical Modeling of Cholera
1146 - A Population Model with Age Structure and Periodically Distributed Time Delay
1139 - Eco-Evolutionary Analysis of a Multi-Strain SIS Model to Quantify the Long-Term Efficacy of Control and Preventive Measures

317 BCH: Partial Differential Equations: Analysis, Modeling, and Applications

Organizer: John Singler

1149 - Recovery of a Boundary Flux Using Far Boundary Data
1151 - Parabolic PDEs for Fluid, Flame, and Plasma Dynamics: When Are Solutions Bounded?
1153 - The Morse and Maslov Indices for Schrodinger Operators

318 BCH: Recent Advances in Numerical Methods for Interface Problems

Organizer: Xu Zhang

1162 - Time Domain Interface Methods for Electromagnetic Wave Propagation in Dispersive Media
1160 - A Simple and Accurate Discontinuous Galerkin Scheme for Modeling Scalar-Wave Propagation in Media with Curved Interfaces
1159 - A New Poisson-Boltzmann Equation Hybrid Solver Intermixing with Solution and Domain Decompositions, Finite Element, and Finite Difference
1154 - An Immersed Discontinuous Q1/Q0 Finite Element Method for the Stokes Interface Problem

Conference Schedule
Saturday Afternoon – April 11, 2015

AFTERNOON SCHEDULE

12:20 p.m. – 1:45 p.m.
Lunch Break
(On your own)

2:00 p.m. – 2:45 p.m.
Plenary Session
125 BCH

Coherent structures in nonlocal equations
Arnd Scheel
Speaker details on page 10

2:50 p.m. – 3:35 p.m.
Plenary Session
125 BCH

Weak Galerkin Finite Element Methods for PDEs
Junping Wang
Speaker details on page 10

3:40 p.m.
Group Photo & Refreshment Break
BCH Atrium

4:10 p.m. – 5:50 p.m.
Parallel Sessions
Details on right

6:00 p.m. – 8:00 p.m.
Banquet & Poster Session
St. Pat's Ballroom, Havener Center
See page 33 for poster session details

Parallel Sessions | 4:10 p.m. – 5:50 p.m.

101 BCH: Discontinuous Galerkin Methods for Partial Differential Equations: Theory and Applications

Organizer: Mahboub Baccouch

1005 - Schwarz Methods for Discontinuous Galerkin Approximations of Elliptic Problems.
1011 - A Curved Boundary Treatment for Discontinuous Galerkin Schemes Solving Time Dependent Problems
1003 - A Discontinuous Galerkin Approximation for Photonic Crystals
1009 - Superconvergence of Discontinuous Galerkin Methods for 2D Linear Hyperbolic Equations

120 BCH: Advances in High-order Computational Methods

Organizer: Huiqing Zhu

1021 - A Riemann-Solver Free Spacetime Discontinuous Galerkin Method for General Conservation Laws
1018 - Solution of Nonlinear Time-Dependent PDE Through Componentwise Approximation of Matrix Functions
1020 - Multiscale Hybridizable DG Methods for Flows in Heterogeneous Media
1020a - Numerical smoothness and optimal –optimal error analysis for time-dependent PDEs

121 BCH: Algorithms and Analysis for Efficient Simulation of Wave Propagation Models

Organizer: Mahadevan Ganesh

1036 - A High-Order Coupled Isoparametric Finite Element and Spectral Method for Heterogeneous Media Wave Propagation
1037 - Time-domain BEM-FEM for Transient Acoustic Scattering
1038 - Comparisons of Integral Equations Formulations for High-Frequency Two-Dimensional Helmholtz Transmission Problems in Domains With Corners
1039 - Imaging Underground Faults Using Displacement Measurements on Earth's Surface

124 BCH: Numerical Modeling of Complex Systems

Organizer: Tianshi Lu

1052 - A Matched Alternative Direction Implicit (ADI) Method for Solving 2D Parabolic Interface Problems
1055 - Phenomenological and First Principle Approaches for Micro, Meso and Macro Scales
1056 - A New RKDG Method with Conservation Constraint to Improve CFL Condition for Solving Conservation Laws
1053 - Numerical Modeling and Simulations of Interaction Between Dusty Disk and Embedded Proto-Planets
1054 - MHD Simulation of Pellet Ablation In Tokamaks

Conference Schedule
Saturday Afternoon – April 11, 2015

Parallel Sessions | 4:10 p.m. – 5:50 p.m. *Session Abstracts on pages 11-32*

125 BCH: Recent Advances in Finite Element Methods

Organizer: Xianping Li

1078 - Nonconforming Generalized Finite Element Method for Dirichlet Boundary Value Problems
1081 - Recent Development of Weak Galerkin Methods
1076 - Banach Space Projections and Petrov-Galerkin Estimates
1080 - A Local Nodal Meshless Method for Pdes--Localized Method of Approximate Particular Solutions Using Thin-Plate Spline Rbfs

215 BCH: Contributed presentations in lecture format

1089 - Research of Live Migration Scheduling Method for the Simulation System based on Cloud Computing
1090 - Forecast Uncertainty Quantification of Return Flow over the Gulf of Mexico Using Monte Carlo, Generalized Polynomial Chaos and Unscented Transform methods
1091 - The Exponential Stability of Wave Equation with Dirichlet Boundary Feedback Control
1084 - A Discrete, Arbitrarily-Oriented, 3D Plane Source Analytical Solution to the Heat Equation for Modeling Reservoir Fluid Flow
1099 - Analytical Solutions of Periodic Motions in a Periodically Forced, Damped, Two-Degree-of-Freedom Oscillator with Nonlinear Spring
1092 - Bifurcation trees of period-1 motions to Chaos in a double-well Duffing oscillator under periodic excitation

216 BCH: Interactions Among Analysis, Optimization and Network Science

Organizer: Nathan Albin and Pietro Poggi-Corradini

1114 - Use of Functions of Bounded Variation in Determining Sobolev Functions with Zero Boundary Values
1104 - Exact Coupling Threshold for Structural Transition in Interconnected Networks
1113 - Generalized Centrality Measures Based on Modulus of Families of Walks

314 BCH: Recent Advances in Numerical Methods for Fluid Flows

Organizer: Zhu Wang

1124 - Time Domain Decomposition Methods for Forward-and-Backward PDEs
1120 - A Stable Leapfrog Scheme for Optimal Control of Wave Equations
1123 - Multiscale Mortar Finite Element Methods for Coupling Stokes-Darcy Flows with Transport on Irregular Geometry Domains

315 BCH: Analytical and Computational Methods in Nonlinear Problems of Solid Mechanics

Organizer: Zemlyanova Anna

1131 - Infinite-Order Laminates in a Crystal Plasticity Model with Two Slip Systems
1132 - Nonuniqueness of Blowup Limits of Solutions to the Obstacle Problem
1138 - Singular Integro-Differential Equations for a New Model of Fracture with a Curvature-Dependent Surface Tension
1133 - Numerical Methods for Riemann-Hilbert Problems in Multiply-Connected Circular Domains

316 BCH: Current Trends in Ecology and Disease Modeling

Organizers: Naveen Vaidya and Majid Bani-Yaghoub

1144 - Mathematical Modeling of Whole-Body Metabolism in Girls With Polycystic Ovarian Syndrome
1142 - Unveiling the Past: Separating the Effects of Genetic Drift and Natural Selection Using a Modification of Tajima's D Statistic
1140 - Delayed HIV Rebound After Cessation Of Treatment: Model Predictions
1145 - Modeling Transmission Dynamics of Avian Influenza under Periodic Environmental Conditions

317 BCH: Partial Differential Equations: Analysis, Modeling, and Applications

Organizer: John Singler

1152 - An Acoustic Eigenvalue Problem Related to Electrochemistry
1147 - Impacts of Allee Effect and Maturation Time Delay on Dynamics of a Nonlocal Delayed Reaction Diffusion Population Model
1148 - Split-Step Method for Nonlinear Schrodinger Equation

318 BCH: Recent Advances in Numerical Methods for Interface Problems

Organizer: Xu Zhang

1156 - A Rescaling Scheme and Its Applications in Moving Boundary Problems
1157 - Weak Galerkin Finite Element Methods and Numerical Applications
1155 - Residual-Based a Posteriori Error Estimate for Interface Problems: Nonconforming Linear Elements
1158 - Interface Problem Arising in Quantifying Mitral Regurgitation
1161 - Partially Penalized Immersed Finite Element Methods for Elliptic Interface Problems

Conference Schedule

Sunday – April 12, 2015

8:00 a.m.
Registration Desk Open
Coffee Station
BCH Atrium

8:30 a.m. – 10:10 a.m.
Parallel Sessions
Details below

10:10 a.m. – 10:30 a.m.
Refreshment Break
BCH Atrium

10:40 a.m. – 12:20 p.m.
Parallel Sessions
Details on right

12:30 p.m.
Meeting Adjourns

Parallel Sessions | 8:30 a.m. - 10:10 a.m.

Session Abstracts on pages 11-32

101 BCH: Discontinuous Galerkin Methods for Partial Differential Equations: Theory and Applications

Organizer: Mahboub Baccouch

1000 - An Immersed Discontinuous Galerkin Method for Acoustic Wave Propagation in Nonhomogeneous Media
1010 - A Linear Finite Element Procedure for the Naghdi Shell Model
1006 - Entropy Satisfying Numerical Methods for Fokker-Planck-type Equations
1007 - Alternating Evolution Discontinuous Galerkin Methods for Hamilton–Jacobi Equations

120 BCH: Advances in High-order Computational Methods

Organizer: Huiqing Zhu

1024 - Kansa's Method for 2D Simulation of Slow-Release Permanganate for Groundwater Remediation Vis Oxidation
1022 - A Fast Explicit Operator Splitting Method for a Multi-Scale Underground Oil Recovery Model
1023 - Positivity Preserving High-Order Local Discontinuous Galerkin Method for Parabolic Equations with Blow-Up Solutions

121 BCH: Infinite Dimensional Dynamical Systems: Analysis and Computation

Organizers: Yu-Min Chung, Erik Van Vleck and Andrew Steyer

1040 - On Computations of Inertial Manifolds—The Newton's Method and the BVP Formulation
1043 - Data Assimilation by Feedback Control and Kalman Filters
1045 - The Distinction of Turbulence from Chaos
1041 - On Certain High-Dimensional Models in Statistical Mechanics

124 BCH: Patterns in Complex Systems

Organizers: Iuliana Oprea and Patrick Shipman

1060 - How Defects are Born
1058 - Elasto-Capillary Systems and Capillary Origami
1063 - Self-Similarity and Fibonacci in Phyllotaxis
1062 - Complex Patterns in Anisotropic Fluids

125 BCH: Recent Advances in Finite Element Methods

Organizer: Xianping Li

1074 - A Multiscale Method for Optical Responses of Nano Structures
1067 - A Hybridizable Discontinuous Galerkin Method for the Incompressible Navier-Stokes Equations
1071 - The Dual-Wind Discontinuous Galerkin Method
1082 - A Novel Weak Galerkin Finite Element Scheme for the Brinkman Model

215 BCH: Contributed presentations in lecture format

1100 - A Second Order Periodic Boundary Value Problem with a Parameter and Vanishing Green's Functions
1094 - A Simple Pure Water Oscillator
1095 - On Positive Increasing Solutions of Emden-Fowler Dynamic Systems on Time Scales
1102 - A Distributed Optimal Control Problem Governed by Stokes Equations with an Energy-Norm-Constraint on the Velocity
1098 - From Period-1 Motions to Chaos in a Time-Delayed, Quadratic Nonlinear Oscillator

216 BCH: Interactions Among Analysis, Optimization and Network Science

Organizers: Nathan Albin and Pietro Poggi-Corradini

1115 - Modulus and Quasiconformality
1105 - The Dirichlet Problem with Prime End Boundary Data for Bounded Domains in Metric Spaces
1110 - Discretizations of Metric Measure Spaces of Controlled Geometry

314 BCH: Recent Advances in Numerical Methods for Fluid Flows

Organizer: Zhu Wang

1118 - Fast and Accurate Algorithms for Simulating Coarsening Dynamics of Cahn-Hilliard Equations
1121 - A CVOD Based Low-Dimensional Approximation to Nonlinear Stochastic Partial Differential Equations
1125 - Any Order Finite Volume Schemes Over Quadrilateral Meshes
1117a - Non-linear Flow Characteristics and Horizontal Well Pressure Transient Analysis for Low-permeability Oil Reservoirs

Conference Schedule
Sunday – April 12, 2015

Parallel Sessions | 10:40 a.m. – 12:20 p.m. *Session Abstracts on pages 11-32*

101 BCH: Matrix Computation and Applications

Organizer: Peizhen Zhu

1015 - Understanding the Optics to Aid Microscopy Image Segmentation
1014 - Rank Minimization and Semidefinite Programming
1013 - Applications and Perturbations of Quantum Walk
1012 - Tiled Krylov Expansion on Multicore Architectures
1016 - New Approaches to Compute Principal Angles Between Subspaces

120 BCH: Numerical Methods for System of Partial Differential Equations

Organizers: JaEun Ku, Abdul Q. M. Khaliq and Qin Sheng

1031 - Fast Structured Spectral Methods
1027 - Numerical Simulation of Coupled Burgers' Equation by Fourth-Order Compact ETD Schemes
1029 - Efficient Computation of Phase and Amplitude in Geometrical Optics
1028 - A New Hybrid Mixed Finite Element Method
1030 - An Analysis of Approximate Fourier-Series Solutions of Modified Stochastic Sine-Gordon Equations

121 BCH: Infinite Dimensional Dynamical Systems: Analysis and Computation

Organizers: Yu-Min Chung, Erik Van Vleck and Andrew Steyer

1042 - Geometric Phase in the Hopf Bundle and the Sability of Non-Linear Waves
1047 - Applications of Orthogonal Integration
1046 - Application of Lyapunov Exponents Theory to the Stability of Time-Stepping ODE Initial Value Problem Solvers
1044 - Finite Dimensionality of the Global Attractor of the Solutions to the 3D Primitive Equations with Viscosity

124 BCH: Patterns in Complex Systems

Organizers: Iuliana Oprea and Patrick Shipman

1057 - Positive Temperature Models of Quasicrystals
1065 - Existence of Pearled Patterns in the Planar Functionalized Cahn-Hilliard Equation
1059 - Highly Ordered Square Arrays of Nanoscale Pyramids Produced by Ion Bombardment of a Crystalline Binary Material
1061 - Topological Measures of Order in Nearly-Hexagonal Lattices
1064 - Self-Assembled Nanoscale Patterns Produced by Ion Bombardment of Binary Compounds

125 BCH: Recent Advances in Finite Element Methods

Organizer: Xianping Li

1066 - A High-Order Discontinuous Galerkin Method for Ito Stochastic Ordinary Differential Equations
1069 - The Fictitious Domain Method Based on Slip Boundary Condition For Simulation of Flow-Body Interaction
1070 - Numerical Performance of Reduction Numerical Methods for Single/Two-Phase Flow in Rough Grids and with Discontinuous Permeability
1068 - 3-D Immersed Finite Element Particle-in-Cell Methods for Modeling Laboratory Experiments of Lunar Plasma Environment
1073 - Anisotropic Mesh Adaptation for 3D Anisotropic Diffusion Problems

215 BCH: Contributed presentations in lecture format

1097 - An Effective High-Order Shock-Capturing Limiter for Discontinuous Galerkin Methods
1101 - Parametric Representation of Boundary Flux in Heterogeneous Potential Flow Problems
1093 - A Feasibility Analysis of Several Numerical Schemes for the Prediction of Two Phase Transient Flow in HTHP
1096 - High Accuracy Combination Method for Solving the Systems of Nonlinear Volterra Integral and Integro-Differential Equations with Weakly Singular Kernels of the Second Kind
1099 - Analytical Solutions of Periodic Motions in a Periodically Forced, Damped, Two-Degree-of-Freedom Oscillator with Nonlinear Spring

216 BCH: Interactions Among Analysis, Optimization and Network Science

Organizers: Nathan Albin and Pietro Poggi-Corradini

1108 - Preservation of Bounded Geometry Under Sphericalization and Flattening: Quasiconvexity and 8-Poincare Inequality
1107 - Inventory Accumulation and Quadrangulations of the Sphere
1109 - Pointwise Quasiminimality of Gibbs-Like Measures

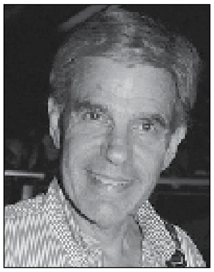
314 BCH: Modeling and Simulation of Turbulence/Hydrodynamics

Organizer: Lian Duan

1126 - Direct Numerical Simulation for Laminar-to-Turbulent Transition Prediction
1127 - Predicting Riblet Performance Using Anisotropy-Resolving Turbulence Models
1129 - New Developments in Fluid Experimental Techniques Provide Benchmark Data for Simulations
1128 - A Mixed Fluid-Kinetic Solver for the Vlasov-Poisson System
1130 - Acoustic Radiation from Tunnel-Wall Turbulent Boundary Layers

Conference Plenary Speakers

Saturday, April 11, 2015 | 125 Butler Carlton Hall (BCH)



Mark J. Ablowitz
University of Colorado
8:30 a.m. - 9:20 a.m.

The Nonlinear Waves—Always Intriguing

The study of nonlinear waves is filled with remarkable discoveries, one of them being `solitons.' Some history, background, and applications in water waves and nonlinear optics, specifically `optical graphene,' will be discussed.

Susanne Brenner
Louisiana State University
9:20 a.m. - 10:05 a.m.

Finite Element Methods for Fourth Order Elliptic Variational Inequalities

Fourth order elliptic variational inequalities appear in obstacle problems for Kirchhoff plates and optimal control problems constrained by second order elliptic partial differential equations. The numerical analysis of these variational inequalities is more challenging than the analysis in the second order case because the complementarity forms of fourth order variational inequalities only exist in a weak sense. In this talk we will present a new approach to the analysis of finite element methods for fourth order elliptic variational inequalities that are applicable to C1 finite element methods, classical nonconforming finite element methods, and discontinuous Galerkin methods.

Arnd Scheel
University of Minnesota
2:00 p.m. - 2:45 p.m.

Coherent Structures in Nonlocal Equations

I'll present recent work on pulses and fronts in systems with nonlocal coupling. I'll first discuss pinning and unpinning of fronts. Near the Maxwell point, that is, when potential energies of the asymptotic equilibria are close, interfaces are often discontinuous and cannot propagate: they are pinned. I'll describe results that characterize pinning regions in parameter space and and show that speeds obey an unusual but universal mu^3/2 asymptotic which is different from conventional mu^1/2 asymptotics in discrete systems. I'll also give some motivation and speculation how speed asymptotics may depend in a universal fashion on kernel regularity properties.

In the second part of the talk, I'll explore some of the techniques involved in the study of such traveling wave problems. In particular, I'll explain how ``spatial dynamics'' can be ``translated'' to traveling-wave problems that cannot be cast as differential equations in a spatial variable. As an application, I'll describe the construction of an excitation pulse in a nonlocal FitzHugh-Nagumo equation.

Junping Wang
National Science Foundation
2:50 p.m. - 3:35 p.m.

Weak Galerkin Finite Element Methods for PDEs

This talk shall introduce a new numerical technique, called weak Galerkin finite element method (WG), for partial differential equations. The presentation will start with the second order elliptic equation, for which WG shall be applied and explained in detail. In particular, the concept of weak gradient will be introduced and discussed for its role in the design of weak Galerkin finite element schemes. The speaker will then introduce a general notion of weak differential operators, such as weak Hessian, weak divergence, and weak curl etc. These weak differential operators shall serve as building blocks for WG finite element methods for other class of partial differential equations, such as the Stokes equation, the biharmonic equation, the Maxwell equations in electron magnetics theory, and div-curl systems. The speaker will demonstrate how WG can be applied to each of the applications, with a discussion on the main features. Furthermore, a mathematical convergence theory shall be briefly given for some applications. The talk should be accessible to graduate students with adequate training in computational methods.

Sessions in 101 BCH

Discontinuous Galerkin Methods for Partial Differential Equations: Theory and Applications

1000 - An Immersed Discontinuous Galerkin Method for Acoustic Wave Propagation in Nonhomogeneous Media

Slimane Adjerid, Virginia Tech

We present an immersed discontinuous Galerkin method for the acoustic interface problem on Cartesian meshes. The method allows elements to be cut by the interface which are equipped with specially constructed piecewise polynomial spaces. We discuss the properties of such immersed finite element spaces and their approximation capability. We solve several acoustic interface problems and show errors and solutions. The proposed method leads to optimal orders of convergence and may be extended to higher degree polynomials and to moving interfaces.

1001 - Recovery-Based Error Estimators for the DG Method for Scalar Conservation Laws

Mahboub Baccouch, University of Nebraska at Omaha

In this talk, we present and analyze robust recovery-based error estimators for the original discontinuous Galerkin (DG) method for linear and nonlinear scalar conservation laws in one and two space dimensions. The proposed error estimators of the recovery-type are easy to implement, computationally simple, asymptotically exact, and are useful in adaptive computations. We prove several optimal L^2 error estimates and superconvergence results. We also provide a very simple derivative recovery formula which gives a superconvergent approximation to the directional derivative. The element-by-element postprocessing of the derivative in the direction of the flow is shown to converge under mesh refinement with order p+1, when piecewise polynomials of degree at most p are used We use these results to prove that the a posteriori DG error estimates at a fixed time converge to the true errors in the L^2-norm under mesh refinement. The order of convergence is proved to be p+1. Finally, we prove that the global effectivity index converges to unity at O(h) rate. Several numerical examples are provided to support our theoretical results and to show the effectiveness of our recovery-based error estimates.

1002 - On a Class of Nonlocal Wave Equations from Applications

Fatih Celiker, Wayne State University

We study equations from the area of peridynamics, which is an extension of elasticity. The governing equations form a system of nonlocal wave equations. Its governing operator is found to be a bounded, linear and self-adjoint operator on a Hilbert space. We study the well-posedness and stability of the associated initial value problem. We solve the initial value problem by applying the functional calculus of the governing operator. In addition, we give a series representation of the solution in terms of spherical Bessel functions. For the case of scalar valued functions, the governing operator turns out as functions of the Laplace operator. This result enables the comparison of peridynamic solutions to those of classical elasticity as well as the introduction of local boundary conditions into the nonlocal theory. The latter is studied in a companion paper.

1003 - A Discontinuous Galerkin Approximation for Photonic Crystals

Aycil Cesmelioglu, Oakland University

Modeling of photonic crystals are done by Maxwell's equations with periodic electric permittivity. Bloch/Floquet Theory for periodic differential operators reduces the problem to a modified Maxwell cavity eigenproblem with periodic boundary conditions on a fundamental cell. We discretize this eigenvalue problem using an interior penalty discontinuous Galerkin method on tetrahedral meshes. Spectral properties of the underlying discrete operator will be discussed.

1004 - HDG Methods For Diffusion: Superconvergence by M-decompositions

Guosheng Fu, University of Minnesota

We introduce the concept of an M-decomposition and show how to use it to systematically construct hybridizable discontinuous Galerkin and mixed methods for steady-state diffusion methods with superconvergence properties on unstructured meshes.

1005 - Schwarz Methods for Discontinuous Galerkin Approximations of Elliptic Problems.

Ohannes Karakashian, University of Tennessee

We consider overlapping and non overlapping Schwarz methods for the solution of the linear systems resulting from interior penalty discontinuous Galerkin discretizations of second and fourth order elliptic problems. We focus on the dependence of the condition numbers of the preconditioned systems on the penalty parameter and give an analytical and experimental study of this dependence.

1006 - Entropy Satisfying Numerical Methods for Fokker-Planck-type Equations

Hailiang Liu, Iowa State University

Kinetic Fokker-Planck equations arise in many applications, and thus there has been considerable interest in the development of accurate numerical methods to solve them. The peculiar feature of these models is that the transient solution converges to certain equilibrium when time becomes large. For the numerical method to capture the long-time pattern of the underlying solution, some entropy satisfying methods have been designed to preserve the entropy dissipation law at the discrete level. I shall explain the main ideas and challenges through several model equations in different applications. Numerical results are reported to illustrate the capacity of the proposed algorithms.

1007 - Alternating Evolution Discontinuous Galerkin Methods for Hamilton–Jacobi Equations

Michael Pollack, Iowa State University

We propose a high resolution Alternating Evolution Discontinuous Galerkin (AEDG) method to solve Hamilton-Jacobi equations. The construction of the AEDG is based on an alternating evolution system of the Hamilton-Jacobi equation, following the previous work of H. Liu, M. Pollack and H. Saran on AE schemes for Hamilton-Jacobi equations. A semi-discrete AEDG derives directly from a sampling of this system on alternating cells. Higher order accuracy is achieved by a combination of high-order polynomial approximation in each cell and a time discretization with matching accuracy. The AEDG methods have the advantage of easy formulation and implementation, and efficient computation of the solution. For the linear equation, we prove the L^2 stability of the method. Numerical experiments for a set of Hamilton-Jacobi equations are presented to demonstrate both accuracy and capacity of these AEDG schemes.

1008 - High Order Maximum Principle Preserving Discontinuous Galerkin Method for Convection-Diffusion Equations

Zhengfu Xu, Michigan Technological University

We will discuss the generalization of the parametrized maximum-principle-preserving

(MPP) flux limiter to the discontinuous Galerkin (DG) method for solving the convection-diffusion equations. The feasibility of applying the proposed MPP flux limiters is based on the fact that cell averages of the DG solutions are updated in a conservative fashion (by using flux difference). The parametrized MPP flux limiter can be applied to DG methods of arbitrary high order. We will address the accuracy issue for scalar one-dimensional problems. Numerical evidence will be presented to show that the proposed MPP flux limiter method does not adversely affect the desired high order accuracy, nor does it require restrictive time steps. Numerical experiments including those for incompressible flow examples will be shown to demonstrate the effectiveness of the MPP flux limiters.

1009 - Superconvergence of Discontinuous Galerkin Methods for 2D Linear Hyperbolic Equations

Yang Yang, Michigan Technological University

We study the superconvergence properties of discontinuous Galerkin (DG) methods for 2-D linear hyperbolic conservation laws over rectangular meshes with upwind fluxes. We prove, under some suitable initial and boundary discretizations, the 2k+1th superconvergence rate of the DG approximation at the downwind points and for the cell average. Moreover, we prove that the gradient of the DG solution is superconvergent with a rate k+1 at all interior left Radau points; and the function value approximation is superconvergent at all right Radau points, with a convergence rate k+2. All theoretical findings are confirmed by numerical experiments.

1010 - A Linear Finite Element Procedure for the Naghdi Shell Model

Sheng Zhang, Wayne State University

A shell deformation could be bending dominated, membrane/shear dominated, or intermediate. We prove the accuracy of a mixed finite element method for bending dominated shells in which a major part of the membrane/shear strain is reduced, to free up membrane/shear locking. When no part of the membrane/shear strain is reduced, the method becomes a consistent discontinuous Galerkin method that is proven accurate for membrane/shear dominated shells and intermediate shells. The two methods can be coded in a single program by using a parameter. We propose a procedure of numerically detecting the asymptotic behavior of a shell, choosing the parameter value in the method, and producing accurate approximation for a given shell problem. The method uses piecewise linear functions to approximate all the variables. The analysis is carried out for shells whose middle surfaces have the most general geometries, which shows that the method has the optimal order of accuracy for general shells and the accuracy is robust with respect to the shell thickness. In the particular case that the geometrical coefficients of the shell middle surface are piecewise constants the accuracy is uniform with respect to the shell thickness.

1011 - A Curved Boundary Treatment for Discontinuous Galerkin Schemes Solving Time Dependent Problems

Xiangxiong Zhang, Purdue University

For problems defined in a two-dimensional domain with boundary conditions specified on a curve, we consider discontinuous Galerkin (DG) schemes with high order polynomial basis functions on a geometry fitting triangular mesh. It is well known that directly imposing the given boundary conditions on a piece-wise segment approximation boundary will render any finite element method to be at most second order accurate. Unless the boundary conditions can be accurately transferred, in general curvilinear element method should be used to obtain the high order accuracy. We discuss a simple boundary treatment for DG schemes defined on triangles adjacent to the curve. Even though integration along the curve is still necessary, integrals over any curved element are avoided. If the domain is convex, or if it is nonconvex and the true solutions can be smoothly extended to the exterior, the modified DG scheme is high order accurate.

Matrix Computation and Applications

1012 - Tiled Krylov Expansion on Multicore Architectures

Henricus Bouwmeester, University of Colorado Denver

We examine non-symmetric matrix eigenvalue problems in the context of HPC via tilde algorithms and the implementation of block Arnoldi expansion in the context of multicore. Pseudocodes of the extension of LAPACK routines into the framework of PLASMA and implementation details are provided along with performance results.

1013 - Applications and Perturbations of Quantum Walk

Chen-Fu Chiang, University of Central Missouri

The hitting time is the required minimum time for a Markov chain-based walk (classical or quantum) to reach a target state in the state space. We investigate the effect of the perturbation on the hitting time of a quantum walk. Quantum walk is the quantum version of random walk that provides speed-up in comparison to its classical counterpart. We obtain an upper bound for the perturbed quantum walk hitting time by applying Szegedy's work and the perturbation bounds with Weyl's perturbation theorem on classical matrix. We further compute the delayed perturbed hitting time and delayed perturbed quantum hitting time (DPQHT). We show that the upper bound for DPQHT is bounded from above by the difference between the square root of the upper bound for a perturbed random walk and the square root of the lower bound for a random walk.

1014 - Rank Minimization and Semidefinite Programming

Fritz Keinert, Iowa State University

A rank minimization problem tries to find the matrix of lowest rank that satisfies some constraints. For example, some of the entries may be known. If the constraints are linear, this can be converted to a semidefinite program, a generalization of a linear program. I will give an overview of some connections between compressed sensing and rank minimization, and between algorithms for linear programming and semidefinite programming.

1015 - Understanding the Optics to Aid Microscopy Image Segmentation

Zhaozheng Yin, Missouri University of Science & Technology

Image segmentation is essential for many automated microscopy image analysis systems. Rather than treating microscopy images as general natural images and rushing into the image processing warehouse for solutions, we propose to study a microscope's optical properties to model its image formation process first, using phase contrast microscopy as an exemplar. It turns out that the phase contrast imaging system can be relatively well explained by a linear imaging model. Using this model, we formulate a quadratic optimization function with sparseness and smoothness regularizations to restore the authentic phase contrast image that directly corresponds to specimen's optical path length without phase contrast artifacts such as halo and shade-off. With artifacts removed, high quality segmentation can be achieved by simply thresholding the restored image.

1016 - New Approaches to Compute Principal Angles Between Subspaces

Peizhen Zhu, Missouri University of Science & Technology

Computing principal angles between subspaces (PABS) is one of the basic important problems in numerical linear algebra. Classical numerical methods for computing the PABS are currently based on their cosines and/or sines. Cosine-based algorithms in principle cannot provide accurate results for small angles. For the same reason sine-based algorithms are in accurate for computing large angles. Combined cosine-sine based algorithms, where small and large angles are computed separately, are being used to cure this problem. However, such algorithms are complicated, costly, and introduce inaccuracies for the computation of the principal vectors corresponding to PABS in the neighborhood of the threshold between the small and large angles. To overcome these problems, we developed new algorithms using the sines of half-PABS through different approaches: algebraic approaches and geometric approaches. New algorithms provide accurate results for all PABS in one sweep and can be implemented simply and efficiently. Furthermore, we generalize our algorithms to compute the principal angles and the principal vectors in an A-based scalar product as well. Perturbation analysis for the sines of half-PABS supports our algorithms.

Sessions in 120 BCH

Advances in High-order Computational Methods

1017 - Incorporating Local Boundary Conditions Into Nonlocal Theories

Fatih Celiker, Wayne State University

We study nonlocal equations from the area of peridynamics on bounded domains. In our companion paper, we discover that, on $\mathbb{R}^n$, the governing operator in peridynamics, which involves a convolution, is a bounded function of the classical (local) governing operator. Building on this, we define an abstract convolution operator on bounded domains which is a generalization of the standard convolution based on integrals. The abstract convolution operator is a function of the classical operator, defined by a Hilbert basis available due to the purely discrete spectrum of the latter. As governing operator of the nonlocal equation we use a function of the classical operator, this allows us to incorporate local boundary conditions into nonlocal theories. We present a numerical study of the solutions of the wave equation. For discretization, we employ a weak formulation based on a Galerkin projection and use piecewise polynomials on each element which allows discontinuities of the approximate solution at the element borders. We study convergence order of solutions with respect to polynomial order and observe optimal convergence. We depict the solutions for each boundary condition.

1018 - Solution of Nonlinear Time-Dependent PDE Through Componentwise Approximation of Matrix Functions

James Lambers, The University of Southern Mississippi

Exponential propagation iterative (EPI) methods provide an efficient approach to the solution of large stiff systems of ODE, compared to standard integrators. However, the bulk of the computational effort in these methods is due to products of matrix functions and vectors, which can become very costly at high resolution due to an increase in the number of Krylov projection steps needed to maintain accuracy. In this paper, it is proposed to modify EPI methods by using Krylov subspace spectral (KSS) methods, instead of standard Krylov projection methods, to compute products of matrix functions and vectors. Numerical experiments demonstrate that this modification causes the number of Krylov projection steps to become bounded independently of the grid size, thus dramatically improving efficiency and scalability.

1019 - A Balanced FEM for a System of Singularly Perturbed Reaction-Diffusion Two-Point Boundary Value Problems

Runchang Lin, Texas A&M International University

A system of linear coupled reaction-diffusion equations is considered, where each equation is a two-point boundary value problem and all equations share the same small diffusion coefficient. A finite element method using piecewise quadratic splines that are globally C^1 is introduced; its novelty lies in the norm associated with the method, which is stronger than the usual energy norm and is balanced, i.e., each term in the norm is $O(1)$ when the norm is applied to the true solution of the system. On a standard Shishkin mesh with N subintervals, it is shown that the method is $O(N^{-1}\ln N)$ accurate in the balanced norm. Numerical results to illustrate this result are presented.

1020 - Multiscale Hybridizable DG Methods for Flows in Heterogeneous Media

Ke Shi, Texas A&M University

In this talk, we will briefly discuss multiscale problems and review some classical multiscale finite element methods for these problems. Then we present a general framework on coupling the hybridization technique with multiscale finite element approach. Several numerical examples will be presented in the end.

1020a - Numerical Smoothness and Optimal –Optimal Error Analysis for Time-Dependent PDEs

Tong Sun, Bowling Green State University

Numerical smoothness is a concept parallel to numerical stability. It means the smoothness properties of numerical solutions. Traditional a priori error analysis uses the smoothness of PDE solutions and the stability of the numerical schemes to estimate error. However, as a new approach, one can also use the smoothness of numerical solutions and the error propagation of PDEs to do error estimation. Moreover, the new approach is better in the sense that it can deliver both optimal convergence rate and optimal error propagation. In this talk, a sequence of error analysis results on nonlinear conservation laws solved with RKDG and WENO schemes will be presented to demonstrate the advantages of the numerical smoothness approach. It will also cover the necessity of numerical smoothness in order to achieve optimal convergence rate.

1021 - A Riemann-Solver Free Spacetime Discontinuous Galerkin Method for General Conservation Laws

Shuang Tu, Jackson State University

A Riemann-solver-free spacetime discontinuous Galerkin method has been developed for general conservation laws. The method integrates the best features of the spacetime Conservation Element/ Solution Element (CE/SE) method and the discontinuous Galerkin (DG) method. The core idea is to construct a staggered spacetime mesh through alternate cell-centered CEs and vertex-centered CEs within each time step. Inside each SE, the solution is approximated using high-order spacetime DG basis polynomials. The spacetime flux conservation is enforced inside each CE using the DG concept. The unknowns are stored at both vertices and cell centroids of the spatial mesh. However, the solutions at vertices and cell centroids are updated at different time levels within each time step in an alternate fashion. Thanks to the staggered spacetime formulation, there is no left and right states for the solution at the spacetime interface. Instead, the solution available to evaluate the flux is continuous across the interface. Therefore, no (approximate) Riemann solvers are needed to provide a unique numerical flux. The current method can be used to solve arbitrary conservation laws including the compressible Euler equations, shallow water equations and magnetohydrodynamics (MHD) equations without the need of any form of Riemann solvers. A set of benchmark problems of various conservation laws are presented to demonstrate the accuracy of the method.

Session Abstracts | 120 BCH

1022 - A Fast Explicit Operator Splitting Method for a Multi-Scale Underground Oil Recovery Model
Ying Wang, University of Oklahoma

In this talk, we propose a fast splitting method to solve a Multi-scale underground oil recovery model which includes a third order mixed derivatives term resulting from the dynamic effects in the pressure difference between the two phases. The method splits the original equation into two equations, one with flux term and one with diffusion term so that the classical numerical methods can be applied immediately. Two different spatial discretizations, second-order Godunov-type central-upwind scheme and WENO5 scheme, are used to demonstrate that higher order method provides more accurate approximation of solutions. The various numerical examples in both one and two dimensions show that the solutions may have many different saturation profiles depending on the initial conditions, diffusion parameter, and the third-order mixed derivatives parameter. The results are consistant with the study of traveling wave solutions and their bifurcation diagram. This is joint work with C.-Y. Kao, A. Kurganov, Z.-L. Qu.

1023 - Positivity Preserving High-Order Local Discontinuous Galerkin Method for Parabolic Equations with Blow-Up Solutions
Yang Yang, Michigan Technological University

We apply positivity-preserving local discontinuous Galerkin (LDG) methods to solve parabolic equations with blow-up solutions. This model is commonly used in combustion problems. However, previous numerical methods are mainly based on a second order finite difference method. This is because the positivity-preserving property can hardly be satisfied for high-order ones, leading to incorrect blow-up time and blow-up sets. In this work, we will apply the LDG method and construct special limiters to keep the positivity of the numerical approximations. Due to the Dirichlet boundary conditions, we have to modify the numerical fluxes and the limiters used in the schemes. Numerical experiments demonstrate that our schemes can capture the blow-up sets, and high-order approximations yield better numerical blow-up time.

1024 - Kansa's Method for 2D Simulation of Slow-Release Permanganate for Groundwater Remediation Vis Oxidation
Guangming Yao, Clarkson University

In Situ Chemical Oxidation (ISCO) with permanganate (MnO_4) has been applied to treat contaminated aquifers. Once injected, the MnO_4 is transported through the aquifer by ambient or induced groundwater flow. Installation of injection points or wells is one of the major capital costs associated with the process. An ISCO diffusion-transport reaction model was developed. The reaction between MnO_4 and a single contaminant is simulated by a coupled system of PDEs in two-dimensional space. Kansa's method is used to simulate different spatial arrangements of the injection points when planning an MnO_4 injection system. The numerical results are consistent with those from the finite difference method. Furthermore, Kansa's method is a complete meshless method which is easy to implement, and works well on a complicated domain with multiple injection points. We can easily extend the Kansa's method to a more realistic model in the future to design an optimal installation of injection points or wells.

1025 - Solving the Yang-Baxter-like Matrix Equation
Chenhua Zhang, University of Southern Mississippi

We give an overview of our research on solving the homogeneous quadratic matrix equation AXA = XAX, called the Yang-Baxter-like matrix equation, for commuting solutions. We hope to attract the attention of linear algebraists to find all solutions of this challenging matrix equation.

1026 - A Hybridizable Discontinuous Galerkin Method for PDE Constrained Optimal Control Problems
Huiqing Zhu, University of Southern Mississippi

In this talk we present error estimates for the discretization of optimal control problems governed by linear diffusion equations and convection-diffusion equations using the hybridizable discontinuous Galerkin method (HDG). Numerical results will also be presented.

Numerical Methods for System of Partial Differential Equations

1027 - Numerical Simulation of Coupled Burgers' Equation by Fourth-Order Compact ETD Schemes
Harish Bhatt, Middle Tennessee State University

This paper introduces two modified higher-order exponential time differencing Runge-Kutta (ETDRK) schemes in combination with a global fourth-order compact finite difference scheme (in space) for direct integration of coupled viscous Burgers' equations. One of them is the modification of the Cox and Matthews fourth-order ETDRK scheme and another one is the modification of Krogstad fourth-order ETDRK scheme. In these schemes, we do not use Hope-Cole transformation or any linearization techniques to handle nonlinearity. For an efficient implementation of the proposed schemes, we have utilized a partial fraction splitting technique in which we just required to solve several backward Euler-type linear systems at each time step. The stability of the schemes is analyzed and the order of convergence of the schemes is examined empirically. Several numerical experiments are carried out in order to demonstrate the performance and adaptability of the proposed schemes. The numerical experiments show that the present schemes provide better accuracy in comparison with those which are already available in the literature.

1028 - A New Hybrid Mixed Finite Element Method
JaEun Ku, Oklahoma State University

A new hybrid mixed finite element method to compute the flux variable accurately and efficiently will be introduced. The method is a two–-step method, based on a system of first-order equations for second-order elliptic partial differential equations. On a coarse mesh, the primary variable is approximated by a standard Galerkin method. Then, on a fine mesh, an H(div) projection is sought as an accurate approximation for the flux variable. The computation on a finer mesh can be carried out very efficiently using well developed preconditioners for the H(div) projection. Also, it will be shown that the mesh size h for the finer mesh can be taken as the square of the coarse mesh size H, or a higher order power with a proper choice of parameter. This means that the computational cost for the coarse-grid solution is negligible compared to that for the fine-grid solution. This is a joint work with Dr. Young Ju Lee and Dr. Dongwoo Sheen.

1029 - Efficient Computation of Phase and Amplitude in Geometrical Optics
Songting Luo, Iowa State University

In geometrical optics approximations to Helmholtz equation, the phase and amplitude must be computed with high accuracy to build reliable waves, which is challenging due to presence of source singularities. We present an efficient factorization approach to resolve this issue. Numerical methods and examples will be presented.

1030 - An Analysis of Approximate Fourier-Series Solutions of Modified Stochastic Sine-Gordon Equations

Henri Schurz, Southern Illinois University

An analysis of the modified stochastic Sine-Gordon equation with homogeneous boundary conditions on the one-dimensional domain [0,l], where l>0 is the length of the vibrating beam, with parameters delta >= 0 as the magnitude parameter of non-linearity, alpha>0 the damping parameter, and sigma > 0 the diffusion intensity. We analyze the properties of the approximate solution u of this SPDE by the eigenfunction approach allowing us to truncate the infinite-dimensional stochastic system (i.e., the SDEs of Fourier coefficients related to the SPDE), to control its energy, existence, uniqueness, continuity and stability of approximate solutions on an appropriate Hilbert space H. The driving noise is supposed to be state-dependent, Q-regular and of sublinear growth. The standard Sine-Gordon source term sin(u) is modified to incorporate a non-global Lipschitz-continuous source term sin(||u||^gamma). Our analysis relies on the investigation of expected Lyapunov-type functional related to the energy in terms of all system-parameters. By this approach we are able to justify both well-posedness and possible adequate simulations of the model with respect to all system-parameters. This is joint work with Abdallah Talafha.

1031 - Fast Structured Spectral Methods

Yingwei Wang, Purdue University

Spectral methods have been used extensively in numerical approximation of partial differential equations due to their bigger accuracy when compared to Finite Differences (FD) and Finite Elements (FE) methods. However, FD and FE usually lead to a sparse linear system while spectral methods often suffer from the huge computational complexity caused by dense matrices. Fortunately, although the matrices arising from spectral methods are dense, they enjoy a hidden nice property, named low-rank structure, i.e. their off-diagonal blocks have small numerical ranks for a given tolerance which is nearly bounded or grows slowly with the sizes of matrices. This property could be exploited to dramatically reduce the computational cost and give birth to direct spectral solvers with nearly optimal complexity and memory, thanks to the hierarchically semiseparable (HSS) representation for structured matrices. The Fast Structured Spectral Methods presented here include fast structured Jacobi transforms, fast structured spectral Galerkin methods for differential equations with variable coefficients, and fast structured spectral collocation methods. Our methods are very attractive for spectral approximations of problems with variable coefficients, especially when the coefficients have steep gradients and/or large variations or are degenerate, and when only matrix-vector products are available.

Sessions in 121 BCH

Algorithms and Analysis for Efficient Simulation of Wave Propagation Models

1032 - Suitable Transmission Conditions for Domain Decomposition Algorithms in the Case of the Helmholtz Equation

Yassine Boubendir, New Jersey Institute of Technology

Our presentation is concerned with the recently proposed non-overlapping domain decomposition algorithm for the Helmholtz equation based on the use of Pade approximants, and whose effective convergence is quasi-optimal. This algorithm combined appropriate choice of transmission conditions with a suitable approximation of the Dirichlet to Neumann operator. In this talk, we proposed to modify this approach in order to reduce the CPU time of the iterative procedure.

1033 - A Class of Staggered-Grid Algorithms and Analysis for Simulation of Time-Domain Maxwell Systems

Alexander Charlesworth, Colorado School of Mines

We consider efficient simulation of time-domain Maxwell systems using a class of finite difference methods in the case of heterogenous, conductive, nondispersive, isotropic, and linear media. These algorithms are based on staggered grids using second-order in time and various low- and high-order approximations in two dimensional space. Unlike standard finite difference methods, for time-domain electromagnetic simulations, staggered grid finite-difference computer models account for various physical behaviors associated with the continuous Maxwell model. A key advantage of the time-domain finite-difference (TDFD) methods is in its simplicity to simulate propagation or scattering Maxwell models. However, standard low-order TDFD methods suffer from large dispersion errors, and hence, it is important to develop high-order FDTD methods with low dispersion errors. We develop dispersion analysis based FDTD computer models and compare results obtained using a (2,2) and a low-dispersion (2,4) scheme.

1034 - High-Order Discretizations for 2D Helmholtz Boundary Layers on Smooth Boundaries

Victor Dominguez, Public University of Navarre

In this talk we present high order discretizations for the Helmholtz boundary layer operators on smooth closed curves. Our approach is based on using high order quadrature methods, combined with appropriate splitting of the kernels of the integral operators, which converge superalgebraically for smooth densities. Our discretizations are sufficiently accurate for providing good approximations even for compositions of different boundary operators (a priori, of different wave-number) as those appearing in regularized formulations in, for example, transmission problems. This is needed to ensure stability of the numerical schemes defined from these approximations. We prove stability and high order convergence in Sobolev norm which provide theoretical support to what has been observed in numerical experiments.

1035 - Sign-Definite Preconditioned Systems for Wave Propagation In Heterogeneous Media: Formulation, Analysis and High-Order FEM

Mahadevan Ganesh, Colorado School of Mines

Development of efficient algorithms to simulate sound wave propagation in heterogeneous media is important for several applications. Celebrated standard finite element method (FEM) algorithms for simulation of the wave model are based on the standard Galerkin variational formulation of the governing variable coefficient Helmholtz partial differential equation (PDE). Such widely used algorithms lead to sign-indefinite systems and hence the Helmholtz equation are termed in the literature as sign-indefinite. An active research area is on the development of efficient preconditioners for such indefinite systems and related solvers. In general sign-definite systems are preferred for efficient simulation using Krylov iterative solvers such as GMRES. In this work, we (i) develop and analyze a new sign-definite variational formulation of the Helmholtz wave propagation heterogeneous model; (ii) introduce and implement efficient high-order FEM approximations for the new formulation; and (iiii) develop novel preconditioners for iteratively solving such systems, with number of the associated GMRES iterations independent of the frequency of the problem. We simulate and demonstrate the sign-definite preconditioned for low to high frequency wave propagation in heterogeneous media with non-smooth, non-convex, and curved boundaries. (This is a joint work with PhD Charles Morgenstern, PhD student, Colorado School of Mines.)

1036 - A High-Order Coupled Isoparametric Finite Element and Spectral Method for Heterogeneous Media Wave Propagation

Charles Morgenstern, Colorado School of Mines

We consider a time-harmonic acoustic wave propagation partial differential equation (PDE) exterior to and interior of a bounded heterogeneous configuration. The model comprises the PDE, the Sommerfeld radiation condition (SRC), and an appropriate boundary condition based on properties of the bounded heterogeneous medium. Standard numerical approaches for simulating PDEs and reformulated boundary integral equations (BIEs) are finite element methods (FEMs) and spectral methods. FEMs for PDEs are well suited for bounded heterogeneous media, and for our model require appropriate artificial truncation of the unbounded region and approximation of the SRC. The BIE based discretizations do not require this artificial truncation, and the BIE ansatz for the exterior region exactly satisfies the SRC. However, BIEs are in general only practical for homogeneous media models. In this work we develop and implement a coupled high-order isoparametric FEM and spectral BIE discretization based computer model for the heterogenous media problem that exactly satisfies the SRC. The spectral BIE method is natural and efficient for high-order coupling in our model compared to coupling based on low-order boundary element methods. We demonstrate the approach and parallel performance for various two dimensional configurations. (This is a joint work with M. Ganesh.)

1037 - Time-domain BEM-FEM for Transient Acoustic Scattering

Francisco Sayas, University of Delaware

In this talk I will address some boundary-field formulations of transient scattering problems by a collection of obstacles with non-homogeneous obstacles immersed in a homogeneous fluid. I will show how the Finite-Boundari Element semidiscrete problem is well-posed and how to obtain error estimates. I will finally show show preliminary numerical examples using an implicit time-stepping method. This is joint work with Matthew Hassell.

1038 - Comparisons of Integral Equations Formulations for High-Frequency Two-Dimensional Helmholtz Transmission Problems in Domains With Corners

Catalin Turc, New Jersey Institute of Technology

We present comparisons between the performance of high-order Nystrom solvers based on various boundary integral formulations of transmission Helmholtz problems in Lipschitz domains in the high-frequency regime. The main formulations under considerations are: (1) the first kind formulation of Costabel and Stephan; (2) the second kind formulations of Kress and Roach; (3) the single integral formulation of Kleinman and Martin; (4) the Multiple Trace Formulation of Claeys, Jerez-Hanckes and Hiptmair; and (5) a direct regularized combined field formulation recently introduced by some of the authors. We also establish the well-posedness of some of the formulations above.

1039 - Imaging Underground Faults Using Displacement Measurements on Earth's Surface

Darko Volkov, Worcester Polytechnique Institute

In this talk we will discuss recent work on the inverse problem consisting of imaging faults and reconstructing slip fields. We use the equations of half space elasticity. We will first (briefly) show that if the slip zone can be approximated by a point source (which is the case during the nucleation phase of an earthquake), then we can compute relevant integrals involving the surface displacement fields to recover that point source. Next, we examine a case with field data. This case is particularly challenging since surface measurements are quite sparse and noisy. Traditionally, most studies first assume a profile for the geometry of the fault and then they determine the slip field on the fault. This is a linear inverse problem. Instead, we were able to solve the nonlinear problem consisting of simultaneously recovering the geometry of the fault and the slip field. We will explain how that was possible using adequate regularization of the forward problem and known physical bounds for faults, slip fields, and, surface displacements. We will show how, in the numerical search for a solution to this inverse problem, it is possible to take advantage of the fact that this problem is linear in the slip on the fault and nonlinear in the geometry of the fault. This is joint work with I. R. Ionescu, C. Voisin, and M. Campillo.

Infinite Dimensional Dynamical Systems: Analysis and Computation

1040 - On Computations of Inertial Manifolds—The Newton's Method and the BVP Formulation

Yu-Min Chung, College of William and Mary

We present recent progress on computing inertial manifolds. First, we show how to apply the Newton's method to this problem, prove convergence results, and illustrate numerically that the Newton's method is significantly more efficient than the existed methods in some cases. Second, we find that the problem of computing inertial manifolds can be viewed as a boundary value problem (BVP). Hence, implementing it becomes elementary in the way that classic methods for BVP can be used, such as shooting, finite difference, and collocation methods, and we demonstrate it by the MATLAB built-in BVP solver.

1041 - On Certain High-Dimensional Models in Statistical Mechanics

Alexander Grigo, University of Oklahoma

We will investigate the macroscopic description of gas-like systems of particles, which interact through binary collisions that conserve momentum and mass, but possibly dissipate energy. In this talk we will consider two possible approaches to obtain a macroscipic description of such gas-like systems: (a) kinetic approach using the Boltzmann equations, (b) a stochastic model that arises in in a certain scaling limit. Special emphasis will be put on the derivation of macroscopic fluid equations. Particular focus will be put on the geometric ideas behind these asymptotic methods, which could be used to reduce the complexity of other models with many degrees of freedom.

1042 - Geometric Phase in the Hopf Bundle and the Sability of Non-Linear Waves

Colin Grudzien, UNC

Building on the Evans function, we have proven a related, alternative form of analysis that uses the Hopf bundle to determine the stability of traveling waves. The total space of the Hopf bundle is S^{2n-1} and it is naturally embedded in $\mathbb{C}^n$. The dynamical system associated with the linearized operator for a PDE induces a winding number through parallel transport in the fibre, S^1. Our method uses parallel transport to count the multiplicity of eigenvalues for the linear operator associated to the wave.

1043 - Data Assimilation by Feedback Control and Kalman Filters
Michael Jolly, Indiana University

We present recent rigorous estimates for data assimilation via feedback control for dissipative systems. The relaxation of the solution to the feedback control system to a reference solution enables the evolution of a determining form, an ordinary differential equation in a space of trajectories. Every solution of the determining form evolves toward a steady state which is a trajectory on the global attractor of the original system. The determining form is employed to synchronize, i.e., remove noise from trajectories. Numerical computations compare the effectiveness of this approach is compared to the method of Kalman filters.

1044 - Finite Dimensionality of the Global Attractor of the Solutions to the 3D Primitive Equations with Viscosity
Ning Ju, Oklahoma State University

The system of 3D Primitive Equations with viscosity is a fundamental mathematical model in Geophysics for large scale fluid motion in atmosphere and ocean. Several years ago, the global existence of the strong solutions to the system was proved independently by Cao-Titi, Kobelkov and Kukavica-Ziane; the existence of the global attractor for the strong solutions was proved by the speaker. In this talk, some new results recently obtained under the cooperation of the speaker and Prof. Roger Temam on the finite dimensionality of the global attractor will be discussed.

1045 - The Distinction of Turbulence from Chaos
Charles Li, University of Missouri Columbia

We proposed a new theory on the physics of turbulence: When the Reynolds number is large, fully developed turbulence is caused by short term unpredictability due to rough dependence upon initial data. When the Reynolds number is moderate, (often) transient turbulence is caused by chaos (long term unpredictability). Numerical evidences support out theory.

1046 - Application of Lyapunov Exponents Theory to the Stability of Time-Stepping ODE Initial Value Problem Solvers
Andrew Steyer, University of Kansas

The most dynamically interesting solutions of differential equations are those that are time-dependent and non-periodic. For ODE initial value problems the solution is typically approximated using either a multistage (Runge-Kutta) or linear multistep method. The numerical stability of these methods is typically characterized by studying the linear stability domain of a method applied to a complex one dimensional time-independent linear test problem. In this talk we use a novel Lyapunov exponents based approach to justify characterizing the stability of Runge-Kutta and linear multistep methods applied to a class of time-dependent, linear, and exponentially decaying ODEs using a real one-dimensional linear time-dependent test problem. We then extend these results to class of nonlinear ODE initial value problems and apply our results to develop an algorithm for selecting step-size using both stability and accuracy.

1047 - Applications of Orthogonal Integration
Erik Van Vleck, University of Kansas

In this talk we survey recent developments that make use of time dependent orthogonal change of variables. This provides a robust moving coordinate system that orders growth and decay in time dependent linear differential equations. Among the application considered are the approximation of Lyapunov exponents and Sacker-Sell spectrum, non-autonomous inertial manifold reduction, time dependent stability of numerical time stepping techniques, and data assimilation.

Sessions in 124 BCH
Mathematical and Computational Issues in Big Data

1048 - Parallel Algorithm for Community Detection Using Multicore Architecture
Rahil Sharma, University of Iowa

One of the most relevant and widely studied structural property of networks is their community structure or clustering. Detecting communities is of great importance in various disciplines where systems are often represented as networks. Previously we designed a sequential bi-level community detection algorithm to identify functional modules of proteins in a PPI yeast network. For this data-set a sequential algorithm was sufficient, but most social and biological networks are very large. Tackling this volume of graph-structured data requires parallel multicore directives to achieve scalable algorithms. We present a multilevel community detection algorithm for multicore computers, which involves pre-processing, where each core computes the edge weights of a fraction of the total edges in the network G based on its topological features. After removing weak edges, we identify a node with high betweeness centrality, and use that to create a coarser graph instance, and recursively apply this idea to find a community. Then we remove this community and recursively apply this step until every node is assigned a community label. We present results showing quality and performance analysis on various bench mark data-sets and input requirements.

1049 - Matrix Optimization for Clustering
David Stewart, University of Iowa

An approach to clustering large datasets via matrix optimization is presented that is based on a formulation of Rao. The optimization problem is non-convex, and yet we present data showing fairly consistent clusterings. Algorithmic techniques are incorporated to make the method efficient for large datasets, which are presented.

1050 - Matrix Completion Algorithms and Recommender Systems
Cole Stiegler, University of Iowa

Many companies use recommender systems to encourage users to purchase further products. One formulation for doing this involves matrix completion: given a set of entries in a large matrix, we want to fill in the other entries under the assumption that the given values are from a low-rank matrix. We propose some algorithms and provide some numerical results for these computations based on convex duality and the nuclear matrix norm.

1051 - Randomized Algorithms in Machine Learning
Tianbao Yang, University of Iowa

In this talk, I will present my recent research work on randomized algorithms in machine learning. Compared to traditional algorithms, the use of randomization could bring us several benefits including (i) it often leads to faster algorithms that can scale to the large size of data; (ii) it can lead to simpler algorithms that are easier to analyze; (iii) it can lead implicitly to regularization and more robust output; and (iv) randomized algorithms can often be organized to exploit modern computational architectures better than traditional algorithms.

Session Abstracts | 124 BCH

Numerical Modeling of Complex Systems

1052 - A Matched Alternative Direction Implicit (ADI) Method for Solving 2D Parabolic Interface Problems

Chuan Li, University of Alabama

A novel Douglas alternating direction implicit (ADI) method was proposed by Dr. Shan Zhao in previous work to solve two-dimensional (2D) heat equations with interfaces by utilizing a novel tensor product decomposition to decouple 2D jump conditions into essentially 1D ones. When enforcing these 1D conditions in rigorous 1D Matched interface and boundary (MIB) schemes, the resulting matched ADI scheme achieves second order of accuracy in space and first order of accuracy in time for all tested 2D interface problems, and well maintains the efficiency of the ADI scheme. However, the proposed scheme is still far from its mature state. Our recent experiments showed that the proposed matched ADI scheme may fail to converge on complex geometries, and the direct application of the MIB spatial discretization with the Peaceman-Rachford ADI method becomes conditionally stable. This work continues the development of the matched ADI scheme with the improvements aiming at overcoming the known difficulties in the scheme and restoring the precious unconditional stability for solving parabolic interface problems on complex 2D geometries.

1053 - Numerical Modeling and Simulations of Interaction Between Dusty Disk and Embedded Proto-Planets

Shengtai Li, Los Alamos National Lab

We present a numerical method and simulation tool for interaction between dusty disk and embedded proto-planets. The disk mainly contains gas and dust and its motion is subject to 3D Navier-Stokes equations, which is solved by directional split Godunov method for the inviscid Euler equations plus operator-split method for the viscous source terms. A semi-Lagrangian method is implemented to remove the background Keplerian motion to alleviate the time step restriction in azimuthal direction. The planets are subject to the Newton's law and solved as an N-body problem. The coupling between the planets and disk is via gravitational force and their interaction is solved using operator-split method. A semi-Lagrangian adaptive mesh refinement is used to enhance the resolution near the planets.

1054 - MHD Simulation of Pellet Ablation In Tokamaks

Tianshi Lu, Wichita State University

We developed a free surface MHD model for the pellet ablation in tokamaks. The conservation laws with electromagnetic terms were solved using MUSCL solvers. We studied the interaction of the pellet ablation flow with the magnetic field. A surface ablation model, a kinetic model for the plasma electron heat flux, and an equation of state accounting for atomic processes in the ablation cloud were developed. Our study indicated that the magnetic field channelled the ablation flow into an extended plasma shield, significantly reducing the ablation rate and thus extending the penetration depth of the pellet. A cloud charging and rotation model was added more recently, and it has been demonstrated that the cloud rotation caused wider ablation channel and increased ablation rate. We also simulated the shrinking process of a tumbling pellet under the experimental parameter profile. When applied to a simplified setting, our code agreed with the prediction of the Neutral Gas Shielding model. However, due to the large density gradient near the pellet surface, the solution around the pellet had big error. To improve the solution we have used a more refined grid near the pellet and replaced the finite volume solver by the DG solver. With the new grid and solver, we studied the properties of the steady state solution and the convergence rate to the steady state solution. The results in 1D and 2D simulations are presented. We plan to use the new method to study striation instabilities in pellet ablation.

1055 - Phenomenological and First Principle Approaches for Micro, Meso and Macro Scales

Sheldon Wang, Midwestern State University (TX)

Concurrent or Hierarchical simulation for complex systems have been proposed and implemented for various material modeling problems. In this talk, we will review some of the successful modeling approaches for complex systems with micro, meso, and macro scales. In addition, we will discuss challenges and new approaches in the study of complex systems. An interesting comparison between the education models in Medical School and Engineering School will also be provided to shed some lights on the training of young professionals who will be tackling different complex systems.

1056 - A New RKDG Method with Conservation Constraint to Improve CFL Condition for Solving Conservation Laws

Zhiliang Xu, Notre Dame University

We present a new formulation of the Runge–Kutta discontinuous Galerkin (RKDG) method for solving conservation laws with increased CFL numbers. The new formulation requires the computed RKDG solution in a cell to satisfy additional conservation constraint in adjacent cells and does not increase the complexity or change the compactness of the RKDG method. Numerical computations for solving 1D and 2D scalar and systems of nonlinear hyperbolic conservation laws are performed with approximate solutions represented by piecewise quadratic and cubic polynomials, respectively. From both numerical experiments and the analytic estimate of the CFL number of the newly formulated method, we find that: 1) this new formulation improves the CFL number over the original RKDG formulation by at least three times or more and thus reduces the overall computational cost; and 2)the new formulation essentially does not compromise the resolution of the numerical solutions of shock wave problems compared with ones computed by the RKDG method.

Patterns in Complex Systems

1057 - Positive Temperature Models of Quasicrystals

David Aristoff, Colorado State University

Quasicrystals are solids with an unusual molecular structure, first discovered experimentally by Shechtman et al (1984), who showed that certain metal alloys have diffraction patterns with rotational symmetries that cannot occur for crystals. Before this discovery it had been believed that all solids in thermal equilibrium were crystalline. Levine and Steinhardt (1984) proposed that clusters of atoms with a particular shape could form the "building blocks" for these quasicrystals. They argued that quasicrystals could then be modeled by aperiodic tilings (first discovered by Berger, 1966): mathematical models of shapes that can tile the plane but only in a non-periodic (i.e., non-crystalline) fashion. This would be a model at zero temperature, since no defects are allowed in a (perfect) tiling. We consider models of quasicrystals at positive temperature, allowing for defects. Some of these models exhibit a first-order phase transition between ordered and disordered phases. The transition parallels the expected solid-liquid transition of crystal-forming materials in thermal equilibrium.

1058 - Elasto-Capillary Systems and Capillary Origami
Nicholas Brubaker, University of Arizona

Elasto-capillary interactions dominate the behavior of many natural systems and cause a wide range phenomena such as the ejection of fungal spores and the clustering of insect bristles. They also play an important role in understanding the morphology of many engineered systems and have led to a number of applications at the micrometer or nanometer scale. One application of particular interest is in the field of micro-scale fabrication, where it has been shown that the folding of a two-dimensional elastic sheet by action of surface tension, known as capillary origami, can produce three-dimensional structures. In this talk, we discuss recent work on modeling capillary origami and the predictions that can be made.

1059 - Highly Ordered Square Arrays of Nanoscale Pyramids Produced by Ion Bombardment of a Crystalline Binary Material
Bahaudin Hashmi, Colorado State University

When the planar surface of a binary material is bombarded with a broad ion beam, generally one of the two atomic species is preferentially sputtered, and, as a consequence a surface layer of altered composition develops. If the solid surface is not flat initially, the spatial variation of the surface height can lead to a surface composition that varies from point to point. Therefore, the dynamics of the surface height and composition are coupled. In this talk, we will study the nanoscale patterns formed when the (100) surface of a crystalline binary material is subjected to normal-incidence ion bombardment. As we will demonstrate, for certain ranges of the parameters, highly ordered square arrays of four-sided pyramids emerge.

1060 - How Defects are Born
Joceline Lega, University of Arizona

Pattern-forming systems typically exhibit defects, whose nature is associated with the symmetries of the pattern in which they appear; examples include dislocations of stripe patterns in systems invariant under translations, disclinations in stripe-forming systems invariant under rotations, and spiral defects of oscillatory patterns in systems invariant under time translations. Numerical simulations suggest that pairs of defects are created when the phase of the pattern ceases to be slaved to its amplitude. Such an event is typically mediated by the build up of large, localized, phase gradients. This talk will describe recent advances on a long-term project whose goal is to follow such a defect-forming mechanism in a system that is amenable to analysis. Specifically, we focus on the appearance of pairs of dislocations at the core of a grain boundary of the Swift-Hohenberg equation. Taking advantage of the variational nature of this system, we show that as the angle between the two stripe patterns on each side of the grain boundary is reduced, the phase of each pattern, as described by the Cross-Newell equation, develops large derivatives in a region of diminishing size. This is joint work with N. Ercolani and N. Kamburov.

1061 - Topological Measures of Order in Nearly-Hexagonal Lattices
Francis Motta, Duke University

Exploiting theory and methods from the field of computational topology, we introduce several quantities which characterize the degree of order in nearly-hexagonal, planar lattices.

1062 - Complex Patterns in Anisotropic Fluids
Iuliana Oprea, Colorado State University

Spatially extended systems driven far from equilibrium may exhibit spatiotemporal complex dynamics manifested through spatiotemporal chaos, intermittency, defects, phase turbulence, etc. We present a comprehensive theoretical framework for the classification and characterization of the spatiotemporal complex chaotic and intermittent dynamics in one of the most challenging pattern forming anisotropic systems, the electroconvection of nematic liquid crystals, based on Ginzburg Landau type amplitude equations.

1063 - Self-Similarity and Fibonacci in Phyllotaxis
Matthew Pennybacker, University of New Mexico

The phenomenon of phyllotaxis, which refers to the regular arrangements of organs such as leaves and petals on a plant, is a singularly impressive example of pattern formation in biological systems. I will discuss a model for phyllotaxis which arises from the biochemistry of plant growth and the remarkable self-similar properties that it possesses.

1064 - Self-Assembled Nanoscale Patterns Produced by Ion Bombardment of Binary Compounds
Patrick Shipman, Colorado State University

When a solid surface is bombarded with a broad ion beam, a plethora of self-assembled nanoscale patterns can emerge, including nanodots arranged in hexagonal arrays of remarkable regularity. We discuss a theory that explains the genesis of the strikingly regular hexagonal arrays of nanodots that can form when binary materials are bombarded at normal incidence. In our theory, the coupling between a surface layer of altered stoichiometry and the topography of the surface is the key to the observed pattern formation. Our theory also that predicts that remarkably defect-free ripples can be produced by oblique-incidence bombardment of a binary material if the ion species, energy and angle of incidence are appropriately chosen. This high degree of order cannot be achieved by bombarding an elemental material. Ion bombardment has the potential to become a cost-effective method to rapidly fabricate large-area nanostructures at length scales beyond the limits of conventional optical lithography. To realize this potentional, however, ways to limit the number of defects in the patterns must be developed. We analyze how a soft mode related to the mean sputter yield can facilitate defect formation and give rise to less ordered patterns.

1065 - Existence of Pearled Patterns in the Planar Functionalized Cahn-Hilliard Equation
Qiliang Wu, Michigan State University

The functionalized Cahn-Hilliard (FCH) equation supports planar and circular bilayer interfaces as equilibria which may lose their stability through the pearling bifurcation: a periodic, high-frequency, in-plane modulation of the bilayer thickness. In two spatial dimensions we employ spatial dynamics and a center manifold reduction to reduce the FCH equation to an 8th order ODE system. A normal form analysis and a fixed-point-theorem argument show that the reduced system admits a degenerate 1:1 resonant normal form, from which we deduce that the onset of the pearling bifurcation coincides with the creation of a two-parameter family of pearled equilibria which are periodic in the in-plane direction and exponentially localized in the transverse direction.

Sessions in 125 BCH

Recent Advances in Finite Element Methods

1066 - A High-Order Discontinuous Galerkin Method for Ito Stochastic Ordinary Differential Equations
Mahboub Baccouch, University of Nebraska at Omaha

In this talk, we present a high order discontinuous Galerkin (DG) method for strong solution of stochastic ordinary differential equations (SDEs) of the Ito type. Motivated by the DG method for deterministic ODEs, we first construct an approximate deterministic ordinary differential equation (ODE) with a random coefficient on each element using the well-known Wong-Zakai approximation theorem. The approximate ODE does not converge to the solution of the original SDE, but converges to the solution of the corresponding Stratonovich SDE. We apply a transformation to the drift term and consider a corrected Wong-Zakai approximation with shifted drift function. The resulting ODE converges to the solution of the original SDE and is discretized using the standard DG method for deterministic ODEs. Our DG method is demonstrated to be strongly convergent, accurate and computationally efficient. More precisely, numerical evidence demonstrate that our proposed DG scheme has a strong convergence order of p, when p-degree piecewise polynomials are used. Several linear and nonlinear test problems are presented to show the efficiency of the proposed method.

1067 - A Hybridizable Discontinuous Galerkin Method for the Incompressible Navier-Stokes Equations

Aycil Cesmelioglu, Oakland University

We present a hybridizable discontinuous Galerkin method to numerically solve the stationary incompressible Navier-Stokes equations. Piecewise polynomials of fixed degree k are used to approximate the velocity gradient, velocity and pressure. The method is well defined under a small data assumption and the global L2-norm of the error in each variable converges with an optimal order of k+1. In addition, we show that the approximate velocity converges with an order of k+2 which can be postprocessed to obtain an H(div)-conforming, divergence-free approximate velocity.

1068 - 3-D Immersed Finite Element Particle-in-Cell Methods for Modeling Laboratory Experiments of Lunar Plasma Environment

Daoru Han, University of Southern California

Understanding the plasma environment near the lunar surface is critical in both scientific and engineering perspectives. Numerical methods such as particle-in-cell (PIC) have been widely used to model such plasma problems. In this study, we use recently developed 3-D immersed finite element (IFE) PIC methods to simulate the plasma flow in a vacuum chamber to model ongoing laboratory investigations. The framework of IFE-PIC will be discussed and numerical results will be presented. Focuses will be given to the integration of a 3-D IFE solver into a standard PIC code to get both homogeneous and non-homogeneous IFE-PIC packages capable of modeling multiple plasma-object interaction problems. Numerical results will be presented to demonstrate the capability of the IFE-PIC methods.

1069 - The Fictitious Domain Method Based on Slip Boundary Condition For Simulation of Flow-Body Interaction

Qiaolin He, Sichuan University

The fictitious domain method is an effective method for simulating flow-body interaction. The method was developed by Glowinski for simulating the particulate flow with no slip boundary condition. In many applications, fluid slip at the solid surface becomes important. The generalization of the fictitious domain method to slip boundary condition is not trivial. As a step in this direction, we discuss a new least-square/fictitious domain method for Navier-Stokes problem with slip boundary conditions. The method is of the virtual control type and relies on a least-squares formulation making the problem solvable by a conjugate gradient algorithm operating in a well-chosen control space. Numerical results are presented. This is a joint work with R. Glowinski and XP Wang.

1070 - Numerical Performance of Reduction Numerical Methods for Single/Two-Phase Flow in Rough Grids and with Discontinuous Permeability

Jiangyong Hou, Xi'an Jiaotong University

In this presentation, we review some popular and recently developed “reduction” methods which are suitable for the single phase Darcy flow problem with full anisotropic and highly heterogeneous permeability on general triangular and quadrilateral grids, and find their application in two phase porous media flow problem. The methods reviewed are Multi-Point Flux Approximation (MPFA), Multi-Point Flux Mixed Finite Element (MFMFE) method, MFE with broken RT method, MPFA-type mimetic finite difference (MFD) method, and mixed-hybrid finite element (MHFE) method. The numerical experiments of these methods on different distorted meshes are compared, as well as their differences in performance of fluxes are discussed. The implementation of some of these methods in two phase porous media flow problem are discussed.

1071 - The Dual-Wind Discontinuous Galerkin Method

Thomas Lewis, The University of North Carolina at Greensboro

A new symmetric discontinuous Galerkin method for second order elliptic problems will be introduced. We show that the numerical method has a unique solution without the introduction of interior or boundary penalizations. Thus, the numerical method features a way to naturally enforce boundary conditions and address the issues associated with a fully discontinuous solution space. The key building block for the method will be the introduction of one-sided discrete derivative operators for piecewise weakly differentiable functions. Using both the up-wind gradient operator and the down-wind gradient operator, we formulate a new discontinuous Galerkin method that is symmetric when written in primal form. We will also summarize the convergence results as well as provide numerical test results that demonstrate the optimal convergence rates for the proposed numerical method.

1072 - Analysis and Approximation of the Dynamic Ginzburg-Landau Equations In Nonconvex Polygons Based on Hodge Decomposition

Buyang Li, Nanjing University

We prove well-posedness of time-dependent Ginzburg–Landau system in a nonconvex polygonal domain, and decompose the solution as a regular part plus a singular part. We see that the magnetic potential is not in H^1 in general, and the finite element method (FEM) may give incorrect solutions. To remedy this situation, we reformulate the equations into an equivalent system of elliptic and parabolic equations based on the Hodge decomposition, which avoids direct calculation of the magnetic potential. The essential unknowns of the reformulated system admit H^1 solutions and can be solved correctly by the FEMs. We then propose a decoupled and linearized FEM to solve the reformulated equations and present error estimates based on proved regularity of the solution. Numerical examples are provided to support our theoretical analysis and show the efficiency of the method.

1073 - Anisotropic Mesh Adaptation for 3D Anisotropic Diffusion Problems

Xianping Li, University of Missouri-Kansas City

Anisotropic diffusion problems arise from many fields of science and engineering. One of the challenge tasks for those problems is to avoid non-physical solutions or spurious oscillations in the numerical computations. A common approach is to design a proper discretization scheme and/or a proper mesh so that the numerical solution satisfies the discrete maximum principle (DMP). In this talk, the mesh adaptation strategies for three-dimensional anisotropic diffusion problems are presented. The results for 2D problems are extended to 3D problems and the conditions on mesh qualities such that numerical solutions satisfy DMP are developed. Some numerical examples are presented.

1074 - A Multiscale Method for Optical Responses of Nano Structures

Di (Richard) Liu, Michigan State University

We introduce a new framework for the multiphysical modeling and multiscale computation of nano-optical responses. The semi-classical theory treats the evolution of the electromagnetic field and the motion of the charged particles self-consistently by coupling Maxwell equations with Quantum Mechanics. To overcome the numerical challenge of solving high dimensional many body Schrodinger equations involved, we adopt the Time Dependent Current Density Functional Theory (TD-CDFT). In the regime of linear responses, this leads to a linear system of equations determining the electromagnetic field as well as current and electron densities simultaneously. A self-consistent multiscale method is proposed to deal with the well separated space scales. Numerical examples are presented to illustrate the resonant condition.

1075 - An Efficient Numerical Method for Acoustic Wave Scattering in Random Media

Cody Lorton, University of West Florida

Wave scattering in random media arises in many scientific and engineering fields including geoscience, materials science and medical science. Computing quantities of interest for the solutions of such wave problems, especially, in the high frequency case, poses a daunting computational challenge because of sheer amount of computations required to solve those problems. Due to their strong indefiniteness, highly oscillatory nature of solutions, and lack of efficient iterative solvers, standard numerical approaches such as brute force Monte Carlo methods and stochastic Galerkin methods are either too expensive to use or do not work well. In this talk we shall present a newly developed multi-resolution approach for the random Helmholtz problem with large wave numbers. In this approach the original random Helmholtz problem is reduced to a finite number of deterministic and non-homogeneous Helmholtz problems with random source terms, which are discretized by some unconditionally stable discontinuous Galerkin methods. An efficient solver with computational complexity of order O(3N3/2) is also proposed to solve the resulting algebraic problems. Convergence analysis and numerical experiments will be presented to demonstrate the potential advantages of the proposed numerical approach.

1076 - Banach Space Projections and Petrov-Galerkin Estimates

Ari Stern, Washington University in St. Louis

The Galerkin and Petrov-Galerkin methods provide the abstract, functional-analytic foundation for the analysis of the finite element method in numerical PDEs. In this talk, I will review these methods and some of the classical estimates, which can be described with few analytical prerequisites beyond the theory of Hilbert and Banach spaces. I will then discuss some recent work showing that one of these classical error estimates, due to Babuska (1971), can be sharpened by considering the relationship between Banach space geometry and projection operators.

1077 - Finite Element Methods for a Fourth Order Curl Operator on Planar Domains

Li-yeng Sung, Louisiana State University

We present theoretical and numerical results for new finite element methods for a fourth order curl operator on planar domains. Both the source problem and the eigenvalue problem will be considered. These finite element methods, which are based on standard Lagrange finite elements for second order scalar problems, are derived through the Hodge decomposition of divergence free vector fields.

1078 - Nonconforming Generalized Finite Element Method for Dirichlet Boundary Value Problems

Nicolae Tarfulea, Purdue University Calumet

In this talk, I will present a method for treating Dirichlet boundary conditions for partial differential equations in the Generalized Finite Element Method (GFEM) framework. The method is based on using approximate Dirichlet boundary conditions and polynomial approximations of the boundary. The sequence of GFEM-spaces consists of nonzero boundary value functions, and hence it does not conform to one of the basic Finite Element Method conditions. I will describe an effective technique for constructing sequences of GFEM-spaces satisfying the required assumptions by using polynomial approximations of the boundary. The method can also be used for treating transmission (or interface) problems.

1079 - BPX Preconditioner for Nonstandard Finite Element Methods for Diffusion Problems

Xiaoping Xie, Sichuan University

We propose and analyze an optimal preconditioner for a general linear symmetric positive definite (SPD) system by following the basic idea of the well-known BPX framework. The SPD system arises from a large number of nonstandard finite element methods for diffusion problems, including the well-known hybridized Raviart-Thomas and Brezzi-Douglas-Marini mixed element methods, the hybridized discontinuous Galerkin method, the Weak Galerkin method, and the nonconforming Crouzeix-Raviart element method. We prove that the presented preconditioner is optimal, in the sense that the condition number of the preconditioned system is independent of the mesh size. Numerical experiments provided confirm the theoretical result. This is a joint work with Binjie Li.

1080 - A Local Nodal Meshless Method for Pdes--Localized Method of Approximate Particular Solutions Using Thin-Plate Spline Rbfs

Guangming Yao, Clarkson University

We will introduce a method that uses radial basis functions to solve partial differential equations---localized method of approximate particular solutions (LMAPS). The method is indeed a generalized finite difference method. The LMAPS was recently developed using strictly positive definite RBFs such as Gasussian, Matern, and Multiquadrics for solving large scale problems in 2D and 3D with even extremely irregular domains. It generates a global sparse linear system using the nodal unknown values without mesh on the domain of the PDE. We will extend the method to a conditionally positive definite RBF---thin-plate spline and compare the numerical efficiency and accuracy of the method with different RBFs on two examples. The LMAPS with thin plate splines is very accurate. The higher the order of the polyharmonic splines, the more accurate the LMAPS is. We can also simply increase the number of points in the local influence domain to improve the accuracy. There is no need to search for shape parameters, so it is efficient as well.

1081 - Recent Development of Weak Galerkin Methods

Xiu Ye, University of Arkansas at Little Rock

Newly developed weak Galerkin finite element methods will be introduced for solving partial differential equations. Weak Galerkin methods have the flexibility of employing discontinuous elements and share the simple formulations of continuous finite element methods at the same time. The Weak Galerkin method is an extension of the standard Galerkin finite element method where classical derivatives were substituted by weakly defined derivatives on functions with discontinuity. Recent development of weak Galerkin methods will be discussed in the presentation.

1082 - A Novel Weak Galerkin Finite Element Scheme for the Brinkman Model

Ran Zhang, Jilin University

The Brinkman model describes flow of fluid in complex porous media with a high-contrast permeability coefficient such that the flow is dominated by Darcy in some regions and by Stokes in others. A weak Galerkin (WG) finite element method for solving the Brinkman equations in two or three dimensional spaces by using polynomials is developed and analyzed. The WG method is designed by using the generalized functions and their weak derivatives which are defined as generalized distributions. The variational form we considered in this paper is based on two gradient operators which is different from the usual gradient-divergence operators for Brinkman equations. The WG method is highly flexible by allowing the use of discontinuous functions on arbitrary polygons or polyhedra with certain shape regularity. Optimal-order error estimates are established for the corresponding WG finite element solutions in various norms. Some computational results are presented to demonstrate the robustness, reliability, accuracy, and flexibility of the WG method for the Brinkman equations.

Sessions in 215 BCH

Contributed presentations in lecture format

1083 - Parallel Simulation of Nonlocal Sub-Diffusion Models

Ahmad Alyoubi, Colorado School of Mines

Anomalous sub-diffusion processes governed by nonlocal operators have been used in various applications. These are recently adapted to model complex single- and multi-phase fluid flow in unconventional reservoirs to understand the long-time behavior of various quantities of interest. Such processes can be described by a class of nonlocal in-time fractional derivative partial differential equations (FPDEs). Standard time-stepping discretization of these continuous models lead to computational bottleneck for long-time simulation. Memory limitations (in each node high performance computing clusters) dictate computational constraints for resolving fine scale spatial structures in the models. We develop multiple message passing interface communicators (MMPIC) based parallel-in-time-and-space computer models for the FPDEs. Our MMPIC framework facilitates efficient simulation of a class of anomalous in-time sub-diffusion models to overcome the time-stepping computational bottleneck and, within the node memory constraints, approximate the continuous models with large degrees of freedom.

1084 - A Discrete, Arbitrarily-Oriented, 3D Plane Source Analytical Solution to the Heat Equation for Modeling Reservoir Fluid Flow

Anqi Bao, The University of Tulsa

A highly accurate and easily computable analytical solution to the heat equation is presented for modeling fluid flow into a 3D, arbitrarily-oriented plane sink within a box-shaped, anisotropic medium with Neumann boundary conditions. The plane sink represents a gathering system for a well stimulated via hydraulic fracturing. Our plane source Neumann function arises from analytic double integration of the point source solution to the heat equation along two vectors forming a parallelogram. A Neumann boundary condition is achieved via the method of images, resulting in triple infinite summations that are reduced using mathematical identities to a combination of closed form expressions and infinite sums with exponential damping. Our solution forecasts time-dependent behavior of fractured wells, useful in interpreting field experiments for characterization of fracturing efficacy, reservoir size, and matrix fluid transport properties. We demonstrate our model with two applications. One is pressure transient analysis with identified flow regimes from a pressure versus time plot. The other is pseudo steady state pressure mapping, simulating inflow from multiple fractures along the trajectory of a single horizontal well, which is achieved using superposition theory and adjustment of flux strength of each plane source to achieve a common pressure at each well-fracture intersection.

1085 - Numerical Solution of Dynamic Electrical Circuits With Diodes

Mario Barela, University of Iowa

Diodes are special components in that they only allow current to flow in one direction. This can be represented by a complementarity condition between the current and the back-voltage on the diode. We present numerical methods for simulating electrical networks with resistors, capacitors, inductors and diodes using complementarity problems. These methods have both high order of accuracy and work directly with the network description of the circuit.

1086 - A Modified Weighting Algorithm for Immersed Finite Element Particle-In-Cell(IFE-PIC) Method

Yuchuan Chu, Harbin Institute of Technology Shenzhen Graduate School

In the plasma simulation community, the Particle-In-Cell (PIC) scheme has been widely used since its noise-reduction capability and moderate computational expense. Immersed finite elements (IFEs) are relatively new and efficient tools to handle interface problems with Cartesian meshes independent of the interface which are required by PIC scheme. Based on immersed finite element (IFE) methods and Particle-In-Cell methods, the recently developed immersed finite element Particle-In-Cell method (IFE-PIC method) provides an outstanding approach to simulate plasma particles with complex interface boundary. However, in current IFE-PIC method, the charge deposit algorithm does not work very well by depositing the particle charge onto mesh nodes located inside the object described by the interface surface. Also, the process of obtaining the electric field on mesh nodes with the potential of those nodes which locate inside the object has the same drawback. This paper is to present a modified weighting algorithm to improve the accuracy of plasma simulation with IFE-PIC method. Numerical examples are provided to demonstrate the accuracy of IFE-PIC method with new modified weighting algorithm.

1087 - Numerical Simulation of an Impact Problem

Benjamin Dill, University of Iowa

Experiments with bouncing steel balls on a steel anvil indicate that there may be some plastic deformation on a very small scale. To investigate this, we perform a large-scale simulation using complementarity for frictionless contact in a finite-element model. In order to carry out this simulation in reasonable computer and human time, we use linearized elasticity in cylindrical polar co-ordinates as a diagnostic method to determine if plastic deformation would occur.

1088 - Simulation of Properties of Acoustic Wave Propagation Configurations

Bradley Dworzak, Colorado School of Mines

The main quantity of interest in wave propagation models is the far-field induced by an incident wave impinging on a configuration of scatterers. We consider sound wave propagation configurations comprising multiple particles with various material properties such as sound-soft, sound-hard, or penetrable. For a given incident wave, the material properties, shape, size, location and orientation of particles in the configuration dictate the intensity of the far-field. In addition to simulation of far-field using efficient forward wave propagation solvers, the far-field can also be measured experimentally. For our application of interest, it is practical to restrict to a single incident wave (with a specific incident direction and frequency). In this work, using the far-field data, we are interested in the nonlinear inverse problem of simulating all of the above properties of the configuration, with the constraint of the data obtained using a single incident wave. We develop computer models to efficiently simulate such properties for a class multiple particle configurations.

1089 - Research of Live Migration Scheduling Method for the Simulation System based on Cloud Computing

Yanfang Fu, Missouri University of Science & Technology

The communication network field has been a strong demand for automatic management of the running of simulation, and the sharing of simulation resources and so on. Aimed at the puzzles in current HLA-based simulation system, and with the combination of a new cloud computing idea, a framework of Cloud Simulation has been presented. This article is absorbed in the aim how to migrate the virtual machine under simulation cloud computing environment and explore the dynamic dispatch to the parallel tasks in the federation entity level. Finally a mended heuristic scheduling algorithm has been designed. This algorithm dynamically adjusted decision-making through using the information of systematical real-time operating status, be able to making a timely response dynamically according to the changes of the characteristics of simulation system, re-achieve balance and improve manageability and fault tolerance, while allowing workload movement with a short service downtime according to the adjustment of the dynamic fluctuations of the loading. Taking the communication network simulation system as an example, simulation results verify that the processes do not need to be aware that a migration is occurring. It allow migrating a simulation federation as it continues to run. Such procedure is termed as "live" or "hot" migration, as opposed to "pure stop-and-copy" or "cold" migration, which involves halting the VM, copying all its memory pages to the destination host and then restarting the new VM.

1090 - Forecast Uncertainty Quantification of Return Flow over the Gulf of Mexico Using Monte Carlo, Generalized Polynomial Chaos and Unscented Transform methods

Junjun Hu, School of Computer Science, University of Oklahoma

Uncertainty in a dynamic model forecast is a result of the combination of uncertainty in initial condition, boundary condition and parameters. Methods for quantifying uncertainty in forecast may be classified into two groups: sampling based and non sampling methods. The classical Monte Carlo methods, the method of unscented transformation, particle filters, to name a few, belong to the sampling based methods. In the non sampling based approach, we approximate the uncertainty using advanced methods such as Wiener's Polynomial Chaos (PC) expansion, generalized polynomial chaos expansion [1]. In this paper, using a model that consists of a system of five coupled ODE that describes the return flow over the Gulf of Mexico that often occurs during cool season, we compare the effectiveness of the Wiener's PC approach using Hermite polynomial, unscented transform and Monte Carlo based approaches. [1] D. Xiu (2010), Numerical Methods for Stochastic Computations: A Spectral Method Approach, Princeton University Press.

1091 - The Exponential Stability of Wave Equation with Dirichlet Boundary Feedback Control

Yan Liu, University of Electronic Science and Technology of China

Using the multiplier method, when $k>0$, we obtain the one-dimensional wave equations with Dirichlet boundary control \begin{eqnarray}\label{a4} \left\{ \begin{array}{ll} w_{tt}(x,t)-w_{xx}(x,t)=0,\,\,\,\,\,00, \\ w(0,t)=0,\,\,\,\\ w(1,t)=-k\int^1_0 xw_t(x,t) dx \end{array} \right. \end{eqnarray} is exponentially stable. In conclusion, we give a numerical example of one-dimensional wave equations with Dirichlet boundary control.

1092 - Bifurcation Trees of Period-1 Motions To Chaos in a Double-Well Duffing Oscillator Under Periodic Excitation

Albert Luo, Southern Illinois University Edwardsville

In this paper, periodic motions of a periodically forced, damped, Duffing oscillator with double-well potential are analytically predicted through discrete implicit mappings. From mapping structures, bifurcation trees of periodic motions of the Duffing oscillator are predicted analytically, and the corresponding stability and bifurcation analysis of periodic motions are carried out through the eigenvalue analysis. Finally, from the analytical prediction, numerical results of periodic motions are performed, and the corresponding harmonic amplitudes are computed through discrete Fourier series of the analytically predicted node points of periodic motions, and the complexity of periodic motions can be measured by the harmonic amplitude.

1093 - A Feasibility Analysis of Several Numerical Schemes for the Prediction of Two Phase Transient Flow in HTHP

Min Luo, Chengdu University of Information Technology

We present a coupled system model of partial differential equations concerning the variation of pressure and temperature, velocity and density at different time and depth in HTHP (high temperature-high pressure) gas-liquid two phase flow wells. LxF (Lax-Friedrichs) method, CE/SE (Space-Time Conservation Element and Solution Element) method and GRP (Generalized Riemann Problem) scheme are modified to solve this set of conservation equations. The basic data of 'X Well' (HTHP well), 7100m deep, located in Sichuan basin, South-West of China, is used for the case history calculations. The comparison of pressures, temperatures along the depth of the well at different time calculated by those methods shows that GRP method is of much higher accuracy.

1094 - A Simple Pure Water Oscillator

Trung Nguyen, School of Computer Science, University of Oklahoma

Welander [1] and Ruddick and Zhang [2] have analyzed the properties of the heat-salt oscillator by considering a well-mixed two layered system of sea water where there is heating and evaporation from the top layer and vertical turbulent mixing between the layers. In this note we examine the presence of oscillation in a system quite like the one described above with the primary difference that the water is pure with no salt component. We are motivated by the observation relating to the overturning of water in pure water lakes that occurs when the seasons change from summer to autumn as the top layer cools and again from winter to spring when the top layer warms. This overturning is largely a consequence of the nonlinear dependence of the density of pure water on the temperature. Our model known as the flip-model has piece-wise smooth and discontinuous right hand side. The location and the magnitude of the discontinuity depend on two parameters. We provide a complete characterization of the bifurcation. In addition, using Filippov's theory [3], we also isolate two cases that exhibit oscillations. [1] Welander, P. (1982). "A simple heat-salt oscillator." Dynamics of Atmospheres

and Oceans 6: 233-242. [2] Ruddick, B., and L. Zhang. (1989). "The mythical thermohaline oscillator?" Journal of Marine Research 47: 717-746. [3] Filippov, A.F. (1988). Differential Equations with Discontinuous Righthand Sides. Kluwer Academic Publications, 304 pages.

1095 - On Positive Increasing Solutions of Emden-Fowler Dynamic Systems on Time Scales

Ozkan Oztruk, Missouri University of Science and Technology

We study the existence and the asymptotic behavior of nonoscillatory solutions of Emden-Fowler dynamic sytems on time scales, we use Schauder, Knaster, Tychonoff Fixed Point Theorems in order to show the existence such solutions. We also illustrate some examples.

1096 - High Accuracy Combination Method for Solving the Systems of Nonlinear Volterra Integral and Integro-Differential Equations with Weakly Singular Kernels of the Second Kind

Lu Pan, Sichuan University

We present a high accuracy combination algorithm for solving the systems of nonlinear Volterra integral and integro-differential equations with weakly singular kernels of the second kind. Two quadrature algorithms for solving the systems are discussed, which possess high accuracy order and the asymptotic expansion of the errors. By means of combination algorithm, we may obtain a numerical solution with higher accuracy order than the original two quadrature algorithms. Moreover an a posterior error estimation for the algorithm is derived. Both of the theory and the numerical examples show that the algorithm is effective and saves storage capacity and computational cost.

1097 - An Effective High-Order Shock-Capturing Limiter for Discontinuous Galerkin Methods

David Seal, Michigan State University

In this work, we present a novel shock capturing limiter for the discontinuous Galerkin (DG) method. It can be viewed as either an extension of the recent maximum principle preserving (MPP) limiter devised by Zhang and Shu to be able to handle shocks, or as an extension of the older finite volume limiter developed by Barth and Jespersen to the DG framework. Our limiter constructs local upper and lower bounds for the solution by sampling nearest neighbors, and then limits the solution to stay within these bounds. It is simple to implement, has minimal communication, is effective at capturing shocks, and retains genuine high-order accuracy of the solution in smooth regimes. Numerical results including problems that require positivity preservation in one and two dimensions on structured and unstructured grids are presented that indicate the robustness of the method.

1098 - From Period-1 Motions to Chaos in a Time-Delayed, Quadratic Nonlinear Oscillator

Siyuan Xing, Southern Illinois University Edwardsville

In this paper, periodic motions in a periodically forced, damped, quadratic nonlinear oscillator are investigated through discretization of its differential equation. Bifurcation trees of periodic motions are predicted analytically and the corresponding stability and bifurcation analysis are completed through eigenvalue analysis. From the analytical prediction, numerical results of periodic motions in the time-delayed quadratic nonlinear systems are illustrated.

1099 - Analytical Solutions of Periodic Motions in a Periodically Forced, Damped, Two-Degree-of-Freedom Oscillator with Nonlinear Spring

Bo Yu, Southern Illinois University Edwardsville

In this paper, analytical solutions of periodic motions of a 2-DOF nonlinear oscillator are obtained through finite Fourier series expansion. The dynamical system of coefficients of the Fourier series is developed by the Generalized harmonic balance. From such a dynamical system, stable and unstable periodic motions are determined analytically, and stability and bifurcations of the periodic motions are carried out through the eigenvalue analysis. Numerical simulations of stable period-1 to period-4 motions in the two degrees of freedom systems are illustrated. The harmonic amplitude spectrums show the harmonic effects on periodic motions.

1100 - A Second Order Periodic Boundary Value Problem with a Parameter and Vanishing Green's Functions

Yangwen Zhang, Missouri University of Science and Technology

We consider a second order periodic boundary value problem with a parameter. By using fixed point theorems in a cone, some existence and nonexistence results for non-negative solutions are established under different combinations of super-linearity and sub-linearity of functions at zero and infinity for an appropriately chosen parameter in the case where the associated non-negative Green's functions may have zeros. The results are illustrated by an example.

1101 - Parametric Representation of Boundary Flux in Heterogeneous Potential Flow Problems

Yiteng Zhang, The University of Tulsa

Material transport is anticipated between adjacent porous media in capillary contact for which we have independent Neumann function solutions to either Poisson's Equation or the Heat Equation. These solutions can be extended by opening the boundary using Green's Theorem, resulting in analytic solutions coupled through a boundary integral. Previously, a parametric representation of the boundary flux was proposed as a linear combination of uniform flux and uniform pressure constituents, which has advantages of analytic evaluation of contributing terms. This boundary flux structure is shown to be exact for cells of identical size and permeability. We highlight the extension to systems of either differing domain size or permeability using prolongation. Prolonged problems allow identification with symmetry of equal cell size problems and an exact solution for flux distribution. Correcting for prolongation requires additional uniform flux and circulation elements that are related to the degree of mismatch in cells in the originally-posed problem. Since lengths are scaled with respect to transport properties, we can claim the new method also allows significant bandwidth reduction in solving the heat equation for heterogeneous systems using parametric representation of flux in boundary integrals.

1102 - A Distributed Optimal Control Problem Governed by Stokes Equations with an Energy-Norm-Constraint on the Velocity

Jianwei Zhou, Purdue University

The Stokes equations model the flows with low velocity, or very viscous fluids, e.g., many biological flows and non-Newtonian flows. We design a distributed optimal control problem (OCP, for short) governed by Stokes equations with an energy-norm-constraint, which reads that the energy-norm of the velocity is not more than a given positive constant. We investigate optimal conditions for the OCP with KKT conditions. The Legendre-Galerkin spectral method is employed to approximate the OCP. The a-priori error estimate is deduced. Meanwhile, an efficient algorithm is designed and the convergence is discussed.

Sessions in 216 BCH

Interactions Among Analysis, Optimization and Network Science

1103 - Modulus of Families of Walks on Graphs

Nathan Albin, Kansas State University

The modulus of a family of curves in a continuum provides a quantitative assessment of the “richness” of the family: large families of short curves have larger modulus than small families of long curves. In the discrete setting, the concept of modulus can be linked to several graph-theoretic quantities including shortest path, minimum cut, and effective resistance. This talk will cover connections among these concepts through the Lagrange dual formulation, some applications, and a numerical algorithm for computing the modulus.

1104 - Exact Coupling Threshold for Structural Transition in Interconnected Networks

Faryad Darabi Sahneh, Kansas State University

We study the structural transition phenomenon in dynamical characteristics of interconnected networks between two regimes: one where the coupled networks are distinguishable, and one where they function as a whole single network. The coupling threshold that determines this structural transition is a singularly crucial property of an interconnected network topology. While existence of a coupling threshold has been demonstrated earlier by Radicchi and Arenas 2013, we present here an analytical expression for the exact value of the coupling threshold, outline network interrelation implications, and extract several aspects of the structural transition. Importantly, we show that the structural transition phenomenon disappears when one of the subnetworks is a scale-free network with vanishing algebraic connectivity.

1105 - The Dirichlet Problem with Prime End Boundary Data for Bounded Domains in Metric Spaces

Dewey Estep, University of Cincinnati

First introduced by Caratheodory in 1913, the prime ends provide a way to define the boundary of a bounded planar domain so that the boundary inherits many properties inherit in the domain itself, rather than the ambient space. In a 2013 paper, Adamowicz et. al. defined prime ends for more general metric spaces. The structure of this prime end boundary is intrinsically related to the accessibility of the normal metric boundary of the domain from its interior. Under this lens, we may view the prime end boundary as a tool to understand from where on the boundary information may be successfully transferred into the interior of the domain. Here, we will solve the Dirichlet problem with such boundary data.

1106 - Three Notions of Parabolicity for Networks

James Gill, Saint Louis University

I will discuss three different notions of parabolicity for networks. They all involve a type problem: one for random walks, one for circle packings, and one for Riemann surface type. There are relationships between these problems, but not everything is known.

1107 - Inventory Accumulation and Quadrangulations of the Sphere

Max Goering, Kansas State University

We discuss a bijection due to Scott Sheffield which is based on the Last-In First-Out (LIFO) model of inventory accumulation. This bijection puts planar maps (e.g. quadrangulations of the sphere) in one-to-one correspondence with words in a specific semi-algebra. It is worthwhile to try and understand the relationship between global geometric properties of the planar maps and local quantitative observations in the corresponding words. Our goal is to design certain modulus computations for some families of walks on the planar maps and then observe how the modulus varies when the corresponding words are varied in an approximately continuous way.

1108 - Preservation of Bounded Geometry Under Sphericalization and Flattening: Quasiconvexity and 8-Poincare Inequality

Xining Li, University of Cincinnati

This is a joint work with Estibalitz Durand-Cartagena. In this work we explore the preservation of quasiconvexity and 8-Poincare inequality under sphericalization and flattening in the metric setting. The results developed in our previous work show that the Ahlfors regularity, doubling property, and the p-Poincare inequality for p < 8 are preserved under the sphericalization and flattening transformations if one assumes the underlying metric space has annular quasicovexity. In this work, we propose a weaker assumption to still preserve quasiconvexity and 8-Poincare inequality, called radial starlike quasiconvexity and meridian starlike quasiconvexity, extending in particular a result by Buckley, Herron and Xie to a wider class of metric spaces and covering the case p = 8 in our previous work.

1109 - Pointwise Quasiminimality of Gibbs-Like Measures

Zijian Li, Kansas State University

We say that a set $E \subset \mathbb{R}$ is (quasisymmetrically) minimal if $\dim_H f(E) \ge \dim_H E$ for every quasisymmetric mapping f of the real line. By a theorem of Kovalev it is known that minimal subsets of the line have to be of Hausdorff dimension 1. In dimension 1 there are set of full Lebesgue measure which are not minimal (first constructed by Tukia in 1989). On the other extreme, there are sets of zero Lebesgue measure which are minimal (first constructed by Hakobyan in 2006). In this talk we will give sufficient conditions for subsets of the line to be quasisymmetricaly minimal. The main novelty of our approach is a notion of pointwise minimality for measures. We use this notion to show that uniform Cantor sets are minimal for quasisymmetric mappings of the line if and only if they have Hausdorff dimension 1. This answers a question of Hu and Wen from 2008.

1110 - Discretizations of Metric Measure Spaces of Controlled Geometry

Marcos Lopez, University of Cincinnati

Let (X,d) be a metric space with a doubling measure μ. If (X,d,μ) is endowed with a Poincar\'e type inequality, then it becomes an element from an essential class of metric spaces in the study of Sobolev spaces. Often, it is difficult to verify that an arbitrary measure metric space, (X,d,μ), carries a Poincar\'e type inequality. I will present a method to discretize the space (X,d,μ) while preserving its doubling property. I will then present a necessary and sufficient condition for (X,d,μ) to carry a $(1,p)$-Poincar\'e Inequality involving a discretized $(1,p)$-Poincar\'e inequality on the constructed discretized space. This condition relies on important results due to Cheeger and Koskela, and the ability of a series of discretized spaces to approximate (X,d,μ). These results are due to joint work with James Gill.

1111 - An Introduction to Modulus of Path Families from a Historical Point Of View

Pietro Poggi-Corradini, Kansas State University

I will try to give an overview of modulus techniques, by describing their historical uses in mathematics. I will select a few results that hopefully will give a flavor of the type of applications modulus has had in pure mathematics.

1112 - Impact of Preventive Responses to Epidemics in Rural Regions

Caterina Scoglio, Kansas State University

Various epidemics have arisen in rural locations through human-animal interaction, such as the H1N1 outbreak of 2009. Through collaboration with local government officials, we have surveyed a rural county and its communities and collected a dataset characterizing the rural population. From the respondents' answers, we build a social (face-to-face) contact network. With this network, we explore the potential spread of epidemics through a Susceptible-Latent-Infected-Recovered (SLIR) disease model. We simulate a stochastic SLIR infection spreading process with disease parameters representing a typical influenza-like illness. We test vaccine distribution strategies under limited resources based on several and novel centrality metrics. We examine global and location-based distribution strategies, as a way to reach critical individuals in the rural setting. We demonstrate that locations can be identified through contact metrics for use in vaccination strategies to control contagious diseases. Furthermore, we explore two models of a susceptible individual's dynamics in response to infections observed among the individuals in his neighborhood, namely preventive behavior adoption and social distancing. Through extensive simulations, our investigation reveals the potentially powerful impacts of social spontaneous responses in rural settings.

1113 - Generalized Centrality Measures Based on Modulus of Families of Walks

Heman Shakeri, Kansas State University

We study different families of walks and use them to introduce measures that quantify different properties of graphs. This is done using the notion of modulus of a family of walks, which represents an assessment of how many short walks are in the family. We compare our proposed measures with other known quantities such as current-flow closeness centrality, out-degree centrality and current-flow betweenness centrality. Examples are provided to show that our method can be used for more general

1114 - Use of Functions of Bounded Variation in Determining Sobolev Functions with Zero Boundary Values

Nages Shanmugalingam, University of Cincinnati

In this talk we will discuss a characterization of Sobolev functions with zero boundary values for a given domain in the metric setting, using the theory of BV functions developed by Miranda Jr. and Ambrosio. This is joint work with Juha Kinnunen, Riikka Korte and Heli Tuominen.

1115 - Modulus and Quasiconformality

Marshall Williams, Kansas State University

Modulus is important in the study of Sobolev regularity, quasiconformality, and metric space analysis. I will define modulus of curves, surfaces, sets, and measures, and discuss a number of results in this area, particularly in connection with quasiconformal maps.

Sessions in 314 BCH

Recent Advances in Numerical Methods for Fluid Flows

1116 - Numerical Methods for Flow in Poroelastic Media

Yanzhao Cao, Auburn University

We are surrounded by poroelastic solid materials: natural (e.g., living tissue: plant or animal, rocks, soils) and manmade (e.g., cement, concrete, filters, foams, ceramics). Because of their ubiquity and unique properties poroelasticity materials are of interest to natural scientists, and engineers. Applications of poroelasticity include reservoir engineering, biomechanics and environmental engineering. In this talk we present models for a steady and quasi-static flow in a saturated deformable porous medium. This is a coupled phenomenon distinguished by the interaction of a porous, deformable, elastic solid matrix and a saturating fluid which occupies and flows through its pores. We will present results on well-posedness, regularity and numerical solutions of the governing PDEs.

1117 - Mimetic and Convergent Discretization of Vector Fields on Unstructured Meshes

Qingshan Chen, Clemson University

In this talk, we present a new theoretical framework for analyzing FD/FV schemes for a wide range of fluid problems. There are two essential ingredients to this framework. The first is the external approximation of function spaces, which seems particular adept in dealing with discontinuous functions. The second is the tracking of divergence and vorticity, instead of individual derivatives. This approach gets rid of the requirement for a Cartesian coordinate system, and makes this framework applicable to unstructured meshes. Once the framework has been presented, we will apply it to the classical incompressible Stokes problem, and prove that the discrete solutions converges to the solution of the continuous system, without assuming that one actually exists.

1117a - Non-linear Flow Characteristics and Horizontal Well Pressure Transient Analysis for Low-permeability Oil Reservoirs

Chaohua Guo, Missouri University of Science and Technology

In this paper, lab experiments have been carried out to study the threshold pressure gradient (TPG) and stress sensitivity which cause the non-linear flow in low permeability oil reservoirs. The investigation of existing conditions of TPG for oil transport in irreducible water saturation low-permeability reservoirs was conducted and discussed. The relationship between TPG and absolute permeability were obtained through experimental results. It was found that TPG increases with absolute permeability decreasing. Then, stress sensitivity experiments were carried out through depressurizing experiments and step-up pressure experiments. Permeability modulus which characterizes stress sensitivity increases with absolute permeability decreasing. Then, a horizontal well pressure transient analysis mathematical model considering TPG and stress sensitivity was established based on mass and momentum conservation equations. The finite element method was deployed to solve the model. Influencing factors, such as TPG, permeability modulus, skin factor, wellbore storage, horizontal length, horizontal position, and boundary effect on pressure and pressure derivative curves were discussed. Results analysis demonstrates that the pressure transient curves are different from the Darcy's model when considering the non-linear flow characteristics. Both TPG and permeability modulus lead to more energy consumption and the reservoir pressure decreases much more compared with Darcy's model.

1118 - Fast and Accurate Algorithms for Simulating Coarsening Dynamics of Cahn-Hilliard Equations

Lili Ju, University of South Carolina

The coarsening dynamics in a binary mixture can be modeled by the celebrated Cahn-Hilliard equations. To perform efficient and accurate long time integration, we develop a fast and stable high-order numerical algorithm for solving CahnHilliard equations. The spatial discretization is carried out by compact difference schemes while the time integration is done through a high-order exponential time differencing multistep approach. We demonstrate the effectiveness of the proposed algorithms by numerical experiments and study computationally the coarsening kinetics corresponding to different choices of the diffusion mobility.

1119 - Magnetohydrodynamic Flows: Boussinesq Conjecture

Alexander Labovsky, Michigan Technological University

The Boussinesq assumption that turbulent fluctuations have a dissipative effect on the mean flow is the basis for most turbulence models used in practical flow simulations. Data from computational tests and experiments has indicated that in 2d fluid flows an inverse energy cascade is expected. However, the Boussinesq assumption has recently been proven to hold in a time averaged sense for the Navier-Stokes equations. In Magnetohydrodynamic (MHD) flows, the dynamo effect suggests an inverse cascade of energy from small to large scales in both 2d and 3d, suggesting its re-evaluation for MHD flows. Here we use the MHD formulation in the Elsasser variables to show that the Boussinesq assumption also holds for MHD turbulence. A short discussion on the choice of eddy viscosity models is presented, as a consequence of the main result.

1120 - A Stable Leapfrog Scheme for Optimal Control of Wave Equations

Jun Liu, Southern Illinois University

We proposed and analyzed a new leapfrog finite difference scheme in time for solving the first-order necessary optimality systems arising in optimal control of wave equations. With a standard second-order central finite difference scheme in space, the full discretization is proved to be unconditionally convergent with a second-order accuracy, which is not restricted by the classical Courant-Friedrichs-Lewy(CFL) stability condition on the spatial and temporal step sizes. Moreover, based on its nicer structure compared to that of the traditional leapfrog scheme, an efficient preconditioned iterative method is provided for solving the discretized unsymmetric sparse linear system. Numerical examples are presented to confirm our theoretical conclusions and demonstrate the promising performance of our proposed preconditioned iterative solver.

1121 - A CVOD Based Low-Dimensional Approximation to Nonlinear Stochastic Partial Differential Equations

Ju Ming, Beijing Computational Science Research Center

Making accurate predictions about the behaviors of complex system described by partial differential equations (PDEs) with incomplete or unreliable data is an important goal of the computational science involving uncertainty quantification, where a significant challenge is to develop and establish an efficient numerical approach to overcome the high computing requirement and provide accurate solutions of the associated stochastic PDEs. Over past decade, reduced-order models have been found increased use to greatly reduce the computational cost in the areas such as flow control and optimization. In this lecture, we will present an effective stochastic reduced-order modeling method that combines the advantages of proper orthogonal decomposition and centroidal Voronoi tessellations. The optimality of such hybrid method for model reduction is discussed and numerical tests are performed to validate our results.

1122 - Predicting Orientation of Fibers in Injection Molded Plastics

Stephen Montgomery-Smith, University of Missouri

Prediction of orientation of short fibers in injection molded plastics has industrial applications, as the final orientation determines material properties of the final part such as strength. Unfortunately results from experiments deviate greatly from theory in that the rate of alignment of orientation can be up to fifty times slower than theory predicts. Current theory, such as the Folgar-Tucker equation, is based upon treating the fiber suspension as a continuum. It uses an equation due to Jeffery from 1923, which models a single fiber, combined with a Laplacian term meant to model interactions between the fibers. In this talk, I present research to test the hypothesis that experimental behavior could still be predicted by a continuum model, by including the effect fiber orientation has upon the non-isotropic viscosity of the suspension. We posit that the coupling of the effect of fluid flow, fiber orientation, and non-isotropic viscosity, creates instabilities. We present numerical evidence demonstrating the existence of these instabilities. We also present recent results in the exact calculation of tensor closure formulas that greatly speed up calculations. Finally I ask for help in creating a finite element numerical model to fully validate the hypothesis.

1123 - Multiscale Mortar Finite Element Methods for Coupling Stokes-Darcy Flows with Transport on Irregular Geometry Domains

Pu Song, University of Pittsburgh

A non-overlapping domain decomposition method is developed for coupled Stokes-Darcy flows in irregular domains. The Stokes region is discretized by standard Stokes finite elements while the Darcy region is discretized by the multipoint flux mixed finite element method. The subdomain grids may not match on the interfaces and mortar finite elements are employed to impose weakly interface continuity conditions. The interfaces can be curved and matching conditions are imposed via appropriate mappings from physical grids to reference grids with flat interfaces. The global problem is reduced to a mortar interface problem, which is solved by the conjugate gradient method. Each iteration involves solving subdomain problems of either Stokes or Darcy type, which is done in parallel. We also investigate DG-DG domain decomposition coupling using mortar finite elements to approximate the solution to the transport equation coupled with Stokes-Darcy flow on irregular geometry domains. Numerical tests are presented for verifying theory derived.

1124 - Time Domain Decomposition Methods for Forward-and-Backward PDEs

Zhu Wang, University of South Carolina

The forward-and-backward partial differential equation system always appears in the optimal control and optimization problems. It is appealing to solve such a system directly since a single solve suffices to determine the optimal states, adjoint states, and controls. However, this approach is computationally expensive. In this talk, we present several time domain decomposition methods, which are based on a decomposition of the time domain into smaller subdomains, and are suited for implementation on parallel computer architectures. The effectiveness of these algorithms are verified by numerical tests.

1125 - Any Order Finite Volume Schemes Over Quadrilateral Meshes

Qingsong Zou, Sun Yat-Sen University

A family of any order finite volume (FV) schemes over quadrilateral meshes is analyzed under the framework of Petrov-Galerkin method. By constructing a special mapping from the trial space to the test space, a unified proof for the inf-sup condition of any order FV schemes is provided under a weak condition that the underlying mesh is an $h^{1+\gamma},\gamma>0$ parallelogram mesh. The optimal convergence rate of FV solutions is then obtained with well-known techniques.

Modeling and Simulation of Turbulence/Hydrodynamics

1126 - Direct Numerical Simulation for Laminar-to-Turbulent Transition Prediction

Lian Duan, Missouri University of Science and Technology

Laminar-to-turbulent transition prediction and control is one of the key enabling technologies for quiet and efficient aircraft. Accurate prediction of transition requires a holistic approach, which accounts for all major stages within transition (namely, receptivity, linear growth, nonlin- ear interactions and secondary instability) in an integrated manner. In this talk, we will focus on direct numerical simulation (DNS) studies of laminar-to-turbulent transition in two aspects. One is to characterize the acoustic freestream fluctuations radiating from supersonic/hypersonic turbulent boundary layers (under supersonic/hypersonic conditions, with adiabatic/cold walls), which is an important step to enable meaningful application of receptivity theory in the con- text of actual wind-tunnel experiments. The other is to investigate the secondary instability and breakdown mechanisms of crossflow vortices in three-dimensional swept-wing boundary layers, which is critical for the development of engineering methodologies for the design and optimization of roughness-based laminar flow control.

1127 - Predicting Riblet Performance Using Anisotropy-Resolving Turbulence Models

Elbert Jeyapaul, Missouri University of Science and Technology

There is need for a computational tool to predict rough wall flows at engineering Reynolds numbers with reasonable accuracy. Previous studies (Djenidi and Antonia, 1995) have shown second-moment RANS closures to hold promise in predicting riblet performance. In this study we use a simpler two-equation anisotropy-resolving model, the Explicit Algebraic Reynolds Stress Model (EARSM) to predict riblet flows. In triangular riblets of sizes $5 10$, however the magnitudes are overpredicted. Tuning of the EARSM coefficients has shown to improve the model's predictive capability.

1128 - A Mixed Fluid-Kinetic Solver for the Vlasov-Poisson System

James Rossmanith, Iowa State University

The dynamics of plasma can be simulated using kinetic or fluid models. Kinetic models are valid over most of the spatial and temporal scales that are of physical relevance in many application problems; however, they are computationally expensive due to the high-dimensionality of phase space. Fluid models have a more limited range of validity, but are generally computationally more tractable than kinetic models. One critical aspect of fluid models is the question of what assumptions to make in order to close the fluid model. A theoretically ideal but practically difficult to achieve model would combine positive aspects from both the kinetic and fluid models. In this work we develop and study an approach to hybridize fluid models with the Vlasov equation. The transfer of information from the kinetic to the fluid model (i.e., restriction) can be readily handled through the computation of moments. How to handle the transfer in the other direction (i.e., prolongation) is much less clear, and we consider a variety of approaches. The resulting model is discretized using a high-order discontinuous Galerkin scheme implemented in the freely available software package DoGPack. The resulting method is applied to several standard numerical test cases for the Vlasov-Poisson system.

1129 - New Developments in Fluid Experimental Techniques Provide Benchmark Data for Simulations

Huixuan Wu, University of Kansas

CFD has made significantly advances over last decades. On the other hand, fluid experimental techniques also experienced a great progress. The researchers have seen increasingly closer collaborations between experimentalist and computation experts. Flow measurement results are not only materials for scientific study, but also benchmark data for numerical colleagues, who can validate their models and explore larger parameter space. A widely used experimental method is particle image velocimety (PIV). It measures flow velocity field by taking a time sequence of images of the seeding particles in a flow. Given that the time interval between successive images are small enough, the flow velocity can be calculated using the particle displacement over this time. The latest PIV technique provides time-resolved 3D velocity field. PIV is more advantageous than single point probing, as it provides information over a 2D or 3D domain. For example, PIV is used in turbomachinery flows, which are very complex due to moving boundaries and 3D curving geometry. The measurements clearly resolve all the flow structures in the rotor passage. Simulation groups used these data to tune up the parameters and finally produced correct simulation with RANS model.

1130 - Acoustic Radiation from Tunnel-Wall Turbulent Boundary Layers

Chao Zhang, Missouri University of Science and Technology

Prediction of laminar-turbulent transition is a critical part of the design of hypersonic vehicles because of the large increase in skin-friction drag and surface heating associated with the onset of transition. Transition testing in hypersonic ground facilities has been an important avenue to understanding the laminar-turbulent transition behavior of hypersonic vehicles. However, most of the existing transition test data using hypersonic wind tunnels are contaminated by facility noise that is radiated from the turbulent boundary layers on the tunnel walls. An understanding of tunnel noise effects is critical to enabling more effective use of the transition data from noisy wind tunnels and permitting more accurate extrapolation of the wind-tunnel results to flight. This talk will focus on high-fidelity simulations of acoustic radiation from the tunnel-wall boundary layers, the genesis of unsteady freestream disturbances in ground facility experiments. Such simulations provide unique information that cannot be obtained using current measurement techniques and, in so doing, open door to rational, holistic modeling of transition in high-speed boundary layers.

Sessions in 315 BCH

Analytical and Computational Methods in Nonlinear Problems of Solid Mechanics

1131- Infinite-Order Laminates in a Crystal Plasticity Model with Two Slip Systems

Nathan Albin, Kansas State University

The macroscopic material response of certain crystalline solids appears to be largely influenced by the spontaneous formation of microstructure as the material responds locally to internal stresses. We'll discuss a variational model for an elastically rigid crystalline structure in which the crystalline lattice can slip in two orthogonal directions. By exploring the generalized convex envelopes of the local energy, we make some qualitative observations related to spontaneous microstructure formation.

1132 - Nonuniqueness of Blowup Limits of Solutions to the Obstacle Problem

Ivan Blank, Kansas State University

When studying the obstacle problem, it seems that having our coefficients in the space of vanishing mean oscillation is the minimum regularity which we can hope to assume while still proving some measure theoretic version of Caffarelli's celebrated regularity theorem. On the other hand, even in cases where we can pose the problem as the minimization of a convex integrand within the calculus of variations, we can still produce an example where the solution has an infinite number of distinct blowup limits (even after modding out by rotations) as a measure theoretically regular free boundary point. This talk is based on joint work with Kubrom Teka and Zheng Hao.

1133 - Numerical Methods for Riemann-Hilbert Problems in Multiply-Connected Circular Domains

Thomas DeLillo, Wichita State University

Riemann-Hilbert problems in multiply connected domains arise in a number of applications, such as the computation of conformal maps. As an example here, we consider a linear problem for computing the conformal map from the exterior of m disks to the exterior of m linear slits with prescribed inclinations. The map can be represented as a sum of Laurent series centered at the disks and satisfying a certain boundary condition. R. Wegmann developed a method of successive conjugation for finding the Laurent coefficients. We compare this method to least squares solutions to the problem. The resulting linear system has an underlying structure of the form of the identity plus a low rank operator and can be solved efficiently by conjugate gradient-like methods. This is joint work with Raja Balu.

1134 - Approximation of DtN Map in a High Contrast Conductivity Problem

Yuliya Gorb, University of Houston

A model of a composite material consisting of a matrix of finite conductivity with ideally conducting almost touching particles is considered, and a discrete network approximation for the Dirichlet-to-Neumann map is constructed and justified.

1135 - Domain Formation in Membranes Near Onset of Instability

Gurgen (Greg) Hayrapetyan, Ohio University

The formation of microdomains, also called rafts, in membranes can be attributed to the surface tension of the membrane. In order to model this phenomenon, an energy functional involving a coupling between the local composition and the local curvature was proposed by Seul and Andelman in 1995. We study the Γ-convergence of this family of energy functionals depending on the size of the sample, involving nonlocal as well as negative terms.

1136 - Qualitative Properties of the Solution of the Equations in Non-Divergent Form with Zaremba Type of Boundary Conditions in Non-Smooth Domain

Akif Ibraguimov, Texas Tech University

In the article I will present (joint with Professor Alexander Nazarov from Saint Petersburg) proof of the Lemma of growth for solution of elliptic equations with mixed boundary condition. We will consider equation in non-divergent form of second order with Neumann, and only local Lipchitz condition on the Neumann boundary. This problem with big details for domain with none—smooth boundary was studied in the series of the paper of professor Vladimir Mazya and his students for equations in divergent form. In contrast to case of in divergent form equation even for Lipschitz domain flattening of the boundary is not applicable to study behavior of the solution near Neumann boundary in general and near junction point of Dirichlet and Neumann Data. We construct a specific barrier to prove Lemma of growth near Neumann boundary and use "by step" algorithms to propagate information from Dirichlet boundary to Neumann boundary. Finally we proved Wiener type test for sufficient condition on the Dirichlet boundary which grantee regularity of the junction point for mixed boundary condition.

1137 - Neutrality of Coated Ellipsoids with a Linear Shell and a Nonlinear Core

Silvia Jimenez Bolanos, Colgate University

The problem of determining nonlinear neutral inclusions in (electrical or thermal) conductivity is considered. Neutral inclusions, inserted in a matrix containing a uniform applied electric field, do not disturb the field outside the inclusions. The well-known Hashin coated sphere construction is an example of a neutral inclusion. In this talk, we consider the problem of constructing neutral inclusions from nonlinear materials. In particular, we discuss assemblages of coated ellipsoids. The proposed construction is neutral for a given applied field.

1138 - Singular Integro-Differential Equations for a New Model of Fracture with a Curvature-Dependent Surface Tension

Anna Zemlyanova, Kansas State University

A new model of fracture mechanics which takes into account interfacial effects due to a curvature-dependent surface tension acting on the boundary of the fracture is discussed. The model is based on a physically valid assumption that the behavior of molecules near a surface of a material is significantly different from those in the bulk and depends on the local curvature of the material surface. The theory will be presented on the examples of interface and non-interface curvilinear fracture. It will be shown that the incorporation of surface effects on the crack boundary eliminates the power and oscillating singularities at the crack tips which are predicted by linear elastic fracture mechanics. The contact problems for a rigid stamp indentation into an elastic half-plane with a surface tension on the boundary will be discussed as well. The mechanical problems will be reduced to the systems of singular integro-differential equations using methods of complex analysis. The regularization and numerical solution of these systems will be addressed and numerical examples will be presented. Potential directions for future research and connections with experimental results will be discussed.

Sessions in 316 BCH

Current Trends in Ecology and Disease Modeling

1139 - Eco-Evolutionary Analysis of a Multi-Strain SIS Model to Quantify the Long-Term Efficacy of Control and Preventive Measures

Majid Bani-Yaghoub, University of Missouri-Kansas City

Joint work with Sharif S Aly (University of California Davis), and Patrick Pithua (University of Missouri-Columbia) Control and preventive measures, such as environmental decontamination (ED) and antimicrobial drug administration (ADA) can affect the stability of host-pathogen systems. These measures can also affect the interactions between ecology and evolution (i.e., eco-evo feedback loops). A fundamental challenge facing public health officials and decision makers is to accurately assess the long-term efficacy of these measures in presence of eco-evo feedback loops. Using a multi-strain SIS-type model we investigate the efficacy of ADA and ED, under the assumption that pathogens develop resistance to antimicrobial drugs and disinfectants. It is shown that pathogen's evolution may destabilize the disease-free equilibrium and give rise to stable single-strain or multi-strain endemic equilibria. We derive conditions for stability of multi-strain co-existence equilibria. Although higher intensities of ADA and ED may eliminate the multi-strain co-existence equilibria, the eradication of infection is not possible without the passage through the stable single-strain equilibria.

1140 - Delayed HIV Rebound After Cessation Of Treatment: Model Predictions

Jessica Conway, Pennsylvania State University

Reports suggest that early initiation of HIV antiretroviral therapy, within a few months of infection, may permit post-treatment control (PTC): control of infection, defined as sustained undetectable viral load, after treatment cessation. In cases of no control, viral rebound (VR) occurs. VR may be immediate, or delayed by months or even years, as was the case for the Boston Patients and the Mississippi baby, respectively. We assume that viral rebound is associated with latent cell activation, and investigate the hypothesis that ART initiated early during primary infection permits PTC or delayed VR by limiting the size of the latent reservoir. A sufficiently small latent reservoir may, at treatment termination, undergo delayed activation or even stochastic extinction, delaying or preventing or viral rebound. We will present a simple, stochastic, model of VR, including generalized dynamics on the latent reservoir. From the model we will derive analytic expressions for probability and time to viral rebound as first passage time calculations. We will then discuss clinically relevant resulting predictions.

1141 - Ideal Treatments for HIV-TB Co-Infected Populations: Modeling and Optimal Control Theory Perspectives

Abhishek Mallela, University of Missouri – Kansas City

HIV-TB co-infected individuals undergoing TB treatment often face the dilemma of initiating HIV treatment either immediately or after the TB treatment course is complete. Initiating HIV treatment early during the TB treatment course has advantages such as fewer AIDS-related deaths and a lower risk of HIV transmission as well as disadvantages such as Immune Reconstitution Inflammatory Syndrome (IRIS) and complications arising from a high pill burden. Here, we develop a mathematical model to explore the effects of early and late HIV treatment initiation on new HIV infections, AIDS-related deaths, and new IRIS cases/complications. We identify that the minimum burden that can be achieved with these treatments depends on both the strength and the timing of initiation of HIV treatment. Thus, we also formulate an optimal control problem based on our model, and determine ideal HIV-TB treatment protocols for these co-infected populations.

1142 - Unveiling the Past: Separating the Effects of Genetic Drift and Natural Selection Using a Modification of Tajima's D Statistic

Pamela Ryan, Truman State University

Many statistical tests have been devised to infer selective processes and demographic structure from the patterns of nucleotide variation within a population. However, interpretation of the results is complicated by the fact that a wide range of population-level processes can yield similar patterns within the data. Here we propose and evaluate a partitioning approach that separately analyzes synonymous and nonsynonymous variation. Using modified versions of Tajima's D statistic, we test the ability of this approach to resolve five distinct evolutionary models: neutral evolution, purifying selection, negative frequency-dependent (NFD) selection, population bottleneck, and population subdivision. We demonstrate that our approach successfully distinguishes data sets simulated under neutral evolution from those simulated under the other four models. An analysis of actual genetic sequences from the V3 loop of HIV similarly rejected models of purifying selection, NFD selection, and population subdivision, but could not rule out the presence of population bottlenecks. Our results suggest that data partitioning approaches have promise but require further refinements to increase their statistical power.

1143 - Mathematical Modeling of Cholera

Zhisheng Shuai, University of Central Florida

Cholera was one of the most feared diseases in the 19th century, and remains a serious public health concern today. It can be transmitted to humans directly by person-to-person contact or indirectly through ingestion of contaminated water. Basic cholera models that include both direct and indirect transmission and assume homogeneous mixing in the host population will be reviewed. Detailed models that incorporate spatial heterogeneity will be applied to understand cholera dynamics on community networks. New biological insights will be derived using results from matrix theory and graph theory. Joint work with Pauline van den Driessche (Victoria), Joseph Tien (Ohio State), and Marisa Eisenberg (Michigan).

1144 - Mathematical Modeling of Whole-Body Metabolism in Girls With Polycystic Ovarian Syndrome

Jacqueline Simens, Colorado School of Mines

Polycystic Ovarian Syndrome (PCOS) affects 6-10% of U.S. women and is a leading cause of infertility. In addition, the metabolic phenotype of PCOS includes higher rates of insulin resistance (IR) and type 2 diabetes. To investigate altered hepatic metabolism in PCOS, we are developing a stable isotope tracer-based Oral Glucose Tolerance Test (OGTT) protocol. As part of this protocol, we use a labelled OGTT mathematical model, originally developed by Dalla Man et al., to describe individualized glucose-insulin dynamics. When estimated reliably, model parameters may be used to quantify hepatic IR. We investigate the identifiability of this model using the Taylor Expansion Method, also called the Power Series Expansion method. Identifiability analysis informs the choice of appropriate numerical approaches for subject-specific parameter estimation. This work contributes to an improved understanding of hepatic IR in PCOS that may help to guide the development of targeted therapeutics.

1145 - Modeling Transmission Dynamics of Avian Influenza under Periodic Environmental Conditions

Naveen Vaidya, University of Missouri - Kansas City

Understanding the Avian Influenza (AI) dynamics in wild aquatic birds is critical to predicting disease risk in wild and domestic birds and preventing transmission to humans. Persistence of AI virus in water is highly sensitive to environmental conditions such as temperature, which varies seasonally and geographically. In this talk, I will present a mathematical model to study the effects of time-varying environmental conditions on AI dynamics. Analyzing our models for the local and the global AI dynamics, we derive mathematical formulations of basic reproductive numbers and AI invasion thresholds. We show that apart from the mean temperature, the amplitude of the periodic temperature profile plays a significant role in the AI invasion as well as the long-term AI persistence in wild birds. Our results show that time-varying environmental temperature predicts several interesting features of avian influenza dynamics, which are observed in real data: peak-time variation, place-to-place variation, and seasonal double peaks (summer and fall).

1146 - A Population Model with Age Structure and Periodically Distributed Time Delay

Xiang-Sheng Wang, Southern Missouri State University

We propose a population model with age structure and periodically distributed time delay. A standard linear chain trick reduces the delay differential equation into an infinitely dimensional ordinary differential system. Asymptotic expansion of the solution and approximate formula of basic reproduction number are obtained.

Sessions in 317 BCH

Partial Differential Equations: Analysis, Modeling, and Applications

1147 - Impacts of Allee Effect and Maturation Time Delay on Dynamics of a Nonlocal Delayed Reaction Diffusion Population Model

Majid Bani-Yaghoub, University of Missouri - Kansas City

We numerically study the dynamics of a nonlocal delayed reaction diffusion population model with respect to maturation time delay and Allee effect growth types. With a weak Allee effect, delay-induced solutions bifurcate from the positive steady state. With a strong Allee effect, the increased time delay first results in two wave solutions traveling in the opposite directions in the spatial domain and thereafter the solution converges to the trivial steady state. Hence, the single species population goes extinct due to increased maturation time delay, only when there is a strong Allee effect. The other implication of a strong Allee effect is the existence of stationary wavefront and wave pulse solutions, where the global stability of these solutions are numerically investigated.

1148 - Split-Step Method for Nonlinear Schrodinger Equation

Siwei Duo, Missouri University of Science and Technology

Split-step methods have been widely used in solving time-dependent PDEs. In this talk, we discuss the numerical stability of the split-step method for solving the (fractional) nonlinear Schrodinger (NLS) equation. The stability conditions are analyzed for the plane wave solutions, and numerical experiments are provided to verify our analytical results. In addition, the performance of the split-step method is studied and compared in solving the standard and fractional NLS.

1149 - Recovery of a Boundary Flux Using Far Boundary Data

Seth Oppenheimer, Mississippi State University

We consider a mold of a uniform material. It is idealized as one-dimensional and of length one. The left endpoint, x=0, will be in contact with cooling molten metal. The right endpoint, x=1, will be exposed to air at a constant temperature. Assuming we know the temperature and heat flux at the right endpoint, we wish to recover the heat flux at the left endpoint. This problem is a relative of the sideways heat equation. We will discuss well-posedness and qualitative properties for the forward problem and some numerical results for the inverse problem. This is Joint work with Mark S. Riggs of Ashland Community and Technical College.

1151 - Parabolic PDEs for Fluid, Flame, and Plasma Dynamics: When Are Solutions Bounded?

John Singler, Missouri University of Science & Technology

Many parabolic PDEs modeling fluid, flame, and plasma dynamics have quadratic, energy-conserving nonlinear terms. If the linear term in such a PDE is coercive, then standard energy estimates show that the energy norm of the solution remains bounded for all time. However, for many models the linear term is not coercive and it is not immediately clear that solutions remain bounded. We present results showing solutions remain bounded for a general class of such PDE models, and we demonstrate that many fluid, flame, and plasma models fall in this framework.

1152 - An Acoustic Eigenvalue Problem Related to Electrochemistry

Gerhard Strohmer, The University of Iowa

If one exposes an electrolyte contained in a small vessel with an open top to ultrasound, one can observe phenomena that are strongly dependent on the shape of the free surface. We introduce a model for the sound propagation incorporating the wave equation with Neumann boundary conditions in part determined by the linearized mean curvature at the top. It turns out that the Laplace operator with these boundary conditions is self-adjoint and the eigenfunctions, which represent standing waves, are dense in the space and can be numerically computed by variational considerations.

1153 - The Morse and Maslov Indices for Schrodinger Operators

Selim Sukhtaiev, University of Missouri Columbia

For Schrodinger operators with matrix valued periodic potentials, we discuss relations between the Morse index, counting the number of unstable eigenvalues, and the Maslov index, counting the number of signed intersections of a path in the space of Lagrangian planes with a fixed plane.

Sessions in 318 BCH

Recent Advances in Numerical Methods for Interface Problems

1154 - An Immersed Discontinuous Q1/Q0 Finite Element Method for the Stokes Interface Problem

Slimane Adjerid, Virginia Tech

We present a finite element method for solving two phase flows modeled by the Stokes interface problem using nonfitted meshes that are cut by the interface. Using the jumps across the interface, we are able to construct special Q1/Q0 finite element spaces on elements cut by the interface which are combined with both NIPG and SIPG finite element formulations. We solved both the two-dimensional and three-dimensional axisymmetric Stokes interface problems with moving interfaces which we track using a set of control points. Extensive numerical results show that the proposed immersed finite element spaces yield optimal convergence rates for the velocity and pressure and show that the proposed methods are conservative and may be used without remeshing steps.

1155 - Residual-Based a Posteriori Error Estimate for Interface Problems: Nonconforming Linear Elements

Cuiyu He, Purdue University

We study the residual-based a posteriori error estimation for the nonconforming linear finite element approximation to the interface problem. We introduce a new and direct approach, without using the Helmholtz decomposition, to analyze the reliability of the estimator. It is proved that a slightly modifed estimator is reliable with the constant independent of the jump of the interfaces, without the assumption that the diffusion coefficient is quasi-monotone. Numerical results for a test problem with interesting interfaces will also be presented.

Session Abstracts | 318 BCH

1156 - A Rescaling Scheme and Its Applications in Moving Boundary Problems

Shuwang Li, Illinois Institute of Technology

In this talk, I will first show a few examples of moving boundary problems. Then I will present an efficient rescaling scheme for computing the moving interface. The scheme is based on the idea of self-similarity that enables one to scale the time and space appropriately and achieve: (1) for slow interface growth problems, one can speed up the computation to gain exponentially fast growth; (2) for rapid interface shrinking problems, one can slow down the calculation to zoom in the details of interface morphology.

1157 - Weak Galerkin Finite Element Methods and Numerical Applications

Lin Mu, Michigan State University

Weak Galerkin finite element methods are new numerical methods for solving partial differential equations that were first introduced by Wang and Ye for solving general second order elliptic partial differ- ential equations (PDEs). The differential operators in PDEs are replaced by their weak forms through the integration by parts, which endows high flexibility for handling complex geometries, interface discontinuities, and solution singularities. This new method is a discontinuous finite element algorithm, which is parameter free, symmetric, and absolutely stable. Furthermore, through the Schur-complement technique, an effective implementation of the weak Galerkin is developed a linear system involving unknowns only associated with element boundaries. In this talk, several numerical applications of weak Galerkin methods will be discussed.

1158 - Interface Problem Arising in Quantifying Mitral Regurgitation

Yifan Wang, University of Houston

Mitral regurgitation (MR) is a disorder of the heart in which the mitral valve fails to close completely during ventricular systole. This causes blood to flow back from the left ventricle into the left atrium and can lead to atrial arrhythmias, congestive heart failure and death. The decision to proceed with surgical valve repair is based on an assessment of symptoms and valve regurgitation severity. Echocardiography is primarily used to assess the severity of MR. However, the accuracy and reproducibility of the method is questionable. A recently proposed clinical 3D color Doppler method to quantify MR is based on measurement of the diameter or area of the regurgitant jet at regurgitant orifice. Clinically this narrow jet region, known as the vena contracta (VC), is mainly dependent on the size of the regurgitant valve orifice. The severity of MR can be estimated by evaluating VC area. As this technique continues to evolve, computational models of mitral valve regurgitant flows are desired to support, quantify and reinforce it. Our simulation model consists of a deformable heart chamber, an orifice and interacting blood fluid, which are coupled through suitable conditions at the interface. The main challenges in our model are the fine resolution of the realistic structure of the heart chamber and relative high Reynolds blood flow. Therefore, different numerical methods, i.e., Discontinuous Galerkin method and conventional finite element method are used to conduct numerical simulations. Large scale simulations are also conducted on stampede at TACC (Texas Advanced Computing Center).

1159 - A New Poisson-Boltzmann Equation Hybrid Solver Intermixing with Solution and Domain Decompositions, Finite Element, and Finite Difference

Dexuan Xie, University of Wisconsin-Milwaukee

The Poisson-Boltzmann equation (PBE) is a singular nonlinear interface problem. It has been widely applied to the calculation of electrostatics for ionic solvated biomolecules. However, PBE was often solved numerically without considering the flux interface conditions to simplify the numerical solution of PBE. Each involved Dirac delta distribution was also simply approximated as a continuous function to overcome the singularity difficulty. Such traditional treatments caused the current popular PBE solvers to suffer the problems of low numerical solution accuracy and poor numerical stability. To develop a PBE solver with numerical convergence and stability, in the past ten years, several solution decomposition schemes were proposed to solve PBE as the interface problem, including our recent work. In this talk, we will present a new PBE hybrid solver, which is constructed by the techniques of solution decomposition, Schwartz's overlapped domain decomposition, finite element, and finite difference. This new hybrid PBE solver has been programmed as a software tool for predicting electrostatics of a protein in a symmetric 1:1 ionic solvent. Numerical results will be given to demonstrate its high performance. This project is a joined work with my student, Jinyong Ying, under the support by NSF award DMS-1226259.

1160 - A Simple and Accurate Discontinuous Galerkin Scheme for Modeling Scalar-Wave Propagation in Media with Curved Interfaces

Xiangxiong Zhang, Purdue University

Conventional high-order discontinuous Galerkin schemes suffer from interface errors caused by the misalignment between straight-sided elements and curved material interfaces. We develop a novel discontinuous Galerkin scheme to reduce the errors. We modify the numerical fluxes to account for the curved interface. Our numerical modeling example demonstrate that our new discontinuous Galerkin scheme significantly suppresses the spurious diffractions seen in the results obtained using the conventional scheme. The computational cost of our scheme is similar to that of the conventional scheme. Our new discontinuous Galerkin scheme is thus particularly useful for large-scale scalar-wave modeling involving complex subsurface structures.

1161 - Partially Penalized Immersed Finite Element Methods for Elliptic Interface Problems

Xu Zhang, Purdue University

In this presentation, we discuss a class of new immersed finite element (IFE) methods for a second order elliptic interface problem. The proposed methods can be used on Cartesian meshes regardless of the interface geometry. Compared to classic IFE methods using Galerkin formulation, these new IFE methods contain extra stabilization terms introduced at interface edges. A priori error estimation shows that the new IFE methods can converge optimally in a mesh-dependent energy norm. Our numerical results demonstrate that these new methods outperform classic IFE methods in the vicinity of interface.

1162 - Time Domain Interface Methods for Electromagnetic Wave Propagation in Dispersive Media

Shan Zhao, University of Alabama

Dispersive media are ubiquitous in nature, such as in biological tissues, rocks, soils, ice, snow, and plasma. In such media, the dielectric permittivity is a function of frequency so that a broadband electromagnetic wave will propagate and attenuate in a frequency dependent manner. The interaction of such a wave with a dispersive interface, which separates a dispersive medium and a non-dispersive medium, is a very complex electromagnetic process. In particular, the electromagnetic field discontinuity across the dispersive interface is known to be frequency-dependent or time-varying in time domain simulations. In order to track these transient jumps, we have developed novel Maxwell systems for both transverse magnetic (TM) and transverse electric (TE) problems. Based on the auxiliary differential equations, both Debye and Drude dispersive materials have been studied. The resulting time-dependent jump conditions are enforced via the matched interface and boundary (MIB) scheme. High order convergences are numerically achieved in treating complex and dispersive interfaces. This is a joint work with my PhD student Duc Nguyen.

Poster Sessions

BCH Atrium and St. Pat's Ballroom, Havener Center

Performance Evaluation of Sweep Implementations for 2-D Discrete-Ordinates Method

Wenkai Fu, Kansas State University

The performance of six different sweep implementations for the 2-D, multigroup, discrete-ordinates method is studied. Each sweep represents a loop over energy groups, angles, and spatial cells, and the order of these loops (e.g., EAS for energy-angle-space) greatly affects the sweep performance under serial, vectorized, and parallel conditions. Several test cases were run using randomized material properties to simulate the heterogeneous geometries characteristic of real nuclear reactors. With efficient use of cache, the time per sweep of the vectorized ASE and SAE sweep functions was approximately half of the time per sweep of the vectorized AES, EAS, ESA and SEA sweep functions. Thread-level parallelism based on OpenMP further improved the relative performance of the ASE sweep function. Specifically, the parallelized and vectorized ASE sweep outperformed the more traditional EAS sweep (as used, e.g., in the Detran code) by as much as a factor of six and the next-best cases by approximately a factor of two. Because modern (e.g., Krylov) solvers can be cast entirely in terms of a sweep over all energy groups, angles, and spatial cells, the results of this study show that any solver can be substantially improved by using an optimally-ordered transport sweep.

Immersed Finite Element Particle-in-Cell Methods for Modeling Plasma Interactions on the Lunar Surface

Daoru Han, University of Southern California

Understanding the plasma environment near the lunar surface is critical in both scientific and engineering perspectives. Numerical methods such as particle-in-cell (PIC) have been widely used to model such plasma problems. In this study, we use recently-developed 3-D immersed finite element (IFE) PIC methods to simulate the plasma flow near the surface of lunar terminator regions. Focuses will be given to the integration and validation of a 3-D non-homogeneous IFE solver into a standard PIC code to get the non-homogeneous IFE-PIC method capable of modeling multiple plasma-object interaction problems. Numerical results will be presented to demonstrate the capability of the non-homogeneous IFE-PIC method.

Age-Dependent Cell Division and Applications to the Luria-Delbrück Experiment

Hesam Oveys, University of Missouri

Populations adapt to their environment by acquiring advantageous mutations, but in the early twentieth century, questions about how these organisms acquire mutations arose. The experiment of Luria and Delbrück that won them a Nobel Prize in 1969 confirmed that mutation occurs at birth, and thus organisms follow Darwinian evolution instead of Lamarckian. Since then, there have been numerous implications that are still being expanded on today. Determining the number of mutants in a large population of cells is one such implication. Probability distributions that determine the number of mutants in a large population have been derived by Lea and Coulson and also Haldane. However, not much work has been done when time of cell division is a function of cell age, and even less so, when mother and daughter cells may grow differently, as is the case in most biological situations. Using probability generating function methods, we rigorously construct a model for how a single cell grows given a life span distribution, and then determine its asymptotic growth rate. We use this to construct a distribution for the number of mutants in a large population of cells.

A New Finite Element and Finite Difference Hybrid Method for Solving Size Modified Poisson Boltzmann Equation

Jinyong Ying, University of Wisconsin-Milwaukee

The uniform size modified Poisson Boltzmann equation (SMPBE) is an important variant of the Poisson Boltzmann equation to reflect the ionic size effect in the prediction of electrostatics for protein in ionic solvent. Recently, an effective SMPBE finite element algorithm and program package were developed in our group. To further improve the performance of this program package, we recently developed a new SMPBE finite element and finite difference hybrid method, which we constructed using domain decomposition and multigrid techniques. In this poster, we report this new hybrid solver with some details of new method and the new program package. Numerical results on a dipole model and six different proteins will be presented to show the high performance of this new program package. Finally, the convergent and stable properties of our hybrid solver will be discussed in the calculation of solvation and binding free energies.

Application of an Optic Disc Finder and Deep Learning to Detect Neo-Vascularization of the Optic Disc

Kasra Zarei, University of Iowa

Retinal neovascularization is characterized by a tangle of blood vessels on the retinal surface commonly caused by diabetes. Retinal neovascularization consists of hastily built blood vessels which lack the typical, bifurcating pattern of normal vessels, and bleed spontaneously. As a result of neovascularization, blood pours into the retina and leads to retinal detachment. Although rare, this condition leads to blindness and is hard for clinicians to detect. Fundus images (i.e. a photograph of the interior of the eye including the retina, optic disc, and other structures) were taken by clinicians. A dataset consisting of 30 fundus images of patients with diagnosed neovascularization of the optic disc, and hundreds of images of healthy, control patients was acquired. An optic-disc finder algorithm was developed and applied to the dataset to exclude all regions of the fundus images except for the optic disc of interest. Deep learning techniques were applied to this dataset using Caffe, a widely-used deep learning framework, in an attempt to classify optic discs as normal (i.e. no neovascularization) or displaying neovascularization. The performance of the deep learning approach was assessed by comparing the results to classifications from clinicians (i.e. expert truth).

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Missouri University of Science and Technology CAMPUS MAP

CLASSROOMS/LABS
1 James E. Bertelsmeyer Hall
2 Butler-Carlton Civil Engineering Hall
3 Computer Science Building
4 Emerson Electric Company Hall
5 Engineering Management Building
6 Fulton Hall
7 Gale Bullman Multi-Purpose Building
8 Harris Hall
9 Humanities and Social Sciences Building
10 IDE Building
11 V.H. McNutt Hall
12 Physics Building
13 Pine Building
14 Rock Mechanics and Explosive Research Center
15 Rolla Building
16 Schrenk Hall
17 Toomey Hall

RESEARCH/SUPPORT FACILITIES
18 Historic Bureau of Mines Building No. 1
19 Engineering Research Laboratory
20 MSTR
21 Technology Development Center
22 Straumanis-James Hall
23 Curtis Laws Wilson Library

STUDENT HOUSING
24 Farrar Hall
25 Miner Village
26 Nagogami Terrace
27 Residential College 1
28 Residential College 2
29 Thomas Jefferson Residence Hall

CAMPUS/STUDENT SUPPORT
30 605 W. 11th Street
31 Allgood-Bailey Stadium
32 Altman Hall
33 Athletic Fields
34 Campus Housing and Dining Services
35 Campus Support Facility
36 Castleman Hall
37 Centennial Hall
38 Chancellor's Residence
39 Custodial and Landscape Services Building
40 Fitness Center
41 General Services Building
42 Golf Course
43 Hasselmann Alumni House
44 Havener Center
45 Kummer Student Design Center
46 Miner Dome Indoor Practice Facility
47 Norwood Hall
48 Parker Hall
49 Power Plant
50 Southwestern Bell Cultural Center
51 Student Health Complex
52 Student Recreation Center
53 Temporary Facility A

CAMPUS LANDMARKS
54 E3 Commons
55 Millennium Arch
56 Observatory
57 The Puck
58 Solar Village
59 Stonehenge