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14. ABSTRACT
The conference was organized by Sigal Gottlieb, Fengyan Li, Jennifer Ryan, and Johnny Guzman. An outstanding group of the world's most distinguished mathematicians gathered to celebrate Professor Shu's legacy by presenting some of their most influential work in the field of applied and computational mathematics.

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Report Title

Final Report: 3.4 Frontiers in Applied and Computational Mathematics Conference

ABSTRACT

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Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received		Paper
05/02/2017	2	Johnny Guzman. Proceedings of Frontiers in Applied and Computational Mathematics Conference, Frontiers in Applied and Computational Mathematics. 04-JAN-17, Brown University, Providence, RI. : ,
05/25/2017	4	Sigal Gottlieb, Fengyan Li, Jennifer Ryan, and Johnny Guzman. Final Report: Frontiers in Applied and Computational Mathematics Conference, Frontiers in Applied and Computational Mathematics Conference. 05-JAN-17, Brown University, Providence, RI. : ,
TOTAL:	**2**	

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received	Paper
TOTAL:	

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received	Paper
TOTAL:	

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:...... 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

The funds from this grant were used to support the international conference, “Frontiers in Applied and Computational Mathematics”, which took place at the Institute for Computational and Experimental Research in Mathematics (ICERM), Brown University on January 4-6, 2017. This was a special conference organized on the occasion of Professor Chi-Wang Shu's sixtieth birthday and was dedicated to pushing the frontiers of scientific computing, mathematical modeling and applications. A notable feature of this conference was the focus on the integration of cutting edge numerical methods and mathematical analysis to tackle important physical applications.
Through this combination of theory, computation, and application we were able to highlight the role of significant mathematics in the design of advanced algorithms applicable to real world problems.

The diverse set of topics represented by the speakers led to a cross pollination of ideas across a variety of fields and aided in pushing forward the frontiers in applied and computational mathematics. To further promote this, we organized a moderated discussion and panel session where participants explored the frontiers of different research areas and possibilities of new connections between areas. We were also able to actively promote participation of young researchers (including students) and provide opportunities and guidance in identifying potential problems for study.

Technology Transfer

Frontiers in Applied and Computational Mathematics Conference
Grant Number: 69181MACF
Proposal Period: 1 April 2016 – 31 March 2017
PIs: Sigal Gottlieb, Fengyan Li, Jennifer Ryan, and Johnny Guzman

1. Objective

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2. Participation

The conference featured 21 invited speakers who have made tremendous contributions in applied and computational mathematics and included members of National Academy of Science and a Fields Medalist. The themes of the talks ranged from the underlying mathematics, including constructing better mathematical models, improving the numerical methods through finite element and discontinuous Galerkin methods, as well as more application oriented discussions such as modeling tsunamis. More specifically, Advances in Numerical Analysis (3.4.1.1), Multi-scale Methods (3.4.1.2), Fractional order methods (3.4.1.3) and Reduce order models (3.4.2.1) were topics strongly represented by the speakers. These themes aligned well with current research goals of the Army. More details are included in the attached conference proceedings. The stellar list of the invited speakers and the diverse set of topics represented by them attracted 124 participants from eleven countries (see attached photo). The participants ranged from graduate students to well-established researchers, who are either numerical analysts with strong interests in application, applied and computational mathematicians, or engineers.

The funds used to support this conference aided in supporting not only invited speakers, but also approximately 30 graduate student and junior researchers.

Attracting so many stellar speakers and attendees to one conference of this size is quite unique and shows the influence Chi-Wang Shu's research has had in our community. The numerical advances done by Chi-Wang Shu and the invited speakers have allowed the scientific computing community to simulate many important real phenomena that are of great interest to different funding agencies. Further, to illustrate the success of this conference, many of the participants were in attendance for the entire meeting.

3. Conference Activities

In addition to the 21 renowned invited speakers, there was a panel discussion session, a poster session, as well as many opportunities for interaction between the participants.

3.1.Invited Talks

The invited speakers have done fundamental work in applied and computational work, and many of them are currently doing cutting edge research that is in the frontiers of what is known. Among the list of research topics represented by the speakers in numerical methods are: computational fluid dynamics, numerical methods for hyperbolic PDEs, multi-scale methods, discontinuous Galerkin methods, stable time discretizations, spectral and high-order methods, finite difference and finite volume ENO and WENO methods, fast-marching and level set methods and computational methods for kinetic problems. Application areas include, tsunami modeling, gas dynamics, astrophysics, modeling of semi-conductor devices, electromagnetic dynamics, fluid dynamics, geophysical problems, image processing, among others.

To ensure that the conference appealed to the wide-ranging audience, we asked the speakers to give an introductory background and context for their talk. Additionally, we had one sequential session in order to enhance the cohesiveness of the conference. We also asked the speakers to look toward the future and present their vision of the new and interesting challenges.

3.2 Poster Session

To promote the cross-pollination of ideas, a poster session was organized with totally 39 presentations. The poster session primarily consisted of graduate student and junior researchers and was well attended. Many of the posters presenters were supported by travel funds from the ARO. The topics are outlined in the conference proceedings.

3.3 Discussion Panel

The purpose of this panel was for leading researchers in applied and computational mathematics to provide guidance to rising generations for their professional and scientific development. The panel provided opportunities to address aspects such as directions and trends of the field, career development, and funding opportunities. Some outcomes of this panel discussion were:

- Recommendation that we take a new perspective on applied and computational mathematics. That is, that the subject presents tools and techniques to solve real-world problems.
- The area of scientific computing can contribute or connect to emerging areas, such as data science. Some panelists expressed that the data aspect can not be neglected by the applied and computational mathematics community, and advocated combining the rapidly progressed data-related developments with the conventional physical models and computational tools.
- Avenues for encouraging young aspiring women mathematicians to pursue research in applied and computational mathematics through women in numerical analysis and scientific computing (WiNASC). This was facilitated by the fact that one of the conference organizers is on the AWM's network building committee and one organizer is building the AWM website for WiNASC. We note that there were three women speakers.
- Persistence is key to success whether it be for a faculty position or grant proposal, etc. As part of this, it was pointed out that research ideas evolve, change in time, and new applications are found.

4. Journal of Scientific Computing Special Issue

Many of the invited speakers have contributed a paper to a special issue in the Journal of Scientific Computing on the occasion of Chi-Wang Shu's 60th birthday. This special issue was open to other participants in the conference, and announced on the website and in all conference materials. Overall, we expect the special issue to have 31 high caliber articles. Even though this special issue is not formally the proceedings of this conference, it will cover many topics of the conference and will help in the promotion of the ideas discussed in the conference to broader audience.

Participants of “Frontiers in Applied and Computational Mathematics”, ICERM, January 4-6, 2017

Proceedings of
Frontiers in Applied and Computational Mathematics
January 4-6, 2017

The conference was organized by Sigal Gottlieb, Fengyan Li, Jennifer Ryan, and Johnny Guzman. An outstanding group of the world's most distinguished mathematicians gathered to celebrate Professor Shu's legacy by presenting some of their most influential work in the field of applied and computational mathematics. The conference took place at ICERM. Many of the talks are available for watching on ICERM's site.

1.Conference Schedule

	January 4	**January 5**	**January 6**
8:00-9:00	coffee and welcome	coffee	coffee
9:00-9:40	Sigal Gottlieb	Gilbert Strang	Jan S. Hesthaven
9:45-10:25	Bernardo Cockburn	Bjorn Engquist	Weinan E
10:30-10:45	coffee	coffee	coffee
10:45-11:25	Irene Gamba	Eitan Tadmor	James Glimm
11:30-12:10	Randy LeVeque	Mary Wheeler	Wai Sun Don
12:10-1:40	lunch	lunch	lunch
1:45-2:25	Marsha Berger	Stanley Osher	Philip Roe
2:30-3:10	Philip Colella	Shing-Tung Yau	Constantine Dafermos
3:15-3:30	coffee	coffee	coffee
3:35-4:15	Thomas Hou	Panel discussion	Remi Abgrall
4:20-5:00	Antony Jameson	Panel discussion	closing remarks
5:00-5:30	Poster session	Panel discussion	
5:30-6:00	Poster session	pre-banquet social	
6:00-8:00		Banquet	

2.Conference Talks: Titles and Abstracts

High order finite element methods for unsteady problems

Remi Abgrall,
Universität Zürich

This talk will deal with the numerical approximation of unsteady hyperbolic problems with continuous finite element methods. It is well known that these methods, as for discontinous galerkin methods, lead a mass matrix that needs to be inverted for applying the method of lines. This can be problematic because the mass matrix is only sparse, in contrast to DG where the mass matrix is block diagonal with small blocks. In this talk I will show how to avoid this problem. Thanks to a particular choice of basis functions and a particular class of integration method, we only need to invert a diagonal 'mass' matrix. I will explain the rational behind this, provide some element of proof and numerical examples.

Simulation and modeling of asteroid-generated tsunamis

Marsha Berger,
Courant Institute

In 1908 a large asteroid exploded in the atmosphere over Tunguska. The resulting blast wave leveled approximately 30 square miles of forest. There is a worry that if such an asteroid were to explode over the ocean, the blast wave could generate a large tsunami that would threaten coastal cities. Modern codes such as GeoClaw can simulate earthquake-generated tsunamis, but airburst-generated waves may be qualitatively different. The shorter length scales of the airburst pressure wave may make the shallow water equation model (which is a long wave approximation) inaccurate. The short time scales may make water compressibility important. We present simulations using GeoClaw for tsunami propagation from asteroid-generated air bursts under a range of conditions, using bathymetry from real coastlines. We also present analytical and semi-numerical studies of a one dimensional model problem to explore the effects of dispersion and compressibility. We compare the shallow water solution with a linearized Euler solution. Our results indicate that due to the short wave lengths of this type of tsunami, the shallow water equations may not be an appropriate model.

Discontinuous reminiscences

Bernardo Cockburn, University of Minnesota

I will provide a personal, completely biased account of the main ideas which drove the evolution of the so-called discontinuous Galerkin methods, from the early seventies, when the method was introduced for the neutron transport equation, to the nineties, when it was extended to nonlinear hyperbolic problems, to the present time, when it is being extended to a wide variety of partial differential equations.

Local Discrete Convolution Methods for Constant-Coefficient PDE on Locally-Structured Grids

Philip Colella,
University of California, Berkeley

The numerical solution of classical constant-coefficient PDE on structured and locally-refined grids is a ubiquitous core component of a broad range of problems in computational physics. However, these problems have the potential for being a significant bottleneck in the development of high-performance and scalable simulations on the coming generations of low-power processor architectures: the classical finite-difference methods that have been customarily used for these problems perform a relatively small number of floating point operations per unit of data transfer, in a setting where data motion is more expensive, and the ratio of floating-point capabilities to the bandwidth through the memory hierarchy is much larger than that of more traditional processor architectures. In this talk, we will discuss approaches to solving such problems based on local Green's function methods on locally structured grids, in which the computational kernels are small discrete convolutions that fit on a single processor and are computed using FFTs and Hockney's method. Such methods can be designed to reduce amount of data traffic at the cost of increasing the amount of floating point operations performed, in a way that leads to a smaller time to solution than more traditional structured-grid methods. We will discuss two examples of this approach: one based on the Method of Local Corrections for Poisson's equation, the other for Maxwell's equations based on a variation of Kirchhoff's method of spherical means.

BV solutions to the Cauchy problem

Constantine Dafermos, Brown University

The lecture will survey a program for constructing BV solutions to the Cauchy problem for hyperbolic systems of balance laws with partially dissipative source.

Recent Development of High Order WENO and Hybrid Finite Difference Schemes

Wai-Sun Don, Ocean University of China

Ever since the development of the high order WENO finite difference scheme by Jiang and Shu, it has been widely adopted for solving hyperbolic conservation laws that captures shocks essentially non-oscillatory while resolving fine scale structures efficiently. Numerous advances have been proposed to reduce the dissipation and dispersion errors by improving/modifying certain critical components of the WENO reconstruction procedure, such as, the definitions of nonlinear weights and the smoothness indicators and the tuning of existing parameters. In this talk, I will present some recent topics and results regarding 1) the role of the smoothness indicators play in the symmetry-preserving property of a symmetrical problem, 2) the positivity-preserving property of the 5th and 7th order WENO FD scheme with global and Local LF flux splitting for some often cited benchmark problems under extreme conditions and 3) the role of the smoothness and power parameters play on functions with critical points. Finally, despite the enhancement of the scheme, hybrid scheme that conjugates the high order linear compact and nonlinear WENO FD scheme can be employed to improve the performance of the scheme in the smooth regions of the solution. I will briefly discuss several key components and enhancements to improve the robustness of the high order shock detection algorithms.

Theory and application of stochastic gradient algorithms

Weinan E, Beijing Institute of Big Data Research and Princeton University

Stochastic gradient algorithms have been very popular in machine learning and have been THE algorithm of choice for very large data sets. We provide a detailed analysis of the dynamical behavior of this algorithm that captures both the details of the initial exponential convergence behavior as well as the final fluctuations. We also analyze the various acceleration schemes, compute the optimal learning rate and mini-batch size. We conclude by showing some novel new application areas for these algorithms.

Fast algorithms for high frequency wave propagation

Bjorn Engquist, University of Texas, Austin

Direct numerical approximation of high frequency wave propagation typically requires a very large number of unknowns and and are computationally very costly. We will discuss two aspects of this type of problem. One is the development and analysis of fast algorithms of optimal computational complexity for boundary integral formulations and variable coefficient differential equations. The other aspect is analysis revealing when algorithms of the type mentioned is possible and when it is not.

Conservative schemes for the Boltzmann and Landau transport equations

Irene Gamba, University of Texas at Austin

These are computational models at the core of collisional plasma theory. In particular we will discuss several aspects of conservative solvers for the kinetic transport equations of particle interactions, that involve either linear or non-linear Boltzmann as well as the non-linear Landau equations, by means of stagger conservative DG schemes for the transport part and DG or spectral solvers for the collisional parts, linked by a projection method that is conservative. In addition, we will discuss the computational aspects of boundary layer formation due to rough boundary effects for insulating conditions.

Scaling laws and stochastic random field equations for turbulent velocity gradients and fluctuations

James Glimm, University at Stony Brook

The Kolmogorov-Obukhov 1962 theory for the turbulent dissipation rate is extended to a space-time theory governed by stochastic random field equations. New scaling laws are derived from a new universality principal, and allow simple parameterization of the stochastic equations. In the context of a large eddy simulation, subgrid time and statistical scales are rescaled by factors depending on the resolved scale flow. The result is a universal statitics for the variance and decay time scale of the turbulent fluctuations, and a stochastic subgrid model for these fluctuations. The covariance and time scale in this theory both satisfy simple power laws. A stochastic subgrid scale model is developed from this theory for particles transported by turbulent flow. Limitations of this theory for a large number of modeled length scales are mentioned, and a renormalization group framework is indicated to address the limitation. This model is applied to the clustering of particles in low turbulent regions. (This is a joint work with Vinay Mahadeo.)

The work of Professor Shu: The first 60 years
Sigal Gottlieb, University of Massachusetts, Dartmouth

In this talk we will review Ch-Wang Shu's major contributions to our field.

Stucture preserving reduced order models
Jan Hesthaven, EPFL

Reduced basis methods have emerged as a powerful approach for the reduction of the intrinsic complexity of parametrized partial differential equations. However, standard formulations of reduced models do not generally guarantee preservation of symmetries, invariants, and conservation laws of the original system. This questions the validity of such models and has a number of unfortunate consequences, e.g., lack of stability of the reduced model. In this talk we discuss the recent developments of reduced methods that ensure the conservation of chosen invariants or key properties of the original problem. We shall pay particular attention to the development of reduced models for Hamiltonian problems and propose a greedy approach to build the basis. The performance of the approach is demonstrated for both ODEs and PDEs. We subsequently discuss the extension of these techniques to ABC flows and, time permitting, point toward different directions and open questions within the development of reduced order models for time-dependent problems. (This is a joint work with Babak Maboudi Afkham)

Sparse operator compression of elliptic operators
Thomas Yizhao Hou, Caltech

We introduce a systematic approach to construct localized finite element basis functions for any (2k)th-order elliptic problems (k>0 is an integer) with heterogeneous and multiscale coefficients without scale separation. The basis functions are energy minimizing functions on local patches. On a regular mesh with mesh size h, the basis functions have supports of diameter h(log(1/h)) and have the optimal convergence rate O(h^k) for (2k)th-order elliptic problems measured by the associated energy norm. From the perspective of operator compression, these localized basis functions approximate accurately the principal eigen-space of the corresponding elliptic operators, and thus provide an efficient and optimal way to compress elliptic operators of any order with localized basis. From the perspective of the Sparse PCA, our results show that a large set of covariance functions can be approximated by a rank-n operator with optimal accuracy, i.e., on the order of its nth eigenvalue, and that the range space of the rank-n operator can be spanned by a localized basis. In contrast to the traditional error analysis of FEM that utilizes the interpolation type polynomial approximation property in the Sobolev Spaces, the projection type polynomial approximation property in the Sobolev Spaces plays an essential role in the error analysis of our new method. Our method provides a solid foundation to build new multigrid methods for solving linear systems and eigenvalue decomposition for elliptic operators. This is a joint work with Mr. Pengchuan Zhang.

Application of Dual Time Stepping to Fully Implicit Runge-Kutta Schemes for Unsteady Flow Calculations & Future Directions in Computational Fluids Dynamics

Antony Jameson, Stanford University

This talk presents the formulation of a dual time stepping procedure to solve the equations of fully implicit Runge-Kutta schemes. In particular the method is applied to Gauss and Radau 2A schemes with either two or three stages. The schemes are tested for unsteady flows over a pitching airfoil modeled by both the Euler and the unsteady Reynolds averaged Navier Stokes (URANS) equations. It is concluded that the Radau 2A schemes are more robust and less computationally expensive because they require a much smaller number of inner iterations. Moreover these schemes seem to be competitive with alternative implicit schemes.

In this talk we will also present some of the key challenges in computational fluid dynamics (CFD) today and outline future directions for the field. Specific issues that we will address include the impact of heterogeneous massively parallel computing hardware, the need for new and novel numerical algorithms, and the increasingly complex nature of methods and their respective implementations. The role of 'grand challenge' problems as a driving force is also considered. (This is a joint work with F. D. Witherden.)

Coupling Seismic and Tsunami Modeling

Randall J. LeVeque, University of Washington

Tsunami modeling is often performed using the two-dimensional shallow water equations, while seismic waves generated by an earthquake can be modeled with three-dimensional elasticity. Both of these are hyperbolic systems of PDEs for which high-resolution finite volume methods based on Riemann solvers are a good choice of numerical method. In both cases, the wide range of spatial scales makes adaptive mesh refinement desirable and highly effective. The open source software Clawpack (Conservation Laws Package) has been designed to solve a very general class of hyperbolic problems with adaptive refinement. The GeoClaw subset of Clawpack has been extensively developed over the past decade for modeling tsunamis and related geophysical hazards such as storm surge and landslides. Typically a homogeneous elastic halfspace solution is used to approximate the static seafloor deformation resulting from a tsunami-generating earthquake. In recent work with Chris Vogl, a seismic earthquake model is being developed to provide better coupling of subduction zone earthquake models to the tsunamis they generate, with potential applications to early warning systems.

Overcoming the Curse of Dimensionality for Hamilton-Jacobi equations with Applications to Control and Differential Games

Stanley Osher, University of California at Los Angeles

It is well known that certain Hamilton-Jacobi partial differential equations (HJ PDE's) play an important role in analyzing control theory and differential games. The cost of standard numerical algorithms for HJ PDE's is exponential in the space dimension and time, with huge memory requirements. Here we propose and test methods for solving a large class of these problems without the use of grids or significant numerical approximation. We begin with the classical Hopf and Hopf-Lax formulas which enable us to solve state independent problems via variational methods originating in compressive sensing with remarkable results. We can evaluate the solution in 10^(-4) to 10^(-8) seconds per evaluation on a laptop. The method is Embarrassingly parallel and has low memory requirements. Recently, with a slightly more complicated, but still embarrassingly parallel method, we have extended this in great generality to state dependent HJ equations, apparently, with the help of parallel computers, overcoming the curse of dimensionality for these problems. The term, "curse of dimensionality" was coined by Richard Bell man in 1957 when he did his classic work on dynamic optimization. (This is a joint work with Jerome Darbon, Yat-Tin Chow, and Wotao Yin.)

Is discontinuous reconstruction really a good idea?

Philip Roe, University of Michigan

Godunov's 1959 paper is the spiritual ancestor of almost all of the numerical methods in use today for the solution of hyperbolic conservation laws. His inspired innovation was to put the initial data in a form to which the exact evolution operator, or a close approximation of it, could be applied. This form was a projection into the class of cellwise constant functions, with discontinuities at the cell boundaries. Although it became apparent early on that this procedure did have drawbacks, such as poor representations of oblique waves and excessive dissipation at low Mach numbers, no other unifying concept has yet enjoyed the same degree of success. The discontinuous Galerkin method continues this kind of representation, and in simple enough situations enjoys the phenomenon of superconvergence, which is often held to flow from use of a discontinuous representation. However, it will be shown that dG methods for linear advection can also be derived from a continuous viewpoint, and that in fact the superconvergence follows from insisting on maximal smoothness, in the sense that as many degrees of freedom as possible should be shared between elements. A scheme for the multidimensional acoustic equations will be described that is based on a continuous FE representation, is upwind, fully discrete, explicit, isotropic, conservative and maximally stable. Results will also be shown for the nonlinear Euler equations.

Lagrange Interpolation is Stable in the Inside Interval

Gilbert Strang, Massachusetts Institute of Technology

The Lax-Wendroff finite difference method for the wave equation is essentially 3-point Lagrange interpolation -- and it is the first in a sequence of increasingly accurate interpolations.

THEOREM: They are all stable for Courant numbers below 1. The limit has infinite accuracy and the familiar Lagrange polynomials approach sinc functions! The spectrally accurate interpolation becomes Shannon's's interpolation formula for band-limited functions. We discuss these Toeplitz and circulant matrices, finite and infinite.

Spectral gap and critical thresholds in two-dimensional hydrodynamic flocking

Eitan Tadmor, University of Maryland and ETH-ITS Zürich

We discuss the question of global regularity for a general class of Eulerian dynamics driven by a forcing with a commutator structure. The study of such systems is motivated by the hydrodynamic description of agent-based models for flocking driven by alignment. For commutators involving bounded kernels, global regularity follows for sub-critical initial data such that the initial divergence is "not too negative" and the initial spectral gap is "not too large". A similar role of the spectral gap appears in the study of two-dimensional pressure-less equations. Here, we develop a new L^1 framework to prove the existence of weak dual solutions for the 2D pressure-less Euler equations. The derivation of these dual solutions as vanishing viscosity limits is based on new BV estimates associated with the spectral gap of the velocity gradient matrix.

Enriched Galerkin finite element methods (EG)

Mary F. Wheeler, The University of Texas at Austin

We present and analyze enriched Galerkin finite element methods (EG) to solve coupled flow and transport system with jump coefficients referred as miscible displacement problems. The EG is formulated by enriching the conforming continuous Galerkin finite element method (CG) with piecewise constant functions. This approach is shown to be locally and globally conservative while keeping fewer degrees of freedom in comparison with discontinuous Galerkin finite element methods (DG). Also, we present and analyze a fast and effective EG solver for flow simpler than DG and whose cost is roughly that of CG and can handle an arbitrary order of approximations. Moreover, to avoid any spurious oscillations for the higher order transport system, we employ an entropy residual stabilization technique. Dynamic mesh adaptivity using hanging nodes is applied to save computational cost for large-scale physical problems. Some numerical tests in two and three dimensions are presented to confirm our theoretical results as well as to demonstrate the advantages of the EG. Computational results for two phase flow in porous media are also discussed. This work was done in collaboration with Sanghyun Lee and Young-Ju Lee.

Efficient numerical method for nonlinear filtering problem

Shing-Tung Yau, Harvard University

In this talk , we shall explain how to solve Zakai equation that appeared in nonlinear filtering problem. The theoretical approach was devised by Stephen Yau and myself more than ten years ago. The numerical method was implemented and discussed in this talk. This is a joint work with Wen Wei Lin and Mei Cheng Yueh

3. Poster Presentations

The concept of the dividing surface in collinear Hydrogen exchange reaction.

Ali Allaham, Qassim University, Saundi Arabia

Transition state theory (TST) describes the elementary chemical reaction rate. There are three main regions in the reaction: reactant, product and the transition state (TS). The transition state must have two properties to make the transition state theory exact: all reactive trajectories must cross the TS (dividing surface) and the reactive trajectories cross it only once. Dynamical effects recrossing is possible from coupling in kinetic energy where TST provides upper bound of the exact reaction rate. Historically, (Wigner 1938) developed the reaction rate theory and extended the idea from con figuration space to phase space. (Pollak et al 1978) found the structure of the dividing surface in the collinear H2 + H reaction. It is well-known as unstable periodic orbit dividing surface (PODS). We are going to talk about the reactivity on the dividing surface of this reaction.

Discontinuity-Driven Mesh Adaptation Method for Hyperbolic Conservation Laws

Mihhail Berezovski, Embry-Riddle Aeronautical University

We developed a highly accurate, efficient, and robust adaptive-mesh computational method for hyperbolic systems of conservation laws, with particular reference to problems with evolving discontinuities. The main idea is to combine the flexibility afforded by a dynamically moving mesh with the increased accuracy and efficiency of a discontinuity tracking algorithm, while preserving the stability of the scheme. Key features of proposed method are accuracy and stability, which will be ensured by ability of the adaptive technique to preserve the modified mesh as close to the original fixed one as possible.

A discontinuous Galerkin method for Schrodinger equation with optimal accuracy

Anqi Chen, Michigan State University

In this work, we study a discontinuous Galerkin scheme for solving Schrodinger equation. The scheme does not introduce any auxiliary variables, and we prove its stability and optimal accuracy for a large class of flux with varying parameter choices. The optimal convergence rate is established based on global and local projection techniques. (Joint work with Yingda Cheng)

A Sparse Grid Discontinuous Galerkin Method for High-Dimensional Transport Equations

Yingda Cheng, Michigan State University

We present a sparse grid discontinuous Galerkin (DG) scheme for transport equations and applied it to kinetic simulations. The method uses the weak formulations of traditional Runge-Kutta DG schemes for hyperbolic problems and is proven to be \$L^2\$ stable and convergent. A major advantage of the scheme lies in its low computational and storage cost due to the employed sparse finite element approximation space. This attractive feature is explored in simulating Vlasov and Boltzmann transport equations. We also discuss extension of the scheme to adaptive sparse grid methods.

Fractally homogeneous, air-sea turbulence and the moment field equations,

Colton Conroy, Columbia University

Abstract: We investigate atmospheric turbulence along with the wind-waves it generates. In particular, we examine the local distribution of turbulence along space-time paths rather than that of traditional spatial distributions. These temporal distributions are unique functions of a set of characteristic variables that represent the large scale dynamics of the space-time path under consideration. More specifically, we utilize a temporal self-similar kernel to "pave" large scale averages and construct a wind curve whose fractal dimension is consistent with theory and observation. The local kernel provides exact perturbation relations for the characteristic frequency and variance of the wind-sea, and immediately gives rise to an expression for the local pressure in terms of the kinetic energy of the atmosphere, which serves as an initiator of the air-sea energy transfer. We cement this energy transfer mechanism in terms of the dispersion relation and group velocity of the wind-waves, providing unambiguous local source terms for a system of moment field equations—equations that preserve discrete spectral fluctuations of the short-crested gravity waves—in which the solution is more tractable than that of traditional frequency-resolving spectral methods. The model is discretized using unstructured RKDG methods, where all the primary variables including the integrated direction of the moment field are discretized with discontinuous polynomial spaces of arbitrary order. Numerical results illustrate the generation and propagation of the waves, while hindcasts over Lake Erie evaluate the wind-sea assumptions inherent to the model.

Multi-dimensional filtering: Reducing the dimension through rotation

Julia Docampo Sanchez, University of East Anglia

Abstract: Over the past few decades there has been a strong effort in the development of Smoothness-Increasing Accuracy-Conserving (SIAC) filters for Discontinuous Galerkin (DG) methods, designed to increase the smoothness and improve the convergence rate of the DG solution through this post-processor. These advantages can be exploited during flow visualization, for example by applying the SIAC filter to the DG data before streamline computations [Steffan {\it et al.}, IEEE-TVCG 14(3): 680-692]. However, introducing these filters in engineering applications can be challenging since a tensor product filter grows in support size as the field dimension increases, affecting the computational costs. As an alternative, [Walfisch {\it et al.}, JOMP 38(2);164-184] proposed a univariate filter implemented along the streamline curves. Until now, this technique remained a numerical experiment. In this work we introduce the {\it SIAC Line filter} and explore how the orientation, structure and filter size affect the order of accuracy and global errors. We discuss how line filtering preserves the properties of traditional tensor product filtering, including smoothness and improvement in the convergence rate. Furthermore, numerical experiments are presented, exhibiting how these

filters achieve the same accuracy at significantly lower computational costs, becoming an attractive tool for the scientific visualization community. Co-authors: Jennifer K. Ryan, Mahsa Mirzargar, Robert M. Kirby.

Time-stepping and the numerical flux in superconvergence of discontinuous Galerkin methods

Daniel Frean, University of East Anglia, UK

Numerical solutions to hyperbolic conservation laws whose spatial discretization is completed by the discontinuous Galerkin (DG) method often profit from a superconvergence property. We consider how superconvergence properties are affected by the pairing of DG with a time-stepping method as well as by the choice of flux function in the spatial discretization. We present theoretical results for linear equations and illustrate nonlinear cases with numerical experiments. This is joint work with Jennifer Ryan.

A high-order targeted ENO scheme for the large eddy simulation of incompressible and compressible turbulence

Lin Fu, Technical University of Munich

Although TENO schemes show promising results for turbulence reproduction, they are unsuitable to function as a reliable subgrid LES model by generating excessive dissipation. Meanwhile, the state-of-the-art implicit LES models, e.g. the localized artificial diffusivity scheme,typically depend on shock sensors, which are case-dependent and fail to retain the monotonicity near discontinuities. The difficulty locates on scale-separating the low-wavenumber smooth regions, high-wavenumber fluctuations and discontinuities sufficiently and incorporating adequate dissipation into numerical schemes correspondingly. In this paper, we propose a new 8-point 6th-order TENO8-A scheme. which is motivated for gas dynamics and physics-consistent for incompressible and compressible turbulence modeling. While the low-wavenumber smooth region is handled by the optimized linear scheme, with the measurement of local flow scales, the high-wavenumber fluctuations and discontinuities are predicted with adaptive nonlinear dissipation. The new scheme is Galilean invariant and free from physics-based sensors rendering its high generality. Benchmark simulations demonstrate that, while the TENO8-A scheme exhibits exceptional performance in gas dynamics, it faithfully reproduces the kinetic energy evolution for incompressible turbulence and predicts the vorticity, entropy and acoustic modes as good as the physics-motivated ILES models for compressible turbulence decay. Co-authors"Lin Fu, Xiangyu Y. Hu, Nikolaus A. Adams".

Resilience Analysis for Multigrid Methods

Christian Glusa, Brown University

We present a framework for the analysis of linear iterative methods in fault-prone environments such as next-generation HPC systems. The effects of failures are taken into account through a probabilistic model involving random diagonal matrices. Using this model, we analyze the behavior of two- and multigrid methods under random node failures. Our results show that while standard multigrid is not resilient, protecting the prolongation leads to a fault-resilient variant. This is joint work with Mark Ainsworth

A hybrid algorithm for shallow water flows with horizontal temperature gradients

Gerardo Hernandez-Duenas, National University of Mexico

In this work, shallow water flows in one and two dimensions with a thermodynamic component are considered. Horizontal temperature gradients are incorporated in the system where a potential temperature is advected by the flow. A two way feedback between the potential temperature, the water's flow and topography is ensured through the pressure and source terms in the momentum equation. The system is hyperbolic with two shock-wave families and a contact discontinuity associated to the potential temperature and the interface between warm and cold water. This new field is degenerate with pressure and velocity as the corresponding Riemann invariants. Numerically recognizing such invariants across contact discontinuities is important to correctly compute the flow near interface regions where the potential temperature jumps. Here we present a numerical algorithm that correctly captures all waves with a hybrid strategy. The method integrates the Riemann invariants near contact discontinuities and switches back to the conserved variables away from it to properly resolve shock waves. For illustration, we use a Roe-type upwind scheme. However, this strategy can be applied to any numerical scheme. Numerical solutions in one and two dimensions are shown to illustrate the advantages of the strategy and the merits of the scheme.

Numerical simulations of the humid atmosphere above a mountain

Youngjoon Hong, University of Illinois, Chicago

New avenues are explored for the numerical study of the two dimensional inviscid hydrostatic primitive equations of the atmosphere with humidity and saturation, in presence of topography and subject to physically plausible boundary conditions for the system of equations. Flows above a mountain are classically treated by the so-called method of terrain following coordinate system. We avoid this discretization method which induces errors in the discretization of tangential derivatives near the topography. Instead we implement a first order finite volume method for the spatial discretization using the initial coordinates x and p. A compatibility condition similar to that related to the condition of incompressibility for the Navier-Stokes equations, is introduced. In that respect, a version of the projection method is considered to enforce the compatibility condition on the horizontal velocity field, which comes from the boundary conditions. For the spatial discretization, a modified Godunov type method that exploits the discrete finite-volume derivatives by using the so-called Taylor Series Expansion Scheme (TSES), is then designed to solve the equations. We report on numerical experiments using realistic parameters. Finally, the effects of a random small-scale forcing on the velocity equation is numerically investigated.

Adaptive High-Order Central ENO Method for Inviscid, Viscous and Magnetized Flows

Lucian Ivan, Canadian Nuclear Laboratories

High-order schemes have been actively pursued in an effort to reduce the cost of large-scale scientific computing applications. Moreover, for numerical simulations of physically complex flows having a wide range of spatial and temporal scales both high-order discretizations and adaptive mesh refinement are often demanded. For hyperbolic conservation laws the challenge has been to achieve accurate discretizations while coping in a reliable and robust fashion with discontinuities and shocks. Essentially non-oscillatory (ENO) schemes and weighted ENO (WENO) methods provide a robust framework for high-order finite-volume discretizations of hyperbolic systems. While successful implementations of this class of finite-volume scheme have been developed, in general the computational costs and complexity of the schemes have somewhat limited their widespread application, especially for multi-dimensional problems and large systems of coupled partial differential equations (PDEs). To address some of the issues, a high-order central essentially non-oscillatory (CENO) finite-volume procedure has been proposed for the solution of hyperbolic systems of equations. The spatial discretization is based on a hybrid solution reconstruction procedure that combines the unlimited high-order k-exact least-squares reconstruction technique of Barth based on a fixed central stencil with a monotonicity preserving limited piecewise linear least-squares reconstruction algorithm. Switching in the hybrid procedure is determined by a solution smoothness indicator that indicates whether or not the solution is resolved on the computational mesh. The limited reconstruction procedure is applied to computational cells with under-resolved and/or non-smooth solution content and the unlimited k-exact reconstruction scheme is used for cells in which the solution is fully resolved. Over the last decade the scheme has been extended and applied in combination with block-based adaptive mesh refinement to a variety of flows, including those governed by the Navier-Stokes, ideal magnetodynamics (MHD) and resistive MHD equations. More recently, the CENO method has been developed for flows pertaining to space physics on three-dimensional cubed-sphere grids with local anisotropic grid adaptivity. This poster provides a comprehensive overview of the development of high-order CENO methods and their application to inviscid, viscous and magnetized flows. Co-authors: Lucie Freret, Hans De Sterck, Clinton Groth

Offline-Enhanced Reduced Basis Method through adaptive construction of the Surrogate Parameter Domain

Jiahua Jiang, University of Massachusetts Dartmouth

Classical Reduced Basis Method (RBM) is a popular certified model reduction approach for solving parametrized partial differential equations. However, the large size or high dimension of the parameter domain leads to prohibitively high computational costs in the offline stage. In this work we propose and test effective strategies to mitigate this difficulty by performing greedy algorithms on surrogate parameter domains that are adaptively constructed. These domains are much smaller in size yet accurate enough to induce the solution manifold of interest at the current step. In fact, we propose two ways to construct the surrogate parameter domain, one through an Inverse Cumulative Distribution Function (ICDF) and the other based on the

Cholesky Decomposition of an error correlation matrix. The algorithm is capable of speeding up RBM by effectively alleviating the computational burden in offline stage without degrading accuracy. We demonstrate the algorithm's effectiveness through numerical experiments. Co-authors: Yanlai Chen and Akil Narayan

A WENO-based Method of Lines Transpose Approach for Vlasov Simulations

Yan Jiang, Michigan State University

A high order implicit Method of Lines Transpose (MOLT) method based on a weighted essentially non-oscillatory (WENO) methodology is developed for one-dimensional linear transport equations and further applied to the Vlasov-Poisson (VP) simulations via dimensional splitting. In the MOLT framework, the time variable is first discretized by a diagonally implicit strong-stability-preserving Runge-Kutta method, resulting in a boundary value problem (BVP) at the discrete time levels. Then an integral formulation coupled with a high order WENO methodology is employed to solve the BVP. As a result, the proposed scheme is high order accurate in both space and time and free of oscillations even though the solution is discontinuous or has sharp gradients. Moreover, the scheme is able to take larger time step evolution compared with an explicit MOL WENO scheme with the same order of accuracy.

An Invariant-Region-Preserving Limiter for the DG Method to Isentropic Gas Dynamics

Yi Jiang, Iowa State University

In this work, we introduce an invariant-region-preserving limiter and apply it to the discontinuous Galerkin (DG) method for isentropic gas dynamics. The reconstructed polynomial preserves the cell average and lies within the invariant region. A rigorous analysis is presented to show that for smooth solutions the high order of accuracy is not destroyed in general cases. Moreover, this limiter is explicit, and easy for computer implementation. Some numerical experiments are provided to illustrate these properties of the limiter. In particular, numerical tests on different Riemann solutions show that the designed limiter is helpful to oppress some oscillations in the numerical solution. Co-author: Hailiang Liu

Error Estimates with Linear Growth in Time for the DG Method Applied to Advective Problems

Vaclav Kucera, Charles University in Prague

When deriving error estimates for numerical methods applied to time dependent PDEs, the final step usually consists of the application of some version of Gronwall's lemma. This however usually yields error estimates which grow exponentially in time. For the DG method applied to advective problems, this can be avoided in some special situations, e.g. when divergence-free flow fields are considered - thus one obtains an estimate that grows only linearly in time. In this work we generalize these results to get, in general, error estimates that grow exponentially not with respect to time T, but in the maximal time that a particle following the flow field has spent in the computational domain up to T. Hence if this time is uniformly bounded for all T one obtains only linear growth in T. More generally, this leads to various possible sub-exponential dependencies of the error on time. Authors: Vaclav Kucera, Chi-Wang Shu

Stable coupling strategy for nonlocal diffusion models

Xingjie Li, University of North Carolina, Charlotte

We developed a new symmetric, consistent, and stable coupling strategy for nonlocal diffusion models, inspired by the quasinonlocal atomistic-to-continuum method for crystalline solids. The proposed coupling model is coercive with respect to the energy norms induced by the nonlocal diffusion kernels as well as the L2 norm, and it satisfies the maximum principle. A finite difference approximation is used to discretize the coupled system, which inherits the property from the continuous formulation. Furthermore, we demonstrated a special example which shows the discrepancy between the fully nonlocal and fully local diffusion, whereas the result of the coupled diffusion agrees with that of the fully nonlocal diffusion. Co-authors: Jianfeng Lu.

Bayesian Learning for High-Dimensional Chaotic Dynamical Models with Application to Two-Dimensional Turbulent Bottom Gravity Currents

Jing Lin, MIT

Bayesian inference in high-dimensional chaotic dynamical systems, such as turbulent fluid flows, is challenging because of the high computational costs in capturing the multiscale dynamics and integrating over high-dimensional state variables to compute posteriors. To overcome this difficulty, we developed a novel hierarchical Bayesian learning methodology for such settings. The methodology propagates uncertainty in a reduced subspace using the dynamically orthogonal (DO) equations, and jointly infers state variables and model parameters by the Gaussian mixture model-DO filter. Based on the evolving statistics and the sequential observations, the underlying models are learned dynamically in a Bayesian way. This methodology is applied to a two-dimensional realistic turbulent bottom gravity current. The learning targets include initial and boundary functional data, domain geometry and model parameters. The numerical results indicate the capability and efficiency of our hierarchical Bayesian learning methodology for capturing non-Gaussian statistics and nonlinear dynamics in high-dimensional chaotic dynamical models.

Efficient Monte-Carlo Methods for Statistical Solutions of Hyperbolic Conservation Laws

Kjetil Lye, ETH Zürich

An open question in the field of hyperbolic conservation laws is the question of well-posedness. Recent theoretical and numerical evidence have indicated that the correct notion of solutions for systems of conservation laws is the notion of measure valued solutions. These have later been extended to include statistical solutions, which incorporates the measure valued solutions along with multi-point spatial correlations measures. We introduce a convergent numerical method for computing the statistical solution of conservation laws, and prove that it converges in the Wasserstein distance through narrow convergence for the case of scalar conservation laws. For the scalar case, we validate our theory by computing the structure functions of the Burgers' equation with random initial data. The results agree well with the theory, and we get the expected convergence rate. We furthermore show that we can get faster computations using Multilevel Monte-Carlo for computing the statistical solutions of scalar conservation laws. In the case of systems of equations, we test our theory against the compressible Euler equations in two space dimensions. We check our numerical algorithm against two ill-behaved initial data, the Kelvin-Helmholtz instability and the Richtmeyer-Meshkov instability, and compute the corresponding structure functions. We furthermore show that in the case of these ill-behaved initial data, Multilevel Monte-Carlo can not improve upon the Monte-Carlo algorithm in computing the statistical solutions. Co-Author (advisor): "Siddhartha Mishra" (ETHZ)

Mathematical treatment and simulation for methane hydrate models.

F. Patricia Medina, Worcester Polytechnic Institute

Abstract: The computational simulation of Methane Hydrates (MH), an ice-like substance abundant in permafrost regions and in subsea sediments, is useful for the understanding of their impact on climate change as well as a possible energy source. In [1], we consider a simplified model of MH evolution which is a scalar nonlinear parabolic PDE with two unknowns, solubility, and saturation, bound by an inequality constraint. This constraint comes from thermodynamics and expresses maximum solubility of methane component in the liquid phase; when the amount of methane exceeds this solubility, methane hydrate forms. The problem can be seen as a free boundary problem somewhat similar to the Stefan model of ice-water phase transition. Mathematically, the solubility constraint is modeled by a nonlinear complementarity constraint and we extend the theory of monotone operators to the present case of a spatially variable constraint. In our fully implicit finite element discretization, we apply recently analyzed semismooth Newton method and show that it converges superlinearly, also for other interesting test cases unrelated to MH but covered by the theory. As concerns error estimates and convergence order, we show that they are essentially of first or half-order, depending on the norm (L2 or L1), or the variable (the smooth solubility variable or the non-smooth saturation). These results are similar to those known for the temperature and enthalpy, respectively, for Stefan problem. In [2], the reduced model for methane hydrate formation in variable salinity conditions was introduced; moreover, the authors provided details in the phase behavior adapted to the case study from Ulleung Basin. In [3], we also consider this model and provide details on the discretization and phase equilibria implementation. We describe three time-stepping variants and the sensitivity of the model to the simulation parameters and in particular to the reduced phase equilibrium model. This is joint work with Malgorzata Peszynska and Ralph E. Showalter

Improving the accuracy of convexity splitting methods for gradient flow equations

Saulo Orizaga, University of Arizona

This paper introduces numerical time discretization methods which significantly improve the accuracy of the convexity-splitting approach of Eyre (1998) [7], while retaining the same numerical cost and stability properties. A first order method is constructed by iteration of a semi-implicit method based upon decomposing the energy into convex and concave parts. A second order method is also presented based on backwards differentiation formulas. Several extrapolation procedures for iteration initialization are proposed. We show that, under broad circumstances, these methods have an energy decreasing property, leading to good numerical stability. The new schemes are tested using two evolution equations commonly used in materials science: the Cahn–Hilliard equation and the phase field crystal equation. We find that our methods can increase accuracy by many orders of magnitude in comparison to the original convexity-splitting algorithm. In addition, the optimal methods require little or no iteration, making their computation cost similar to the original algorithm.

Arbitrarily high order (weighted) essentially non-oscillatory finite difference schemes for incompressible flows on staggered meshes

Carlos Parés Pulido, ETH Zürich

We will present recently derived arbitrarily high-order accurate (essentially) non--oscillatory finite difference schemes for the incompressible and anelastic Euler equations in both two and three space dimensions. These equations are the fundamental governing equations for atmospheric flows and their numerical approximation is an essential component of all modern climate dynamics codes. Most of these codes use very high-order finite difference schemes, based on central stencils to solve these equations ([1, 2] and references therein). However, these central schemes suffer from several defects - namely, they can produce spurious oscillations when the solution contains sharp gradients, such as in shear layers. Consequently, combining these schemes with sub-grid scale models for atmospheric turbulence leads to large numerical errors. Moreover, some of these schemes are only second-order accurate. Finally, the behavior of these schemes on problems with long time scales is inadequate on account of dispersive errors. Given these defects, WENO schemes have been recently proposed as the suitable simulation framework for some atmospheric flows (see [3]). These schemes have been developed and integrated into the PYCLES simulation code. Although these schemes have many desirable properties, one can show that they are necessarily limited to only second order accuracy, even though arbitrary high order piecewise polynomial functions may be used in the WENO interpolation step. We propose a variant of the scheme of [3] where the interpolations, based on ENO stencils, are used to augment WENO finite differences for approximating cross-terms in the momentum equations. The resulting scheme is provably arbitrarily high order accurate and non-oscillatory. We present many numerical experiments to illustrate the behavior of the scheme.

High order Semi-Lagrangian Methods for Transport Problems with Applications to Vlasov Simulations and Global Transport

Jingmei Qiu, University of Houston

The semi-Lagrangian (SL) scheme for transport problems gains more and more popularity in the computational science community due to its attractive properties. For example, the SL scheme, compared with the Eulerian approach, allows extra large time step evolution by incorporating characteristics tracing mechanism, hence achieving great computational efficiency. In this talk, we introduce a family of high order SL methods coupled with the finite element discontinuous Galerkin (DG) method. The proposed SL schemes are applied to transport problems, the Vlasov model arising from the plasma physics and the global transport problems based on the cubed-sphere geometry from the operational climate model. The methods have been extensively tested and benchmarked with classical test problems in the literature.

Towards Efficient Multiscale Numerical Methods for Kinetic Models of Gases

James Rossmanith, Iowa State University

The dynamics of gases 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. The approach we consider in this work for handling the fluid closure problem is based on the micro-macro partition approach of [Bennoune, Lemou, and Mieussens, J. Comp. Pays., 2008]. In particular, we develop a wave-propagation version of their scheme that handles the microscopic portion of the distribution function via a Hermite spectral method [Grad, 1949]. This formulation has important advantages over the original micro-macro decomposition approach; most notably, no mesh ever needs to be constructed in the velocity variables and no cut-off velocities need to be introduced. Several numerical examples are shown to demonstrate the viability, efficiency, and accuracy of the proposed numerical method

Diagonally Implicit Runge-Kutta Schemes Devoid of Order Reduction

Benjamin Seibold, Temple University

Order reduction is a generic phenomenon that arises for time-dependent PDE boundary value problems, as well as for stiff ODEs. One existing approach to avoid order reduction is to construct schemes with high stage order. Unfortunately, high stage order is incompatible with diagonally implicit Runge-Kutta (DIRK) schemes. We show that a relaxed property, called weak stage order, can also achieve the goal. Even more, it is compatible with DIRK schemes. We finish with a systematic discussion of DIRK schemes (up to fourth order) that are devoid of order reduction. Joint work with Dong Zhou, Rodolfo Ruben Rosales, David Shirokoff

Unconditional stability for multistep ImEx schemes

David Shirokoff, NJIT

We present a new class of high order linear ImEx multistep schemes with large regions of unconditional stability. Unconditional stability is a desirable property of a time stepping scheme, as it allows the choice of time step solely based on accuracy considerations. Of particular interest are problems for which both the implicit and explicit parts of the ImEx splitting are stiff. Such splittings can arise, for example, in variable-coefficient problems, or the incompressible Navier-Stokes equations. To characterize the new ImEx schemes, an unconditional stability region is introduced, which plays a role analogous to that of the stability region in conventional multistep methods. Moreover, computable quantities (such as a numerical range) are provided that guarantee an unconditionally stable scheme for a proposed implicit-explicit matrix splitting. The new approach is illustrated with several examples. Coefficients of the new schemes up to fifth order are provided. This is a joint work with R. R. Rosales, B. Seibold and D. Zhou

Numerical study of linear multistep methods based on Gaussian radial basis functions

Jacob Sousa, UMass, Dartmouth

We investigate the possibility of using non-polynomial functions as bases of interpolants for deriving linear multistep methods. In this work, our focus is on Gaussian radial basis functions. We compute the weights for Adams-Bashforth, Adams-Moulton, and the backward differentiation formula using Mathematica and study the consistency, accuracy, and stability of the methods. Our goal is to see if this method can be a viable choice or if it turns out that polynomial-based methods are always superior. Numerical experiments will be presented. This is joint work with Alfa Heryudono at UMass Dartmouth and Akil Narayan at University of Utah.

Kinetic Monte Carlo Simulations of Traffic Flows: Comparison of Two Look-ahead Rules

Yi Sun, University of South Carolina

We employ an efficient list-based kinetic Monte Carlo (KMC) method to study traffic flow models on one-dimensional (1D) and two-dimensional (2D) lattices based on the exclusion principle and Arrhenius microscopic dynamics. This model implements stochastic rules for cars' movement based on the configuration of the traffic ahead of each car. In particular, we compare two different look-ahead rules: one is based on the distance from the car under consideration to the car in front of it, the other one is based on the density of cars ahead. The 1D numerical results of these two rules suggest different coarse-grained macroscopic limits in the form of integro-differential Burgers equations. The 2D results of both rules exhibit a sharp phase transition from freely flowing to fully jammed, as a function of initial density of cars. However, the look-ahead rule based on the density of the traffic produces more realistic results. The KMC simulations reported in this paper are compared with those from other well-known traffic flow models and the corresponding empirical results from real traffic.

Theory, Implementation, and Applications of Large Scale Particle Simulations of Mesoscopic Phenomena

Yu-Hang Tang, Brown University

The successful application of computer simulation techniques for solving problems in physical sciences requires interdisciplinary effort spanning theory, software implementation, and application. I will present algorithms and strategies for the optimization and efficient utilization of mesoscopic particle solvers that can utilize and push for the limit of thousands of current generation massively parallel processors. I will also talk about how to apply petascale DPD simulations to model the separation of rare circulating cancer cells from millions of normal blood cells, as well as the non-equilibrium dynamics of self-assembled structures called vesicles and micelles whose affinity to water changes nonlinearly with respect to system temperature. The presented work demonstrates that a close interplay between computation and science is critical to facilitate the development and adoption of high performance computing for solving realistic problems.

A Stable FSI Algorithm for Rigid Bodies and Incompressible Flows.

Qi Tang, Rensselaer Polytechnic Institute

A stable added-mass/added-damping partitioned algorithm is developed for fluid-structure interaction (FSI) problems involving viscous incompressible flow and rigid bodies. The algorithm remains stable, without sub-iterations, even for light rigid-bodies when added-mass and viscous added-damping effects are large. A fully second-order accurate implementation of the scheme is developed based on a fractional-step method for the incompressible Navier-Stokes equations using finite difference methods and overlapping grids to handle the moving geometry.

Author: Qi Tang, J.W. Banks, W.D. Henshaw, D.W. Schwendeman

Piecewise Parabolic Method for Propagation of Shear Shock Waves

Bharat B. Tripathi, University of North Carolina, Chapel Hill

We have recently observed a new biomechanical phenomenon: that shear waves generated by an impact develop into shock waves as they propagate into the brain. At the steep shock front the acceleration is magnified by a factor of 8.5. For example, a relatively mild 30 g impact at the brain surface develops into a destructive 255 g wave, deep in the brain. We hypothesize that this local amplification at the shear shock front can tear and damage neurons and may be responsible for a wide range of traumatic brain injuries. Unlike compressional waves the shock behavior of shear waves in the brain is relatively unstudied because we have only just discovered this phenomenon. There are currently no simulation tools that model shear shock wave propagation in the entire head. The most recent numerical tool models a paraxial approximation of a linearly polarized nonlinear shear scalar wave propagation in soft solids [1]. A more general numerical representation of shear shock waves is necessary to accurately describe brain motion during a traumatic event. We think that by accurately modeling shear shock behavior we can establish a clear link between shear brain motion and injury. Here we present a Piecewise Parabolic Method based 2D numerical solver which models the propagation of linearly-polarized nonlinear shear full-wave in soft solids.

Curvature-Augmented Numerical Methods for Interfaces

Chris Vogl, University of Washington

Robust numerical methods for interfaces are required to successfully solve models involving surface tension at a fluids interface, bending resistance of a surface, electric potential on a surface, or diffusion across a surface. When that interface/surface is smooth, the curvature likely plays a role and can be used to improved the involved numerical methods. Here, the curvature is used to augment the level set method and the closest point method. For the level set method, the traditional velocity extension is augmented with curvature information, leading to substantially improved mass conservation. For the closest point method, the surface operator embedding is augmented, resulting in better accuracy and sparsity than the traditional method. To tie these two augmented methods together, some results from vesicle simulations are presented.

Multiwavelets and outlier detection for troubled-cell indication

Mathea Josina Vuik, Delft University of Technology

Algorithm for sensitivity analysis of chaotic fluid dynamics simulations

Qiqi Wang, MIT

This poster will present numerical methods for computing derivatives of long time averages, a.k.a. statistics, in chaotic fluid flow simulations. The algorithm modifies the conventional tangent and adjoint methods, which fail in this case because of the ill conditioned initial value problem. Numerical results on several flow problems will be demonstrated.

Direct discontinuous Galerkin methods for Keller-Segel Chemotaxis equations

Jue Yan, Iowa State University

We develop direct discontinuous Galerkin (DDG) methods to solve Keller-Segel Chemotaxis equations. Different to available DG methods or other numerical methods in literature, we introduce no extra variable to approximate the chemical density gradients and solve the system directly. With P^k polynomial approximations, we observe no order loss and optimal (k+1)th order convergence is obtained. The reason behind is related to the solution gradients' super convergence phenomena. With Fourier analysis technique, we prove the DDG solution's spatial derivative is super convergent with at least (k+1)th order under momentum norm or in weak sense. We show the cell density approximations are strictly positive with at least third order of accuracy. Blow up features are captured well.

An immersogeometric fluid-structure interaction framework for heart valve simulations

Yue Yu, Lehigh University

In this work, we developed a computational method for fluid-thin structure interaction, where a divergence-conforming B-spline fluid discretization is employed, and the bio-prosthetic heart valve is modeled as immersed Kirchoff-Love thin shell structures. An augmented Lagrangian formulation is used for fluid-structure interaction that enforces kinematic constraints with a combination of Lagrange multipliers and penalty forces. On the other hand, in this application there is a large pressure jump across the leaflets, reveals the limitation of the penalty approach. To counteract steep pressure gradients through the structure without the conditioning problems that accompany strong penalty forces, the Lagrange multiplier field is resurrected. To study the convergence of the proposed immersogeometric method as well as to provide guidance for choosing the correct penalty, error analysis is carried out on a simplified linear parabolic model problem with Dirichlet boundary conditions applied along immersed boundaries. The convergence rates for numerical errors in H^1 norm as well as in L^2 norm are provided. We have verified the error estimates with numerical examples, and validated this framework on a computational model by comparing the simulation results with an in vitro experiment that pumps water through an artificial valve. Joint work with: David Kamensky, Ming-Chen Hsu, John A. Evans, Thomas J.R. Hughes

Positivity-preserving high order discontinuous Galerkin schemes for compressible Navier-Stokes equations

Xiangxiong Zhang, Purdue University

For gas dynamics equations such as compressible Euler and Navier-Stokes equations, preserving the positivity of density and pressure without losing conservation is crucial to stabilize the numerical computation. The L1-stability of mass and energy can be achieved by enforcing the positivity of density and pressure during the time evolution. However, high order schemes such as DG methods do not preserve the positivity. It is difficult to enforce the positivity without destroying the high order accuracy and the local conservation in an efficient manner for time-dependent gas dynamics equations. For compressible Euler equations, a weak positivity property holds for any high order finite volume type schemes including DG methods, which was used to design a simple positivity-preserving limiter for high order DG schemes in Zhang and Shu, JCP 2010. Generalizations to compressible Navier-Stokes equations are however nontrivial. We show that weak positivity property still holds for DG method solving compressible Navier-Stokes equations if a proper penalty term is added in the scheme. This allows us to obtain the first high order positivity-preserving schemes for compressible Navier-Stokes equations.

Computational Methods to study the Pattern Formation in Tissue

Xueping Zhao, University of South Carolina

We present a computational model to study the pattern formations in tissues with stem cells and differentiated cells. Our model is derived based on the Generalized Onsager Principle, combining one energy dissipative system and several active factors, such as spontaneous polarity states, birth and death of cells, self-propelled motion of differentiated cells and ATP hydrolysis. Firstly, linear stability analysis is conducted to reveal the long-wave instability inherent in the neighborhood of the constant steady states. Secondly, 2D and 3D experiments simulates the process of various pattern formation in the tissues. To solve this complex model, we develop an efficient energy stable numerical scheme and implement it on GPU clusters for high-performance computing. Our model introduces a novel way to investigate the interplay of stem cell division, differentiated cell migration and other active factors from enviroments. Using our methodology we observe new spatial patterns with spontaneous polarity and study the relations between those new patterns with various active terms in the system. Co-author: Qi Wang (University of South Carolina)

Order Reduction in High-Order Implicit Runge-Kutta Time-stepping for Initial Boundary Value Problems.

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When advancing a time-dependent PDE forward via Runge-Kutta methods, one may observe a convergence order that is less than the actual order of the scheme. We demonstrate that this order reduction phenomenon is in fact the norm, and not the exception. Geometrically, it stems from boundary layers, produced by the fact that the scheme is too accurate near the boundary. A modal analysis reveals under which circumstances boundary layers persist over many time steps. Moreover, a systematic derivation of modified boundary conditions is presented, which remedy the order reduction phenomenon. Co-authors: Rodolfo Ruben Rosales, Benjamin Seibold, David Shirokoff.