Book of Abstracts

NAHOMCon 2019

North American High-Order Methods Conference

June 2-5, San Diego State University, San Diego, CA

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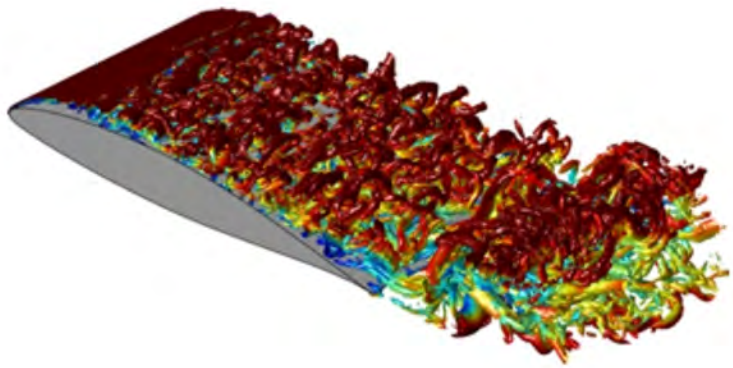

Letter from Lead-Chairs

Dear NAHOMCon Participants,

Welcome to the *first* North American High Order Methods Conference (NAHOMCon) held at San Diego State University from June two to five, 2019!

We created NAHOMCon to have an inclusive and diverse North American centered forum so that computational scientists, mathematicians, scientists and engineers could share ideas and techniques on, and further the state of the art of, high order methods for the solution of partial differential equations with applications to a broad range of scientific and engineering applications. We felt that American research on high order methods has been at a disadvantage when compared to that in European or other nations due to the lack of conferences devoted to the subject. With over ninety talks and distinguished plenary speakers, the response to NAHOMCon has been overwhelming and clearly confirmed the desire for researchers to have this forum.

The conference could not have been organized without the help of the members of the organizing and scientific committees. We also are deeply indebted to the strong financial and non-financial support given by the SDSU's Department of Aerospace Engineering, the College of Engineering, the Computational Science Research Center, and the College of Science at San Diego State University. We are also grateful for the funding from the National Science Foundation to support travel awards for students and early career scientists.

We hope you enjoy getting together with the members of the high-order community, have fruitful scientific discussions, meet old friends, and perhaps make some new ones. We further hope that you will enjoy the beautiful campus of San Diego State University, excellent California weather and the sunset and skyline on the conference dinner cruise.

With the success of the first NAHOMCon, we seek to have a second NAHOMCon in 2021. We invite you to think about organizing it and welcome you to an informal lunch on June 5 with all that are interested.

With warm regards,

Gustaaf Jacobs and David Kopriva (Co-Founders and Lead-Chairs of NAHOMCon)

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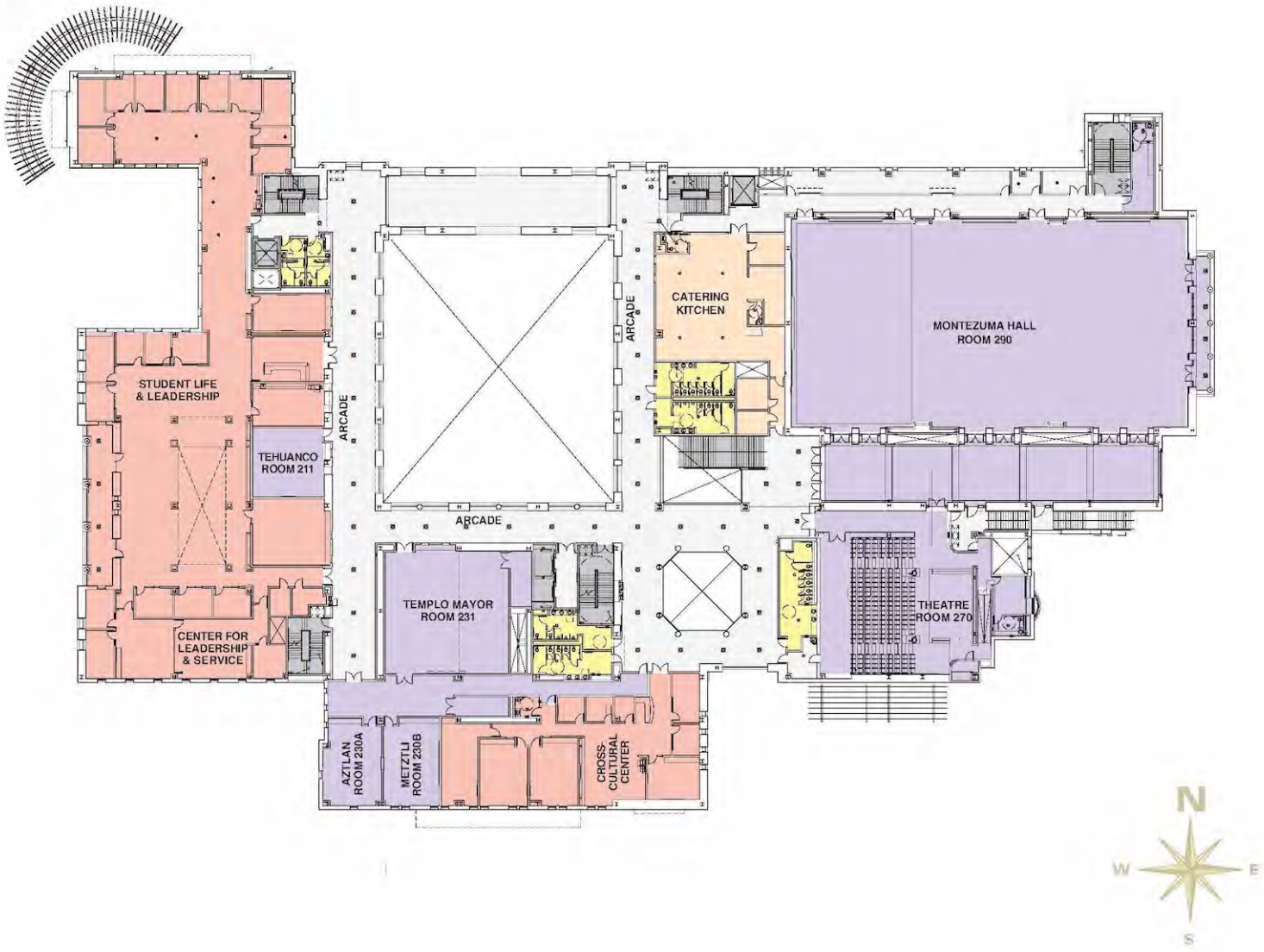

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ASSOCIATED STUDENTS

SAN DIEGO STATE UNIVERSITY

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Plenary Talks (Room: Templo Mayor)

Optimal energy-conserving discontinuous Galerkin methods for wave equations

Chi-Wang Shu*

Energy conservation is an important property for many time dependent PDEs, such as linear hyperbolic systems, linear and nonlinear dispersive wave equations including KdV equations, etc. Discontinuous Galerkin (DG) methods are often used to solve such problems, especially when adaptivity is desired. However, it is difficult to design energy conserving DG methods for such problems with optimal convergence in the L^2-norm. In this talk we will describe our recent work in designing such DG schemes, which involves the technique of possible doubling of unknowns. Optimal a priori error estimates of order $k+1$ are obtained for the semi-discrete scheme in one dimension, and in multi-dimensions on Cartesian meshes when tensor-product polynomials of degree k are used, for linear hyperbolic and dispersive wave equations. Computational results for linear and nonlinear problems including those in aeroacoustics, Maxwell equations and KdV equations, on both structured and unstructured meshes, demonstrate the excellent performance of these energy conserving schemes. This is joint work with Guosheng Fu.

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Exascale applications of high-order methods

Misun Min*

This talk will present recent advances in spectral element simulation efforts that are critical to address important exascale application problems arising in areas such as nuclear reactor design, wind turbine analysis, and urban environment modeling. Computational challenges are driven by multiscale features in thermal hydraulics and heat transfer, accurate modeling of highly turbulent flows, and meshing for complex large-scale geometries.

Numerical strategies to overcome these issues at exascale are discussed. Topics include steady and unsteady solutions of the Navier-Stokes, Reynolds-averaged Navier-Stokes, and drift-diffusion equations, with particular attention to preconditioning and Jacobian-free Newton Krylov methods for the steady-state nonlinear systems.

The talk will also address high-performance computing aspects for efficient and rapid turn-around of application simulations and demonstrate high performance at scale on current leadership computing platforms including accelerator-based architectures. The work is part of a collaborative effort at ANL, LLNL, and several universities that is funded by ECP Co-Design CEED project and the DOE applied math research program.

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Scalable high-order finite elements for compressible hydrodynamics

Tzanio Kolev*

The discretization of the Euler equations of gas dynamics ("compressible hydrodynamics") in a moving material frame is at the heart of many multi-physics simulation codes. The Arbitrary Lagrangian-Eulerian (ALE) framework is frequently applied in these settings in the form of a Lagrange phase, where the hydrodynamics equations are solved on a moving mesh, followed by a three-part "advection phase" involving mesh optimization, field remap and multi-material zone treatment.

This talk presents a general Lagrangian framework[3] for discretization of compressible shock hydrodynamics using high-order finite elements. The use of high-order polynomial spaces to define both the mapping and the reference basis functions in the Lagrange phase leads to improved robustness and symmetry preservation properties, better representation of the mesh curvature that naturally develops with the material motion and significant reduction in mesh imprinting. We will discuss the application of the curvilinear technology to the "advection phase" of ALE, including a DG-advection approach for conservative and monotonic high-order finite element interpolation (remap), as well as to coupled physics, such as electromagnetic diffusion. We will also review progress in robust and efficient algorithms for high-order mesh optimization, matrix-free preconditioning, high-order time integration and matrix-free monotonicity, which are critical components for the successful use of high-order methods in the compressible ALE settings.

In addition to their mathematical benefits, high-order finite element discretizations are a natural fit for modern HPC hardware, because their order can be used to tune the performance, by increasing the FLOPs/bytes ratio, or to adjust the algorithm for different hardware. In this direction, we will present some of our work on scalable high-order finite element software that combines the modular finite element library MFEM [5], the high-order shock hydrodynamics code BLAST [1] and its miniapp Laghos [4], where we will demonstrate the benefits of our approach with respect to strong scaling and GPU acceleration. Finally, we will give a brief update on related efforts in the co-design Center for Efficient Exascale Discretizations (CEED) in the Exascale Computing Project (ECP) of the DOE [2].

References

[1] *BLAST: High-order shock hydrodynamics.* URL: `http://llnl.gov/casc/blast`.

[2] *Center for Efficient Exascale Discretizations.* URL: `http://ceed.exascaleproject.org`.

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[3] Veselin A. Dobrev, Tzanio V. Kolev, and Robert N. Rieben. "High-order curvilinear finite element methods for Lagrangian hydrodynamics." In: *SIAM Journal on Scientific Computing* 34.5 (2012), B606–B641.

[4] *Laghos: Lagrangian high-order solver*. URL: `https://github.com/CEED/Laghos`.

[5] *MFEM: Modular finite element library*. URL: `http://mfem.org`.

What's new with the wave equation?

Daniel Appelö*

Two defining features of waves are their finite speed of propagation and their ability to propagate over large distances without changing shape. It is these properties that allow them to localize in space-time and to carry information so that they can be used to probe and image e.g. the interior of the earth, the human body or engineering structures.

These properties also guide the design of accurate discretizations of wave equations. First, to minimize dispersive errors that alter the shape of waves, high order accurate methods must be used. Second, the finite speed of propagation suggests that optimal discretizations should be explicit and allow for time steps whose size is set only by the speed of sound and the grid size and not by the order of the method.

In this talk we discuss challenges in designing methods for wave equations in second order form that are of arbitrary order and can time march with large time steps. We present some discretizations that overcome these challenges and demonstrate their use for select applications.

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An efficient and high order accurate direct solution technique for variable coefficient elliptic partial differential equations

Adrianna Gillman*

For many applications in science and engineering, the ability to efficiently and accurately approximate solutions to elliptic PDEs dictates what physical phenomena can be simulated numerically. In this talk, we present a high-order accurate discretization technique for variable coefficient PDEs with smooth coefficients. The technique comes with a nested dissection inspired direct solver that scales linearly or nearly linearly with respect to the number of unknowns. Unlike the application of nested dissection methods to classic discretization techniques, the constant prefactors do not grow with the order of the discretization. The discretization is robust even for problems with highly oscillatory solutions. For example, a problem 100 wavelengths in size can be solved to 9 digits of accuracy with 3.7 million unknowns on a desktop computer. The precomputation of the direct solver takes 6 minutes on a desktop computer. Then applying the computed solver takes 3 seconds. A parallel implementation of the solution technique reduces the precomputation time to roughly 30 seconds and halves the time it takes to apply the solver. Applications of the solution technique to inverse scattering problems and time dependent partial differential equations will also be presented.

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Nonlinear stability and the discrete equations of fluid mechanics

Mark H. Carpenter*

A high-level overview of the Summation-By-Parts (SBP) entropy stability literature is presented. Nonlinearly (entropy) stable discretizations of arbitrary order exist for the compressible Navier-Stokes (NS) equations for diagonal norm, tensor-product and multi-dimensional, summation-by-parts (SBP) operators. Recent developments are discussed:

1. Curvilinear brick elements,
2. generalized SBP extensions (triangles, prisms, tets),
3. nonconforming interfaces that enable hp-refinement,
4. arbitrary Lagrangian-Eulerian operators,
5. staggered operators resembling classical FEM,
6. extension to fully discrete operators (SBP in time),
7. nonlinearly stable boundary conditions,
8. dissipation: finite-difference and spectral collocation WENO operators,
9. other related equations.

Impediments are identified that currently hinder/preclude a general and complete nonlinear stability theory for arbitrary discretizations and equations.

BIO: Broad research interests include 1) temporal discretizations, 2) spatial discretizations and 3) linear and nonlinear solvers. Recent efforts include 1) nonlinear stability of spatial and 2) temporal operators for the compressible Navier-Stokes equations, 3) error estimators for IMEX Runge-Kutta schemes, 4) DIRK temporal schemes, 5) retooling DRP schemes, 6) preconditioners for high-order DG schemes ($p \geq 7$), 7) chaotic systems.

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Monday, June 3, Morning Session I (Room: Aztlan)

Modal formulations of entropy stable discontinuous Galerkin methods

Jesse Chan*

High order discontinuous Galerkin (DG) methods are known to be unstable when applied to nonlinear conservation laws with shocks and turbulence, and traditionally require additional filtering, limiting, or artificial viscosity to avoid solution blow up. Entropy stable schemes address this instability by ensuring that physically relevant solutions satisfy a semi-discrete entropy inequality even in the presence of under-resolved solution features and inexact quadrature.

The construction of entropy stable DG methods has traditionally relied on equivalences between "collocation" DG methods and summation-by-parts (SBP) finite differences. We present a framework for constructing high order entropy stable schemes based instead on a "modal" DG formulation and apply it towards the construction of entropy stable schemes on both tetrahedral and hexahedral meshes. We also discuss extensions of this framework to hybrid and non-conforming meshes.

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Energy stable higher order space-time hybridizable and embedded discontinuous Galerkin methods for incompressible flows

Tamas Horvath*, Sander Rhebergen†

The Space-time Discontinuous Galerkin (ST-DG) method is an excellent method to discretize problems on deforming domains. This method uses DG to discretize both in the spatial and temporal directions, allowing for an arbitrarily high order approximation in space and time. Furthermore, this method automatically satisfies the geometric conservation law which is essential for accurate solutions on time-dependent domains. We present a higher-order accurate Hybridizable or Embedded Discontinuous Galerkin (DG-H or DG-E) method for incompressible flows. This discretizations are energy stable and guarantee a pointwise divergence-free velocity field on simplicial meshes. The numerical tests were carried out using the MFEM library.

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Provably conservative and energy-stable finite difference dissipation operators with spectral tunability

Ayaboe Edoh* Venkateswaran Sankaran†

Numerical dissipation operators that are capable of preserving the native stability and conservational properties of finite-difference Summation-by-parts (FD-SBP) schemes are studied in the context of solution filtering (SF) and artificial dissipation (AD), wherein spectral attenuation is tailored to the resolvability of the underlying base scheme. The ability to employ such tuning thus allows one to shift the role of numerical dissipation towards the aim of precisely reducing numerical error effects, which in turn can enable accurate unsteady calculations on coarse grids.

The current study compares the use of general (i.e., explicit and implicit) finite difference SF and AD operators whose spectral damping characteristics can be manipulated. Construction of these schemes is presented via a simplified "cascading" procedure that naturally ensures provable conservation and energy-stability[2]. Respective merits of employing numerical dissipation in SF versus AD forms[1] are explored in the SBP context for time-accurate calculations, noting the potential effect of filtering on stability estimates[3] and the potential influence from the AD contribution on integration stiffness.

References

[1] Ayaboe K. Edoh, Nathan L. Mundis, Charles L. Merkle, Ann R. Karagozian, and Venkateswaran Sankaran. "Comparison of artificial-dissipation and solution-filtering stabilization schemes for time-accurate simulations." In: *Journal of Computational Physics* 375 (Dec. 2018), pp. 1424–1450. DOI: 10.1016/j.jcp.2018.08.019. URL: https://doi.org/10.1016/j.jcp.2018.08.019.

[2] Ayaboe Edoh and Venke Sankaran. "Boundary prescriptions for spectrally-tunable discrete filters." In: *2019 AIAA Aerospace Sciences Meeting*. 2019, p. 2170.

[3] Jan Nordström and Viktor Linders. "Well-posed and stable transmission problems." In: *Journal of Computational Physics* 364 (July 2018), pp. 95–110. DOI: 10.1016/j.jcp.2018.03.003. URL: https://doi.org/10.1016/j.jcp.2018.03.003.

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An energy-based discontinuous Galerkin method with Galerkin difference basis for second-order wave equations

Lu Zhang* Thomas Hagstrom* Daniel Appelö†

The Galerkin difference basis, proposed by J. Banks and T. Hagstrom in 2016, is a set of continuous, piecewise polynomials defined using a finite difference grid of degrees of freedom. In 2015, D. Appelo and T. Hagstrom proposed an energy-based discontinuous Galerkin method that features a direct, mesh-independent approach to define interelement fluxes. To apply the energy-based discontinuous Galerkin method with the standard Galerkin difference basis to solve a scalar second-order wave equation, one usually requires a nonlinear computational cost with respect to the total degrees of freedom even in a simple geometry. In this talk, we propose a new basis derived from the standard Galerkin difference basis, which reduces the nonlinear computational cost to depend linearly on the total degrees of freedom. We compute the spectral radius of the operator to find that the CFL number is proportional to the degree of the approximation space. Our numerical experiments demonstrate the stability of the proposed scheme and the desired optimal convergence rate in L^2.

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A free-energy stable nodal discontinuous Galerkin approximation with summation-by-parts property for the Cahn-Hilliard equation

Juan Manzanero* Gonzalo Rubio David A. Kopriva Esteban Ferrer
Eusebio Valero

We present a nodal Discontinuous Galerkin (DG) spectral element method (DGSEM), which satisfies the summation-by-parts simultaneous-approximation-term (SBP–SAT) property, for the Cahn-Hilliard equation [2]. The SBP property permits us to show that the discrete free-energy is bounded and, as a result, the scheme is provably stable. The scheme and the stability proof are presented for general curvilinear three-dimensional hexahedral meshes and both exact and fully discrete integration in time. We use the Bassi–Rebay 1 (BR1) [3,4] scheme to compute interface fluxes, and an IMplicit–EXplicit (IMEX) scheme [1] to integrate in time for the fully discrete approximation. The Cahn–Hilliard equation in an arbitrary domain, Ω, with phase field φ, interfacial energy coefficient k, chemical potential $w = \psi'(\phi) - k\nabla^2\phi$ (with gradient $\vec{f} = \nabla w$) where $\psi(\varphi)$ is the chemical free-energy, which is a polynomial function in φ, is

$$\phi_t = \nabla \cdot \left(M\vec{f} \right) \tag{1}$$

The free-energy,

$$\mathcal{F}\left(\phi, \nabla\phi\right) = \int_\Omega \left(\psi\left(\phi\right) + \frac{1}{2}k|\nabla\phi|^2 \right) d\vec{x}, \tag{2}$$

of the system satisfies a bound in time

$$\mathcal{F}(T) = \mathcal{F}(0) - \int_0^T \left\langle M\vec{f}, \vec{f} \right\rangle \mathrm{d}t \leqslant \mathcal{F}(0) \tag{3}$$

which can be viewed as a continuous statement of its stability. We will show that the DGSEM approximation for the Cahn–Hilliard equation satisfies the discrete counterpart

$$\mathcal{F}^{T,N} \leqslant \mathcal{F}^{0,N} - \Delta t \sum_{E,n} \left\langle M\vec{F}, \vec{F} \right\rangle_{E,N} \leqslant \mathcal{F}^{0,N} \tag{4}$$

where $\mathcal{F}^{i,N}$ and $\vec{F}$ are the approximations of $\mathcal{F}(T)$ and $\vec{f}$, respectively. In contrast to the continuous energy, the discrete statement is an inequality as a result of both the temporal and spatial dissipation introduced by the discretization. We complement the analysis with two– and three–dimensional numerical experiments that assess the capabilities and convergence of the scheme.

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These experiments show that the approximation is spectrally accurate in space and design order accuracy in time. Fig. 1 shows an example of the time evolution of a mixture of two phases in three space dimensions using the code presented in [5] using the scheme analyzed here.

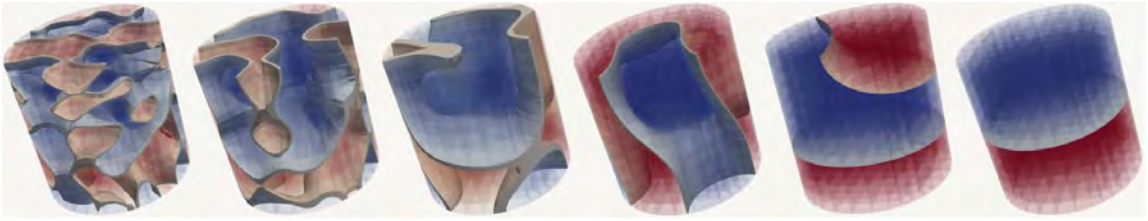

Figure 1: Evolution of the phases with time in a three–dimensional spinodal decomposition inside a cylinder

References

[1] Dong, S. (2018). Multiphase flows of N immiscible incompressible fluids: A reduction- consistent and thermodynamically-consistent formulation and associated algorithm. Journal of Computational Physics, 361, 1-49.

[2] Cahn, J. W., Hilliard, J. E. (1958). Free energy of a nonuniform system. I. Interfacial free energy. The Journal of chemical physics, 28(2), 258-267.

[3] Bassi, F., Rebay, S. (1997). A high-order accurate discontinuous finite element method for the numerical solution of the compressible Navier–Stokes equations. Journal of computational physics, 131(2), 267-279.

[4] Manzanero, J., Rueda-Ramírez, A. M., Rubio, G., Ferrer, E. (2018). The Bassi Rebay 1 scheme is a special case of the Symmetric Interior Penalty formulation for discontinuous Galerkin discretisations with Gauss–Lobatto points. Journal of Computational Physics, 363, 1-10.

[5] Manzanero J, Redondo, Carlos, Rubio G, Ferrer E, Valero E, Gómez-Álvarez, Susana, Rivero, Ángel (2019) A high–order discontinuous Galerkin solver for multiphase flows. (Submitted to) ICOSAHOM 2018

Monday, June 3, Morning Session II (Room: Templo Mayor)

Stable and accurate filtering procedures

Jan Nordström* Tomas Lundquist†

The study of so called transmission problems in [2] revealed that successful numerical filtering may include a delicate balance between the need to remove high frequency oscillations (filter often for accuracy) and the need to avoid possible growth (filter seldom for stability). In this talk we investigate this contradiction, and propose different avenues for improved functionality.

The filter operators derived in [1] are the basic building blocks. We demonstrate that explicit use of the basic filter operators guarantee accuracy but lead to instabilities, while an implicit implementation preserve stability but degrade accuracy. We also prove that a specific accuracy condition is necessary for stability, and that the basic operators do not satisfy that condition.

Finally, new modified filter operators that satisfy the specific accuracy conditions, are stable in combination with summation-by-parts operators [3], and can be used both explicitly and implicitly are constructed. The new operators are shown to efficiently damp the highest frequencies on the grid, including the π-mode.

References

[1] Christopher A Kennedy and Mark H Carpenter. "Comparison of several numerical methods for simulation of compressible shear layers." In: *NASA Technical Paper 3484* (1997).

[2] Jan Nordström and Viktor Linders. "Well-posed and stable transmission problems." In: *Journal of Computational Physics* 364 (2018), pp. 95–110.

[3] Magnus Svärd and Jan Nordström. "Review of summation-by-parts schemes for initial–boundary-value problems." In: *Journal of Computational Physics* 268 (2014), pp. 17–38.

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Entropy stable spectral collocation schemes for the 3-D Navier-Stokes equations on dynamic unstructured grids

Nail K. Yamaleev* David C. Del Rey Fernandez† Jialin Lou*
Mark H. Carpenter‡

New entropy stable spectral collocations schemes of arbitrary order of accuracy are developed for the unsteady 3-D Euler and Navier-Stokes equations on dynamic unstructured grids. An arbitrary Lagrangian-Eulerian (ALE) formulation is adopted to deal with the grid motion and deformation. Therefore, a one-by-one mapping from the moving and deforming hexahedral grid elements onto a cube in the fixed reference system of coordinates is constructed. The proposed scheme is constructed by using the skew-symmetric form of the Navier-Stokes equations, which are discretized by using summation-by-parts spectral collocation operators that preserve the conservation properties of the original governing equations. Furthermore, the metric coefficients are approximated such that the geometric conservation laws (GCL) are satisfied exactly on both static and dynamic grids. A new entropy conservative flux is derived for the 3-D Euler and Navier- Stokes equations on dynamic unstructured grids to ensure the entropy stability of the developed scheme. The new flux preserves the design order of accuracy of the original spectral collocation scheme and guarantees the entropy conservation on moving and deforming grids. Several numerical results are presented to demonstrate design order of accuracy and free stream preservation properties of the new schemes for both the Euler and Navier-Stokes equations on moving and deforming unstructured grids.

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Combining finite element and finite difference methods for isotropic elastic wave simulations in an energy-conserving manner

Longfei Gao* David Keyes†

We consider numerical simulation of the isotropic elastic wave equations arising from seismic applications with non-trivial land topography. The more flexible finite element method is applied to the shallow region of the simulation domain to account for the topography, and combined with the more efficient finite difference method that is applied to the deep region of the simulation domain. We demonstrate that these two discretization methods, albeit starting from different formulations of the elastic wave equation, can be joined together smoothly via weakly imposed interface conditions. Discrete energy analysis is employed to derive the proper interface treatment, leading to an overall discretization that is energy-conserving. Numerical examples are presented to demonstrate the efficacy of the proposed interface treatment.

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Entropy stable discontinuous Galerkin method for shallow water equation *

Wai Sun Don† Zhen Gao† Xiao Wen† Yulong Xing‡

The nonlinear shallow water equations (SWEs) are widely used to model the unsteady water flows in rivers and coastal areas, with extensive applications in ocean and hydraulic engineering. In this work, we propose entropy stable, well-balanced and positivity-preserving discontinuous Galerkin (DG) methods, under more arbitrary choices of quadrature rules, for the SWEs with non-at bottom topography. In [1], a SBP-like differentiation operator is introduced to construct the discretely entropy conservative DG methods. We extend this idea to the SWEs and establish an entropy stable scheme by adding additional dissipative terms. Careful approximation of the source term is included to ensure the well-balanced property of the resulting method. A simple positivity-preserving limiter, compatible with the entropy stable property, is added to guarantee the non-negative water heights during the computation. One- and two-dimensional numerical experiments are presented to demonstrate the performance of the proposed methods.

References

[1] Jesse Chan. "On discretely entropy conservative and entropy stable discontinuous galerkin methods." In: *Journal of Computational Physics* 362 (2018), pp. 346–374. DOI: 10.1016/j.jcp.2018.02.033.

*This document has been approved for public release; its distribution is unlimited.

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Monday, June 3, Morning Session III (Room: Tehuanco)

A particle tracking methodology for spectral high order element methods in Nektar++

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This work presents a particle tracking methodology to simulate laden flows within the context of spectral high order element based methods. As emphasized by Coppola [2], Jacobs [4], Shotorban et. al [5], and Dutta [3], the use of this type of methods could allow an accuracy increment in the simulation due to the potential to consider smaller scales of the turbulence phenomena. This research aims is to assess the impact of higher resolution methods on the prediction of erosion wear rate and distribution. The numerical framework used to implement this methodology is Nektar++, which solves partial differential equations using spectral/hp element methods [1].

The problem of predicting particle movement in a fluid flow has the form of an evolution equation in time (see Eqn. 1)

$$\frac{d\vec{v}_p}{dt} = F(\vec{u}, \rho, \rho_p, C_d, \dots); \quad \frac{d\vec{x}_p}{dt} = \vec{v}_p \tag{1}$$

Where $\vec{v}_p$ represents the particle velocity in a certain point $\vec{x}_p$. The rate of $\vec{v}_p$ change of is a function of external forces (F) over the particle, such as drag, buoyancy, gravity, among others.

To begin with is necessary to obtain the particle velocity on a certain point from an eulerian velocity field. This process consists of three steps: Find the element which contains the particle, interpolate a velocity value to the particle position, and evaluate the next particle position.

The proposed implementation in Nektar++ uses a searching algorithm to evaluate the container element. Then, velocity is evaluated using a built in optimized high-order interpolation function. Finally, the new position is assessed using a multistep Adams-Bashforth method for particle velocity, and an Adams-Moulton method for the particle position.

The proposed methodology is tested with two cases: the cavity flow, and an elbow pipe flow. The performance of each test case, for different searching strategies, and interpolation order and the integration order, is assessed.

A discussion is posed about the potential improvements that can be done on each of the three steps previously explained.

In addition to that, a domain decomposition approach for the parallel version of the particle tracking algorithm is presented, where a discussion about communication, scalability and performance is presented.

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References

[1] Chris D Cantwell, David Moxey, Andrew Comerford, Alessandro Bolis, Gabriele Rocco, Gianmarco Mengaldo, Daniele De Grazia, Sergey Yakovlev, J-E Lombard, D Ekelschot, et al. "Nektar++: an open-source spectral/hp element framework." In: *Computer Physics Communications* 192 (2015), pp. 205–219.

[2] G Coppola, SJ Sherwin, and J Peiró. "Nonlinear particle tracking for high-order elements." In: *Journal of Computational Physics* 172.1 (2001), pp. 356–386.

[3] Som Dutta. "Bulle-effect and its implications for morphodynamics of river diversions." PhD thesis. University of Illinois at Urbana-Champaign, 2017.

[4] Gustaaf Jacobs. "Inertial particle behavior in a an unsteady separated flow." In: *46th AIAA Aerospace Sciences Meeting and Exhibit*. 2007, p. 1159.

[5] Babak Shotorban. "Preliminary assessment of two-fluid model for direct numerical simulation of particle-laden flows." In: *AIAA journal* 49.2 (2011), pp. 438–443.

Efficient and highly accurate semi-Lagrangian discontinuous Galerkin method for convection-diffusion problems *

Mingchang Ding † Xiaofeng Cai † Wei Guo ‡ Jingmei Qiu †

We propose to organically combine Semi-Lagrangian Discontinuous Galerkin (SLDG) method with local DG (LDG) approximations to diffusion terms for convection-diffusion problems. In particular, we apply a weak formulation of the SLDG method for the convection term [1], and along characteristics using high order implicit Runge–Kutta method for a LDG discretization of the diffusion term. The proposed scheme is shown to be mass conservative, high order accurate in both space and in time, and highly efficient due to large time stepping sizes allowed from the semi-Lagrangian and implicit nature of time discretization. The scheme can be straightforwardly extended to 2D problems in the truly multi-D SLDG framework previously proposed. The performance of the scheme will be showcased by several classical linear test problems such as rigid body rotation, swirling deformation, as well as the guiding center Vlasov models.

References

[1] Xiaofeng Cai, Wei Guo, and Jing-Mei Qiu. "A high order conservative semi-lagrangian discontinuous Galerkin method for two-dimensional transport simulations." In: *Journal of Scientific Computing* 73.2-3 (Sept. 2017), pp. 514–542. DOI: 10.1007/s10915-017-0554-0.

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Efficient Lagrangian particle tracking for high-order CFD in complex geometries

Som Dutta* Ketan Mittal† James W. Lottes‡ Paul Fischer§

Lagrangian particle tracking, and the related point-particle models are an efficient and effective way to track coherent structures in a flow, and model transport of particulate matter. Applications of point-particle models range from sediment transport in rivers, to atomization of fuel in an internal combustion engine. The most important and computationally expensive step for any Lagrangian particle tracking calculation is the interpolation step, where the velocity field (and others fields) from the Eulerian grid is interpolated to the location of the particle. In Nek5000 a general interpolation algorithm has been implemented, which is part of the communication library *gslib*[2]. The algorithm has been used in various applications, like efficient overset-grid calculations[3], Lagrangian particle tracking[1], etc. The interpolation algorithm has two major parts; first in which for a given set of arbitrary points (particle locations) the process, and element containing the point is returned along with the physical to local coordinate mapping. The second part uses the information from the preceding step, to interpolate the fields from the Eulerian grid at the prescribed polynomial order. Time required to perform the first-step in the algorithm is directly proportional to the polynomial-order of the element within which the particle/point is present, with substantial reduction in computational cost (at least 10x) when the element is linear/quadratic instead of order seven and above[1]. Most meshes in CFD calculations have relatively low-order elements, this provides us a way to reduce computational time required for the interpolation step. In the current presentation, first we provide a general overview of the interpolation algorithm, and then discuss a method through which the order of the element containing the particle/point is assessed in order to reduce the computational cost of the interpolation step.

References

[1] S. Dutta, P. Fischer, and M.H. Garcia. "Fast semi-implicit Lagrangian transport of polydisperse particles." (under-preparation). 2019.

[2] P. F. Fischer, J. W. Lottes, and S. G. Kerkemeier. *Nek5000*. 2008. URL: `https://nek5000.mcs.anl.gov/`.

[3] Ketan Mittal, Som Dutta, and Paul F. Fischer. "Nonconforming Schwarz-spectral element methods for incompressible flow." In: *under review after revisions for Computer & Fluids* (2018).

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Solving a reduced ocean model using high order spectral element and finite volume methods

Siddhartha Bishnu [*], Joseph Schoonover [†], William Dewar [‡]

Energy is introduced into the oceans primarily at large scales by means of wind, tides and surface buoyancy forcing. This energy is transferred to the smaller mesoscale field through the geostrophic instability processes. The mesoscale field appears not to have accelerated appreciably over the last several decades, so we can assume that the mesoscale loses energy at roughly the same rate it receives energy. Interestingly, how the mesoscale loses energy is not quite clear. We have been exploring topographic interaction as a pathway by which the mesoscale may lose energy to unbalanced forward cascading flows. To demonstrate this phenomenon, an approximate model theory is developed that solves a reduced set of the Navier-Stokes and continuity equations in density coordinates ($xy\rho$ space) for any topographic configuration. Applying the principle of conservation of potential vorticity and scaling analysis, we split these 3D equations into (a) a set of 2D elliptic equations for the perturbation Montgomery (equivalent of pressure in density coordinates) field in the $\rho - x$ plane for every meridional (y) grid point and (b) a set of 1D hyperbolic advection equations on the topography for the perturbation meridional velocity (v) and the fluctuation of isopycnals (i.e. surfaces with constant density) from their background state (z). Equations (a) are solved using Continuous Galerkin Spectral Element Method with polynomial order seven while equations (b) are solved using Colella and Woodward's Piecewise Parabolic Finite Volume Method with third order reconstruction. One complication that arises in density coordinates is the slight time evolution of the topography in the $\rho - x$ plane for every meridional grid point. It is taken care of by regenerating the spectral elements in these planes only along the topography at every time step, so that the computational time and cost are not affected appreciably. The results of these numerical experiments are similar to already published MITGCM (MIT General Circulation Model) simulations.

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A high order multidimensional residual distribution scheme for Lagrangian hydrodynamics

Svetlana Tokareva * Remi Abgrall † Nathaniel Morgan*
Konstantin Lipnikov *

We discuss the multidimensional Staggered Grid Residual Distribution (SGH RD) scheme for Lagrangian hydrodynamics and its extensions to higher than second orders. The SGH RD scheme is based on the staggered finite element discretizations. However, the advantage of the residual formulation over more classical FEM approaches consists in the natural mass matrix diagonalization which allows one to avoid the solution of the linear system with the global sparse mass matrix while retaining the desired order of accuracy. This is achieved by using Bernstein polynomials as finite element shape functions and coupling the space discretization with the deferred correction type timestepping method. Moreover, it can be shown that for the Lagrangian formulation written in non-conservative form, our residual distribution scheme ensures the exact conservation of the total energy. We shall also discuss stabilization techniques for the SGH RD schemes allowing to reduce the dissipation of the numerical solution. Our approach to stabilizing the method consists in adding artificial viscosity terms to the first-order residuals which are then used to generate their high order versions. Therefore, it can be proven that only first-order artificial viscosity term is sufficient to obtain a formally high-order method. Thanks to the generic formulation of the staggered grid residual distribution scheme, it can be directly applied to both single- and multimaterial and multiphase models. We shall demonstrate computational results obtained with the proposed residual distribution scheme for several challenging test problems.

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Monday, June 3, Afternoon Session I (Room: Aztlan)

Enabling performance portability for high-order entropy stable compressible flow simulations

Jerry Watkins* Travis Fisher*

High-fidelity Direct Numerical Simulations of high-speed compressible turbulent flows play a crucial role in the development of multi-fidelity design tools in modern aerospace systems. These simulations often require a massive amount of memory and computation from large, heterogeneous supercomputing clusters to provide sufficient accuracy and resolution. High-order methods have the potential to reduce the execution time for these simulations by benefiting more from the high computational throughput on modern hardware compared to traditional second-order methods. Unfortunately, modern hardware is changing rapidly and refactoring a code to work efficiently on the latest hardware is becoming increasingly infeasible. In an effort to avoid architecture specific programming, programming models such as Kokkos are becoming increasingly important to obtain efficient implementations. In this work, we describe the performance portable implementation of the high-order entropy stable finite difference and spectral collocation methods within the Sandia Parallel Aerodynamics and Reentry Code (SPARC) through the use of the Kokkos programming model. We also provide a detailed performance analysis of the explicit, Navier-Stokes solver on structured meshes on multiple architectures including Intel Haswell CPUs, Intel Xeon Phi Knights Landing and IBM POWER9/NVIDIA V100 GPUs.

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A highly efficient large eddy simulation method for DGSEM using non-linearly optimized relaxation filters

David Flad * Andrea Beck †

Discontinuous Galerkin (DG) methods and closely related flux reconstruction high order methods have recently become popular for large eddy simulation (LES). The paper adds on a recent paper by the author, in which discussed we some limitations in the applicability of the often used implicit or no model large eddy simulation (iLES) [1]. Here the sole mechanism acting as a sink for kinetic energy and hence as a sub grid model surrogate is the cell interface flux coupling by dissipative Riemann solvers. It was shown that under typical, coarse resolution these methods become inaccurate. It was further argued that this deficiency can be overcome by using kinetic energy preserving flux functions, that were recently introduced for DGSEM by Gassner et al. [2], in combination with a low Mach number/low dissipation Riemann solver. By that choice, a simple Smagorinsky model leads to excellent results for the test case of homogeneous isotropic turbulence (HIT), a result that was previously impossible to obtain. While this is the de-facto standard when using finite difference methods, this is an important extension to DG.

In this work, we aim at replacing the Smagorinsky model by a specifically designed, dissipative spatial filter, fully exploiting the high order spectral character of the DG-method. To optimize the filter kernel, data from direct numerical simulation is filtered and used as a ground truth to fit overall kinetic energy and dissipation rate over time. The optimization is carried out for polynomial degree 3 to 10. The found kernels are then tested in the limit of infinite Reynolds number flow (HIT and Taylor Green Vortex flow). A brief extension to plane turbulent channel flow is given. We find the method to give very promising results for all test cases considered. We believe the method to be especially attractive in combination with wall modeled LES, as it can avoid the computation of second order derivatives for very high Reynolds number flows.

References

[1] David Flad and Gregor Gassner. “On the use of kinetic energy preserving dg-schemes for large eddy simulation.” In: *Journal of Computational Physics* 350 (2017), pp. 782–795.

[2] Gregor J Gassner, Andrew R Winters, and David A Kopriva. “Split form nodal discontinuous galerkin schemes with summation-by-parts property for the compressible euler equations.” In: *Journal of Computational Physics* 327 (2016), pp. 39–66.

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A simple Eulerian finite-volume method for compressible fluids in domains with moving boundaries

Alina Chertock* Alexander Kurganov†

We introduce a simple new Eulerian method for treatment of moving boundaries in compressible fluid computations. Our approach is based on the extension of the interface tracking method recently introduced in the context of multifluids. The fluid domain is placed in a rectangular computational domain of a fixed size, which is divided into Cartesian cells. At every discrete time level, there are three types of cells: internal, boundary, and external ones. The numerical solution is evolved in internal cells only. The numerical fluxes at the cells near the boundary are computed using an interface-tracking technique combined with a solid wall ghost-cell extrapolation and an interpolation in the phase space. The proposed computational framework is general and may be used in conjunction with one's favorite finite-volume method. The robustness of the new approach is illustrated on a number of one- and two-dimensional numerical examples.

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A parallel high-order solver for linear elasticity problems using a weak Galerkin finite element method on unstructured quadrilateral grids

Yunze Li* Chunlei Liang† Lin Mu‡

Weak Galerkin Finite Element Method (WGFEM) is a high-order discontinuous method for unstructured grids. In this work, we use a domain decomposition method to create a WGFEM solver for parallel solutions of linear elasticity equations on unstructured quadrilateral grids. In particular, we employ a Balancing Domain Decomposition by Constraints (BDDC) to effectively reduce the computational cost of the global problem for the interface unknowns in the primal space. The standard continuous Galerkin Finite Element Method solves unknowns on nodal points. After domain decomposition, the nodal points on subdomain interfaces may connect to multiple elements. The WG-BDDC method does not need to involve solutions on the nodal points. Therefore, the communication between two adjacent subdomains only requires to collect information over their common faces.

A unique feature of the WGFEM method is the use of weak gradient operator to differentiate basis functions. WGFEM employs two kinds of basis functions including one kind on the edges of each element and the other inside the element. These two kinds of basis functions can be chosen independently. In order to have continuous solution in each element given that two different spaces are used, a stabilizer is introduced at element interfaces. For 2D problems, an integration by parts was used to change surface integrals to line integrals. In the BDDC method, the unknowns are grouped to interior, dual and primal spaces for each subdomain by the technique of Schur complement. Unknowns in dual spaces are on the boundaries of subdomains but only need to compute locally. Unknowns in primal spaces will constitute a new global problem to solve. The size of this new global problem is significantly smaller than that of the global problem involving all unknowns on subdomain boundaries.

We first tested the WG-BDDC method on uniform grids. Both 2nd-order and 3rd-order WG-BDDC methods are able to obtain optimal orders of accuracy on these grids. Excellent scalability performance was obtained for the WG-BDDC method on uniform grids by testing over 16 CPUs. In the final paper, we plan to report the scalability of the WG-BDDC solver on both structured and unstructured grids by testing over several hundred computer cores. Finally, the WG-BDDC method is successfully extended to fully unstructured grids of all quadrilateral elements. Our preliminary tests show that the 2nd-order WG-BDDC method has similar speedup performance on fully unstructured grids comparing with that on uniform grids. The WG-BDDC method is robust and its solution accuracy is insensitive to grid quality.

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Efficient high-order discontinuous Galerkin solution strategies for implicit unsteady flow simulations

Matteo Franciolini*

The work reports on the comparison between efficient implementations of high-order discontinuous Galerkin methods [1]: a modal, matrix-free discontinuous Galerkin (DG) method, a hybridizable discontinuous Galerkin (HDG) method, and a primal formulation of HDG, applied to the implicit solution of unsteady compressible flows. With respect to standard techniques and implementations, the matrix-free strategy allows for a reduction in the memory footprint when dealing with implicit time-accurate discretization. On the other hand, HDG reduces the number of globally-coupled degrees of freedom relative to DG, at high order, by introducing additional face unknowns and statically condensing element-interior degrees of freedom out of the global system in favor of face unknowns. The primal formulation of HDG reduces the element-interior degrees of freedom by eliminating the gradient as a separate unknown, ensuring stability by adding an additional symmetry term involving jumps at the mesh element interfaces.

The effects of several parameters on the computational efficiency will be investigated, with particular interest to the preconditioning strategy. To deal with stiff linear systems arising from a high-order discretization of low-Mach number turbulent flows, the use of p-multigrid will be consider to speed-up the solution process. While standard-inherited approaches are employed for DG [2], the work reports also on the development of an approximate-inherited approach for HDG discretizations [3]. Special attention will be given to the memory footprint of the solver, as well as an assessment of the parallel efficiency considering both the scalability of the algorithm, in terms of number of iterations, as well as the computational time.

Numerical experiments will consider test cases of growing complexity. First, the solution of simple two- dimensional cases involving the laminar compressible flow equations, such as unsteady flow past a circular cylinder and the flow around a heaving and pitching airfoil. Second, the discretizations will be compared on three dimensional turbulent flow simulation cases.

References

[1] Krzysztof J Fidkowski. “A hybridized discontinuous galerkin method on mapped deforming domains.” In: *Computers & Fluids* 139 (2016), pp. 80–91.

[2] Matteo Franciolini, Lorenzo Botti, Alessandro Colombo, and Andrea Crivellini. “P-multigrid matrix-free discontinuous galerkin solution strategies for the under-resolved simulation of incompressible turbulent flows.” In: *arXiv preprint arXiv:1809.00866* (2018).

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[3] Matteo Franciolini, K.J. Fidkowski, and A. Crivellini. "P-multigrid preconditioners applied to high-order dg and hdg discretizations." In: *7th European Conference on Computational Fluid Dynamics, Glasgow, Scotland.* 2018.

Monday, June 3, Afternoon Session II (Room: Templo Mayor)

libParanumal: portable highly optimized high-order finite element implementations for GPU computing

Tim Warburton* Anthony P. Austin† Noel Chalmers‡ Ali Karakus§
Kasia Swirydowicz¶

The U.S. Department of Energy Summit leadership compute facility at Oak Ridge National Lab is currently the fastest system on the Top500 list. Summit is composed of over four thousand compute nodes each equipped with six NVIDIA Volta V100 graphics processing units. In turn each Volta GPU has 2560 64-bit floating point units grouped in eighty logical cores. To run efficiently on Summit requires algorithms and implementations that can fully exploit this deep multilevel parallel hierarchy.

The Parallel Numerical Algorithms group at Virginia Tech started developing the libParanumal library in 2017 to specifically experiment with high-order finite elements that can potentially exploit Summit and successor exascale systems. The library includes reference implementations for compressible and incompressible Navier-Stokes, Galerkin-Boltzmann gas dynamics, elliptic problems, and Stokes flows. The library supports high-order triangles, quadrilaterals, tetrahedra, and hexahedra with continuous or discontinuous Galerkin discretizations in space and a range of time stepping methods. The spatial discretizations, time steppers, and linear solvers included within libParanumal are all implemented using the portable Open Concurrent Compute Abstraction (OCCA).

In this talk I will discuss both the on-node optimality and the strong and weak scaling characteristics of libParanumal on the Summit system for model incompressible flow calculations. I will highlight the remaining challenges that will be compounded as we seek to deploy on upcoming exascale capable systems.

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A GPU-accelerated high-order finite element solver for the stokes equations

Anthony P. Austin* Timothy Warburton*

We present a GPU-accelerated high-order finite element solver for the steady Stokes equations. We show experimentally that our solver attains appropriate h- and p-convergence rates and illustrate its performance on a variety of problems. In particular, we demonstrate that our GPU kernels operate close to the empirically-determined roofline limit on the NVIDIA V100 platform.

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The automatic sparse spectral discretization of tensorial PDEs

Keaton J. Burns* Geoffrey M. Vasil† Daniel Lecoanet‡ Jeffrey S. Oishi§
Benjamin P. Brown¶

Developing efficient global spectral discretizations of PDEs such as the Navier-Stokes equations in a variety of geometries is a challenging task. For instance, the analytical behavior of scalar, vector, and tensor quantities differ near the coordinate singularities in spherical and cylindrical coordinates so care must be taken to maintain accuracy in spectral representations of quantities in these frames. Spectral methods based on Jacobi polynomials have recently been developed for the disk and ball that incorporate these different analytical behaviors and posses sparse and banded representations of differential operators similar to sparse Chebyshev methods [2, 3, 1]. These new bases therefore enable the efficient and systematic discretization of broad ranges of tensorial partial differential equations in cylinders and spheres. Here we will discuss these bases and their implementation in the open-source spectral framework Dedalus (`http://dedalus-project.org`) that automates this discretization process. In particular, we have developed a parsing system that allows users to enter PDEs in plain text using a coordinate-free notation. The parser then transforms these equations into sparse, banded, and well-conditioned matrices using Fourier, Chebyshev, and Jacobi-based spectral methods, depending on the specified geometric domain of the problem. The separability of the resulting discretization is automatically detected and the problem is automatically parallelized over distributed-memory architectures using MPI. This system allows users to easily define systems of scalar, vector, and tensorial PDEs in a domain-independent fashion and to efficiently simulate these equations at scale. We will show several examples of this system applied to multiphase and hydrodynamical PDEs arising in geophysics and astrophysics.

References

[1] Daniel Lecoanet, Geoffrey M Vasil, and Benjamin P Brown. "Tensor calculus in spherical coordinates using Jacobi polynomials. Part-II: Implementation and examples." In: *Journal of Computational Physics: X* (Mar. 2019), p. 100012.

[2] Geoffrey M Vasil, Keaton J Burns, Daniel Lecoanet, Sheehan Olver, Benjamin P Brown, and Jeffrey S Oishi. "Tensor calculus in polar coordinates using Jacobi polynomials." In: *Journal of Computational Physics* 325 (Nov. 2016), pp. 53–73.

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[3] Geoffrey M Vasil, Daniel Lecoanet, and Benjamin P Brown. "Tensor calculus in spherical coordinates using Jacobi polynomials. Part-I: Mathematical analysis and derivations." In: *Journal of Computational Physics: X* (Mar. 2019), p. 100013.

IMEX HDG-DG: a coupled implicit hybridized discontinuous Galerkin and explicit discontinuous Galerkin approach for shallow water systems

Shinhoo Kang* Francis X. Giraldo† Tan Bui-Thanh‡

We propose IMEX HDG-DG schemes for planar and spherical shallow water systems. Of interest is subcritical flow, where the speed of the gravity wave is faster than that of nonlinear advection. In order to simulate these flows efficiently, we split the governing system into a stiff part describing the gravity wave and a non-stiff part associated with nonlinear advection. The former is discretized implicitly with the HDG method while an explicit Runge-Kutta DG discretization is employed for the latter. The proposed IMEX HDG-DG framework: 1) facilitates high-order solutions both in time and space; 2) avoids overly small time-step sizes; 3) requires only one linear system solve per time stage; 4) relative to DG generates smaller and sparser linear systems while promoting further parallelism; and 5) suppresses the fast modes in the system with a large time-step size. Numerical results for various test cases demonstrate that our methods are beneficial for applications where slow modes are accurately treated while fast modes are inaccurately handled, i.e., a fast and stable solution is more important than an accurate solution.

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Monday, June 3, Afternoon Session III (Room: Tehuanco)

Fast algorithms for the evaluation of layer and volume potentials

Andreas Klöckner*

I will present new, asymptotically fast algorithms with high-order error bounds for the evaluation of layer and volume potentials in two and three dimensions. The efficient evaluation of both types of potentials and their effective coupling is essential in the development of efficient integral-equation-based solvers for inhomogeneous elliptic BVPs. I will demonstrate the performance and accuracy of these methods through a number of application examples drawn from electromagnetics and fluid flow.

For the case of layer potentials, I will discuss a guaranteed-accuracy fast algorithm for Quadrature by Expansion (QBX), accelerated through the use of target-specific expansions. QBX is a systematic, high-order approach to Nyström-discretized singular quadrature that applies to layer potential integrals with general kernels on curves and surfaces with high-order unstructured discretizations. Target-specific expansions permit a substantial cost reduction in the fast algorithm, through a decrease of the number of floating point operations required for the evaluation of near-field interactions. Combined with adaptive refinement based on geometric criteria enforced through a tree-based geometry processing method, our fast algorithm, termed GIGAQBX-TS, is governed by a simple, additive error model that robustly controls the truncation, quadrature and acceleration error components while obtaining approximately linear scaling of cost with the size of the geometry.

I will further discuss the coupling of the layer potential scheme with a volume potential evaluation method in two and three dimensions in the presence of complex geometry. Volume potential evaluation is accelerated by a table-driven Fast Multipole algorithm. Time permitting, I will further discuss the automated synthesis of low-complexity expansion and translation operators for a symbolically-supplied kernels.

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High-order hybridized discontinuous Galerkin method and scalable solution strategies for incompressible magnetohydrodynamics

Sriramkrishnan Muralikrishnan* Stephen Shannon† Tan Bui-Thanh‡
John Shadid§

We present a high-order hybridized discontinuous Galerkin (HDG) method and scalable linear and nonlinear solution strategies for incompressible resistive magnetohydrodynamics (MHD). Incompressible resistive MHD presents several challenges in terms of nonlinearity, coupled fluid and magnetic physics, incompressibility constraints in both velocity and magnetic fields to name a few. As a step forward to addressing these challenges in the context of high-order methods, we present an IMEX-HDG-DG nonlinear solution strategy (compared against a Picard iteration strategy) for various benchmark problems in incompressible MHD including, but not limited to, the island coalescence problem which is of significant interest to the MHD/plasma physics community. For linear solvers, we will explore block preconditioning strategies and also show the applicability of a newly developed multilevel solver for HDG trace system in the context of incompressible MHD. Various large scale numerical results in both 2D and 3D will be presented.

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Adaptive mesh refinement on graphics processing units for applications in gas dynamics

Andrew Giuliani* Lilia Krivodonova†

We present novel algorithms for cell-based adaptive mesh refinement on unstructured meshes of triangles on graphics processing units for the discontinous Galerkin method. Our implementation makes use of an edge coloring algorithm for avoiding race conditions when evaluating surface integrals and improved memory management techniques. Both the solver and AMR algorithms are entirely implemented on the GPU, with negligible communication between device and host. We show that the overhead of the AMR subroutines is small compared to the high order solver and that the proportion of total runtime spent adaptively refining the mesh decreases with the order of approximation. We apply our code to a number of benchmark problems as well as more recently proposed problems for the Euler equations that require extremely high resolution. We present the solution to a shock reflection problem that addresses the von Neumann triple point paradox with an accurately computed triple point location.

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A fast high-order solver for high Reynolds number stratified flows on massively multi-cored architectures *

Kristopher Rowe[†‡] Nidia Cristina Reyes Gil[‡] Greg Thomsen[§]
Peter Diamessis[‡]

The simulation of high Reynolds number stratified flows has important applications in atmospheric science, physical oceanography, marine engineering, and wind energy. Present in many of these applications is strongly-stratified turbulence, characterized by the formation of thin, horizontal patches of vertical shear — highly intermittent in both space and time. Fluid motions can persist for greater durations than their unstratified turbulent counterparts, owing to a stifling of the inter-scale transfer of kinetic energy by buoyancy. In addition, stratified fluids support the generation of internal waves capable of transporting energy great distances from their source. Therefore, numerical simulation of strongly-stratified turbulent flows requires long-time integrations on large computational domains using high-resolution spatial grids.

We will present a fast, high-order solver for stratified flows utilizing a Fourier pseudo-spectral discretization in the horizontal and a spectral element method (SEM) in the vertical. An IMEX time-integration scheme is used, requiring the solution of many 1D Helmholtz equations during each time-step. Basis functions for the SEM are constructed using ultraspherical polynomials; subsequently, application of static condensation results in a very large number of small tridiagonal systems – and an algorithm that is as inexpensive as second-order finite difference schemes. Coarse, medium, and fine grain parallelism are exploited to achieve optimal performance on massively multi-cored processors prevalent in today's high-performance computing environment. The wake of a sphere towed through a linearly stratified fluid — a canonical model for more complex flows in oceanographic and marine engineering applications — is used as a numerical example and motivation throughout.

*This document has been approved for public release; its distribution is unlimited.

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Alternating direction implicit modeling of wave motion using compact and mimetic finite differences

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Finite difference (FD) simulations of wave propagation in acoustic media, subject to appropriate boundary conditions, continuous to be insightful and relevant for seismic modeling, room acoustics, electromagnetics, among others applications. Main reasons include their low computation times and satisfactory accuracy even for highly heterogeneous materials. Reductions of simulation times can be achieved by using implicit or semi-implicit time integrations that allow large CFL stepping, and accuracy can be improved by applying high-order stencils that allow high grid sampling of modeling wavelengths. This work is a comparative analysis on the accuracy, stability and computational complexity of two fourth-order FD methods. Both schemes share a semi-implicit time integration derived from a Crank-Nicolson discretization subject to an efficient one-dimensional alternating direction implicit splitting. In space, the first method uses standard compact FD on nodal meshes that require solving banded linear systems along each grid line, whereas the second method employs staggered-grid mimetic FD operators for an explicit differentiation. Our theoretical studies revise the Fourier stability and the arithmetic operational complexity of these methods, and our numerical results assess their empirical accuracy and actual simulation times.

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Tuesday, June 4, Morning Session I (Room: Aztlan)

A parallel high order hp-adaptive discontinuous Galerkin solver for incompressible flow

Catherine Mavriplis* Gilou Agbaglah* Noel Chalmers*†

We present a parallel hp-adaptive high order (spectral) discontinuous Galerkin method for approximation of the incompressible Navier-Stokes equations. We use an interior penalty discontinuous Galerkin method to ensure stability and invertibility for the viscous terms, explicit Runge-Kutta time discretization for the nonlinear convection (flux) terms, and a splitting procedure to efficiently enforce the incompressibility condition at each time step. Poisson problems for pressure and viscous terms are solved implicitly. We detail our implementation consisting of a tensor product basis of high order Legendre polynomials on quadrilateral elements, Lax-Friedrichs numerical fluxes, and p-multigrid and pressure projection techniques to accelerate the conjugate gradient linear solvers. We implement hp-adaptivity using an inexpensive a posteriori error estimator to determine where refinement or coarsening is necessary.

The discontinuous Galerkin spatial discretization allows for simple hp-adaptivity as well as direct parallelization of the scheme due to its discontinuous nature and local flux calculations. Parallelization is implemented using a hybrid MPI and OpenMP approach to allow for greater flexibility of parallelism during adaptive refinement.

Numerical tests validate both the temporal and spatial accuracy of the method and benchmarks indicate that the implementation scales well as parallelism is increased. We present several numerical tests to demonstrate the efficacy of the method, in particular in reducing the number of degrees of freedom needed and allocating computing resources to regions of sharp variation in transient incompressible Navier-Stokes flows. Comparisons with spectral element solutions are provided.

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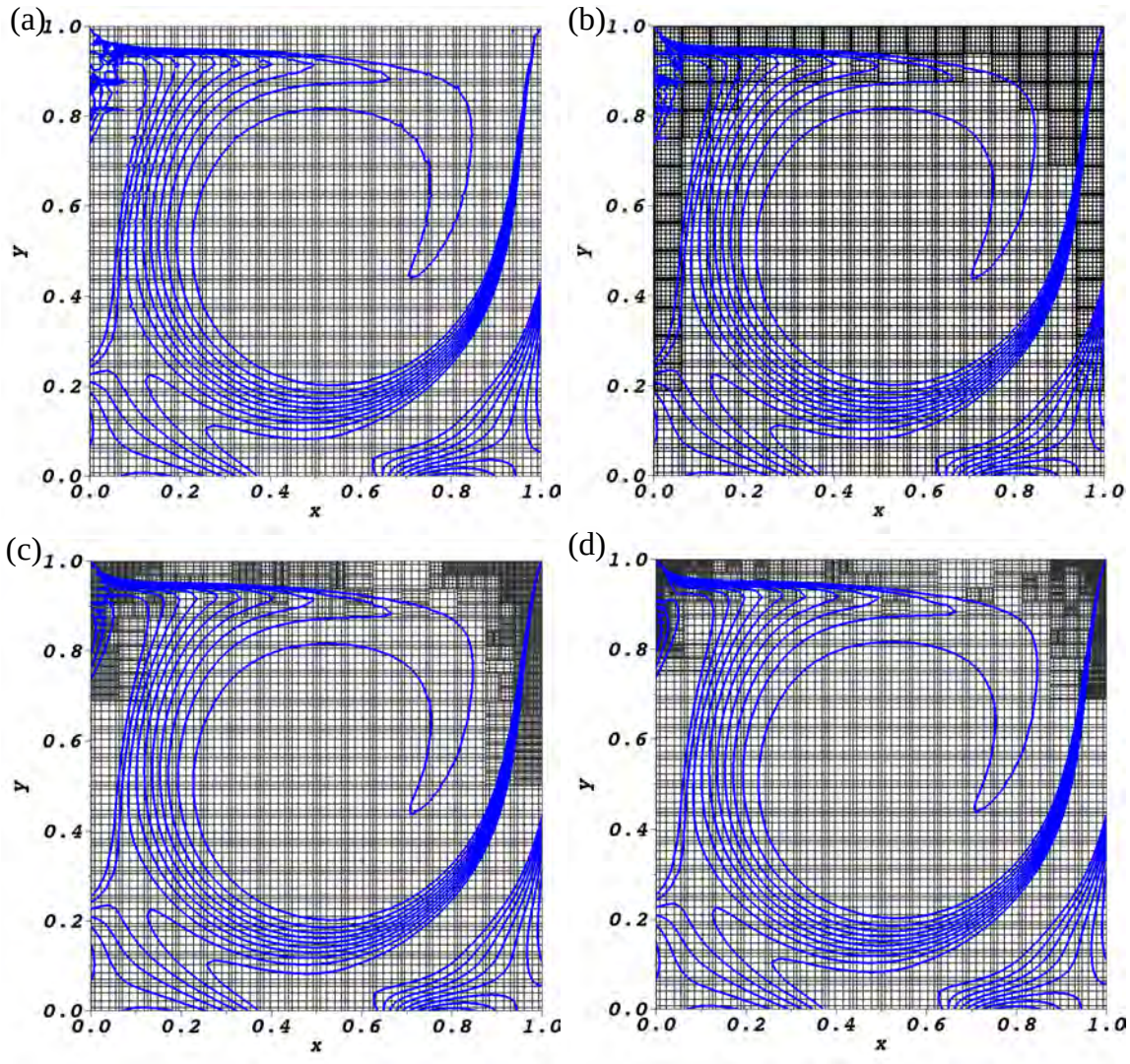

Figure 1: Vorticity contours computed using uniform and adaptive refinement meshes in the driven cavity at $t = 60$ and $Re = 10^3$. (a): uniform elemental mesh with $K = 16 \times 16 = 256$ elements, polynomial orders in x and y of $N = M = 5$, (b): p-adaptive with $K = 16 \times 16 = 256,\ 5 \leq N, M \leq 9$, (c): h-adaptive with $256 \leq K \leq 1024,\ N = M = 5$ and (d): hp-adaptive with $256 \leq K \leq 1024,\ 5 \leq N, M \leq 9$.

Adaptive space-time discontinuous Galerkin methods for solutions of steady and transient partial differential equations

Reza Abedi* Alireza Mazaheri† Robert Haber‡

The asynchronous Spacetime Discontinuous Galerkin (aSDG) method [2] can be used directly, without relaxation, to solve hyperbolic problems. It has proven very effective in this role due to its local conservation properties, linear computational complexity, unconditional stability, powerful adaptive meshing capabilities, and other favorable properties. Here we focus on extensions of aSDG solution technology to address elliptic and parabolic PDEs using hyperbolic pseudo-time relaxations.

In the case of elliptic PDEs, the role of pseudo-time in the relaxed system is analogous to physical time in a conventional hyperbolic system, and the steady limit of the relaxed problem corresponds to the solution of the original elliptic system. We compare three pseudo-time solution schemes for the relaxation: (i) the scheme presented in [3], where we use a discontinuous Galerkin (DG) discretization in space and a finite difference scheme in pseudo-time; (ii) an implicit space-time DG method in which a spatial mesh is extruded in time to form the space-time mesh; and (iii) the aSDG method [2] in which a special asynchronous space-time meshing procedure constructs unstructured spacetime meshes that satisfy a special causality constraint defined in terms of the pseudo wave speed in the relaxed system. The aSDG pseudo-time solver exploits powerful adaptive meshing procedures [1] to ensure accuracy and expedite convergence to the steady limit. For parabolic problems, the relaxed problem comprises a system of PDEs in space, physical time, and pseudo-time that we cast in first-order form. For each increment in physical time, we seek the steady solution of a transient hyperbolic problem in pseudo-time.

In contrast to time-marching schemes that use finite difference operators in time, we can easily introduce arbitrarily high-order space-time polynomial bases to balance and simultaneously improve the aSDG method's order of accuracy with respect to element spatial diameter and temporal duration. We present numerical results for problems involving nonlinear advection-diffusion and the wave equation including studies of asymptotic convergence rates obtained with aSDG and pseudo-time aSDG methods.

References

[1] Reza Abedi, Robert B. Haber, Shripad Thite, and Jeff Erickson. "An h-adaptive spacetime-discontinuous galerkin method for linear elastodynamics." In: *European Journal of Computational Mechanics* 15.6 (2006), pp. 619–642. DOI: 10.3166/remn.15.619-642.

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[2] Reza Abedi, Boris Petracovici, and Robert B Haber. "A space–time discontinuous galerkin method for linearized elastodynamics with element-wise momentum balance." In: *Computer Methods in Applied Mechanics and Engineering* 195.25-28 (2006), pp. 3247–3273.

[3] Alireza Mazaheri and Hiroaki Nishikawa. "Efficient high-order discontinuous galerkin schemes with first-order hyperbolic advection–diffusion system approach." In: *Journal of Computational Physics* 321 (2016), pp. 729–754.

An unsteady and anisotropic p-adaptation method based on truncation error estimations for high-order discontinuous Galerkin schemes

Andrés Mauricio Rueda-Ramírez* Gonzalo Rubio* Esteban Ferrer*
Eusebio Valero*

Truncation error estimators based on the τ-estimation method have been used as efficient indicators to drive locally adaptive simulations for steady-state boundary value problems. Their main advantages are that they are cheaper to compute than adjoint-based error estimators and that they are highly accurate (minimizing the truncation error minimizes the numerical error of all functionals at once). However, there is a lack of scientific literature on their use for unsteady cases.

In this work, we present a p-adaptation algorithm for unsteady problems that targets the truncation error for p-anisotropic Discontinuous Galerkin (DG) discretizations. In order to achieve that, different alternatives for estimating the truncation error of unsteady problems are analyzed and a new methodology is introduced that makes use of a cheap-to-evaluate decoupled truncation error estimator for tensor-product DG methods.

The proposed method is tested for two different compressible flow problems: the convection of an inviscid vortex and the vortex shedding past a circular cylinder. A thorough study of the accuracy and computational cost (both in storage and CPU-time) of the method is presented when different truncation error thresholds and adaptation intervals are used, as well as a comparison with uniform refinement techniques and details on how to efficiently implement the proposed methodology. Significant reductions in the number of degrees of freedom (DOFs) and computational times are observed for the same levels of accuracy (dispersion and dissipation errors), as compared to uniform refinement techniques.

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Using p-refinement to increase boundary derivative convergence rates

David Wells* Jeffrey Banks†

Simulation of many important physical problems, such as fluid structure interaction and conjugate heat transfer, requires numerical methods that compute boundary derivatives or fluxes to high accuracy. In some circumstances the only desired result of a calculation is a quantity derived from the boundary derivatives, such as a flux or stress: this problem has long been recognized as one of importance, and a variety of methods have been proposed that allow reconstruction of an accurate boundary flux from less accurate interior data. Accurate boundary derivatives are also required for some numerical boundary conditions.

A variety of algorithms have been proposed for calculating higher order derivative values from lower order data calculated by a finite element method: most of these algorithms rely on data post-processing, where one uses interpolation or a finite difference formula to compute derivatives from data. In this talk we discuss a novel alternative to these techniques based on local Lagrange-type p-refinement [1] that improves the accuracy of various derivatives of the approximation itself (without the need for any postprocessing) at isolated points along the boundary. We develop a basic theory for such discretizations in a single spatial dimension and then utilize a technique based on the Fourier transform to extend the theory to higher dimensions for elliptic problems. Finally, we demonstrate with numerical experiments that these convergence rates are achieved in practice with some simple test problems.

References

[1] D. Wells and J. Banks. *Using p-refinement to increase boundary derivative convergence rates.* URL: https://arxiv.org/abs/1711.05922.

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A robust and efficient wave-structure interaction solver for high-density ratio multiphase flows

Amneet Pal Singh Bhalla*

We present a robust, adaptive numerical scheme for simulating high-density ratio and high shear multiphase flows on locally refined staggered Cartesian grids that adapt to the evolving interfaces and track regions of high vorticity. The algorithm combines the interface capturing level set method with a variable-coefficient incompressible Navier-Stokes solver that is demonstrated to stably resolve material contrast ratios of up to six orders of magnitude. The solver employs a hybrid preconditioner that solves velocity and pressure degrees of freedom simultaneously and without using any operator-splitting approach. The discretization approach ensures second-order pointwise accuracy for both velocity and pressure with several physical boundary treatments, including velocity and traction boundary conditions. The paper includes several test cases that demonstrate the order of accuracy and algorithmic scalability of the flow solver. To ensure the stability of the numerical scheme in the presence of high density and viscosity ratios, we employ a consistent treatment of mass and momentum transport in the conservative form of discrete equations. This consistency is achieved by solving an additional mass balance equation, which we approximate via strong stability preserving Runga-Kutta time integrator and by employing the same mass flux (obtained from the mass equation) in the discrete momentum equation. The scheme uses higher-order total variation diminishing (TVD) and convection-boundedness criterion (CBC) satisfying limiter to avoid numerical fluctuations in the transported density field. The high-order bounded convective transport is done on a dimension-by-dimension basis, which makes the scheme simple to implement. We also demonstrate through several test cases that the lack of consistent mass and momentum transport in non-conservative formulations, which are commonly used in practice, or the use of non-CBC satisfying limiters can yield very large numerical error and very poor accuracy for convection-dominant high-density ratio flow.

We then combine the aforementioned robust two-phase flow solver with a distributed Lagrange multiplier based immersed boundary method to simulate practical three-phase wave-structure interaction (WSI) problems. An effective wave generation and absorption techniques for a numerical wave tank are presented and used to simulate a benchmark case of water wave distortion due to a submerged structure. The numerical scheme is tested on several benchmarking WSI problems from numerical and experimental literature in both two and three dimensions to demonstrate the applicability of the IB/WSI method to practical marine and coastal engineering problems.

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Tuesday, June 4, Morning Session II (Room: Templo Mayor)

Invariant domain preserving approximation of hyperbolic systems: beyond second-order

Jean-Luc Guermond * Bojan Popov *

We introduce an approximation technique for nonlinear hyperbolic systems with sources that is invariant domain preserving. The method consists of blending a low-order method and a high-order method. The low-order method is formally first-order accurate in space and invariant domain preserving. The high-order method may violate the invariant domain properties, but this defect is corrected a posteriori by a limiting technique that we call convex limiting. After limiting, the resulting method satisfies all the invariant domain properties that are imposed by the user and is formally high-order accurate. The key novelties are as follows: (i) the stencil of the low-order method is restricted to the next neighbors only; (ii) the low-order and the high-order methods carry exactly the same mass; (iii) limiting is done by enforcing bounds on quasiconcave functionals; (iv) the bounds that are enforced on the high-order solution at each time step are necessarily satisfied by the low-order approximation. The method is illustrated with triangular Lagrange elements up to degree three (i.e. fourth order in time and space).

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High-order shock fitting using a discontinuous Galerkin method

Luke D'Aquila* Brian Helenbrook * Alireza Mazaheri †

One-dimensional, moving-grid, shock-tracking, discontinuous Galerkin finite element methods have been implemented to test approaches for obtaining high-order accuracy for flow simulations with shocks. In these approaches, an element edge in the computational mesh is fitted to the shock front and moved with the shock throughout the computation. The one-dimensional Euler equations are solved on the moving mesh in an arbitrary Lagrangian-Eulerian framework. Three different methods for evaluating the shock velocity have been implemented, and the order of accuracy of the resulting solutions were verified using the method of manufactured solutions. The first method computes the shock velocity using a Riemann invariant propagating upstream from behind the shock along with the Rankine-Hugoniot (RH) jump conditions [3]. The second method computes the shock acceleration using an equation for the momentum immediately downstream of the shock along with the RH jump conditions [1]. Finally, the third method computes the shock acceleration using a characteristic relation immediately downstream of the shock along with the RH jump conditions [2]. It was found that all three methods converge to the expected solution. When using a DG method with polynomial degree, p, of 1 and 2, all methods converged with the expected order of accuracy $(p+1)$. For $p=3$ methods one and two obtained the expected 4^{th} order of accuracy but the third approached 3^{rd} order accuracy on fine grids. Based on the results, method one has been deemed the most effective for evaluating the shock velocity, as it is the easiest to implement and achieves the expected order of accuracy.

With the basic methods implemented in one dimension, a 2D implementation has been initiated. The two dimensional simulations use an unstructured triangular mesh and unstructured mesh adaptation techniques to prevent mesh degradation when solving problems with significant shock movement. Viscous forces are also included. Planned demonstration cases include bow shocks and shock boundary layer interaction simulations.

References

[1] A. Henrick, T. Aslam, and J. Powers. "Simulations of pulsating one-dimensional detonations with true fifth order accuracy." In: *Journal of Computational Physics* (2006).

[2] Xiaolin Zhong. "High-order finite-difference schemes for numerical simulation of hypersonic boundary-layer transition." In: *Journal of Computational Physics* (1998).

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†Aerothermodynamics Branch, NASA Langley, Hampton, VA.

[3] Dongyang Zou, Chunguang Xu, Haibo Dong, and Jun Liu. "A shock-fitting technique for cell-centered finite volume methods on unstructured dynamic meshes." In: *Journal of Computational Physics* 345 (2017), pp. 866–882.

Shock-wave boundary layer interactions simulations with a implicit Discontinuous spectral/hp element method

Giacomo Castiglioni* Zhengou Yan* Yu Pan* Joaquim Peiro*
Spencer J. Sherwin*

Shock wave boundary layer interaction (SWBLI) is a phenomena encountered in many industrial devices such as transonic and supersonic external aerodynamic applications, supersonic air intakes, transonic and supersonic cascades, and over-expanded nozzles.

SWBLI plays a critical role to the design of such devices due to its importance for both efficiency and structural integrity, often being the limiting factor to the design envelope.

Although SWBLIs have been extensively (Dolling, 2001) there are still many open questions and they remain a very active research area. Of particular interest are turbulent SWBLIs and SWBLIs in non-trivial geometries.

Lately discontinuous Galerkin spectral element methods (DGSEM) have gained popularity for the solution of the turbulent compressible flows due to their spectral accuracy, geometrical flexibility, and scalability.

These characteristics make of DGSEM a promising candidate to be the platform for a new generation of computational fluid dynamics software.

Several different approaches are proposed in literature to tackle shocks in conjunction with DGSEM including limiters, artificial viscosity, and filtering procedures.

On the other hand, it is noteworthy that so far most methods have been applied only to two-dimensional inviscid flows, see brief overview in Chaudhuri et al. (2017).

The aim of the present work is to evaluate a newly developed implicit in time DGSEM in combination with existing artificial viscosity approaches to accurately simulate two and three-dimensional SWBLI problems.

The solver is implemented in the spectral/hp element framework of the open-source software Nektar++.

A diagonally implicit Runge-Kutta method together with a Jacobian-Free Newton-Krylov (JFNK) method are used for the time integration. The efficiency and robustness of the implicit DGSEM solver are further improved by a thorough restructuring of the solver which includes the non-dimensionalization of the equations, the co-design of a shock-capturing strategy and the development of preconditioners.

The long term objective is to improve the efficiency, and robustness of the existing solver in order to tackle turbulent SWBLIs in industrially relevant geometries.

As a test case for SWBLI we selected a laminar SWBLI problem which has been extensively studied experimentally and numerically. Here we present a comparison between the explicit and

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implicit solvers in terms of accuracy, robustness, and time to solution.

Multi-level static condensation for the simulation of internal solitary waves over an actual bathymetry

Theodoros Diamantopoulos* Kristopher Rowe* Peter Diamessis*
Greg Thomsen†

Internal Solitary Waves (ISWs) are ubiquitous oceanic phenomena found on continental slopes and shelves, in submarine canyons, and over oceanic topographic features. These large amplitude internal waves propagate long distances with nearly unchanging form, transporting energy from the deep ocean into shallower coastal waters. Commonly embedded within the propagating ISWs is finer-scale turbulence, resulting from localized instabilities. The resulting dissipation and mixing are critical drivers of larger-scale shelf energetics and the associated ecosystem balance.

The coherent nature of ISWs is due to a precarious balance between nonhydrostatic dispersion and nonlinear steepening – therefore, the use of high-order methods is necessary to minimize any artificial dissipation or dispersion that may affect the physical properties of these waves. The Spectral Element Method (SEM) is a high-order technique used extensively for the solution of the Incompressible Navier-Stokes Equations (INSE). Performing a realistic simulation of ISW's over an actual bathymetry necessitates the use of highly elongated domains, causing great difficulty in the solution of elliptic problems arising in many popular time-splitting schemes for the INSE. Nevertheless, the compactness of the bases used in the SEM leads to an algebraic structure which can be leveraged to achieve a robust solution of the INS equations.

Field observations suggest that shoaling ISWs frequently propagate in a direction which is normal to isobaths. As such, one may regard the along-shore/transverse direction as homogeneous in the context of any associated wave-induced turbulence. Efficient simulation of ISWs can therefore be realized through the combination of a Fourier-Galerkin and a SEM. Discretization of the transverse coordinate using the Fourier-Galerkin method results in a large number of independent 2D elliptic problems: one for each wavenumber.

Multilevel static condensation, based on repeated calculation of the Schur complement matrix, is a domain decomposition technique which seeks to separate the computational domain into a hierarchy of smaller problems. First, the degrees of freedom interior to each element are eliminated, resulting in a system of equations for the horizontal and vertical edges of the computational domain. Next, further reduction of the problem size takes place by performing a second static condensation – decoupling the horizontal edges from the vertical ones – leading to a block tridiagonal system for the vertical edges amenable to direct solvers. Finally, subsequent independent solves are performed for the degrees of freedom on the horizontal edges, then the element interiors, leading to a highly parallelizable algorithm.

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The focus of this talk will be the development, implementation, and performance of this algorithm on many-cored architectures.

An optimization-based discontinuous Galerkin approach for high-order accurate shock tracking

Matthew J. Zahr*, Per-Olof Persson†

We introduce a high-order accurate, nonlinearly stable numerical framework for solving steady conservation laws with discontinuous solution features such as shock waves. The method falls into the category of a shock tracking or r-adaptive method and is based on the observation that numerical discretizations such as finite volume or discontinuous Galerkin methods that support discontinuities along element faces can perfectly represent discontinuities and provide appropriate stabilization through approximate Riemann solvers. The difficulty lies in aligning element faces with the unknown discontinuity. The proposed method recasts a discretized conservation law as a PDE-constrained optimization problem whose solution is a (curved) mesh that tracks the discontinuity and the solution of the discrete conservation law on this mesh. The discrete state vector and nodal positions of the high-order mesh are taken as optimization variables. The objective function is a discontinuity indicator that monotonically approaches a minimum as element faces approach the shock surface. The discretized conservation law on a parametrized domain defines the equality constraints for the optimization problem. A full space optimization solver is used to simultaneously converge the state vector and mesh to their optimal values. This ensures the solution of the discrete PDE is never required on meshes that are not aligned with discontinuities and improves nonlinear stability. The method is demonstrated on a number of one- and two-dimensional transonic and supersonic flow problems. In all cases, the framework tracks the discontinuity closely with curved mesh elements and provides accurate solutions on extremely coarse meshes.

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Tuesday, June 4, Morning Session III (Room: Tehuanco)

Overlapping Schwarz based spectral element method for incompressible flow in complex domains

Ketan Mittal* Som Dutta† Paul F. Fischer‡

We have developed a robust and scalable method for overlapping grids based on the spectral element method (SEM)[5]. SEM features Lagrangian bases on Gauss-Lobatto-Legendre (GLL) points for representing the geometry and the solution using Nth-order tensor-product polynomials on each spectral element in the mesh. This leads to efficient storage and fast operator evaluation as compared to the classic finite element methods. Additionally, it also enables stable and exponentially-convergent solutions.

SEM has been used to solve incompressible flow and heat transfer problems in complex domains[1], and has strong-scaled to over a million MPI ranks[2]. Since SEM relies on all-hex meshes, complex geometric configurations can require signifcant user input for mesh generation. Overlapping-Schwarz based methods helps users circumvent this problem with simpler overlapping grids where data for interior boundaries is obtained via interpolation from the surrounding domains at each time-step.

Our overlapping-Schwarz based method for solving incompressible flow features a predictor-corrector scheme that was implemented in Nek5000[3]. High-order extrapolation in time is used for the spatially interpolated boundary data to generate an initial solution, followed by corrector iterations where the boundary data is updated using the most recent solution in the surrounding domain. The number of corrector iterations depends on the desired accuracy and the extrapolation order of the boundary data for the predictor step.

Central to this implementation is a fast and robust interpolation and general communication library, gslib, which handles all communication with at most $\log P$ complexity (where P is the number of processors or MPI ranks), and has scaled to over six million MPI ranks. We have introduced gslib in the overlapping Schwarz implementation to ensure scalability, and extended its capability to allow for more than two overlapping meshe[4].

Here, we present new developments for extending the overlapping Schwarz framework to solve a broad range of problems. Recent improvements include techniques to ensure global mass-conservation by imposing an L^2-minimizing correction on the interpolated boundary data, enabling fixed flow-rate through periodic overlapping domains to model engineering applications featuring internal flows, and global weighted integration to compute global quanities such as mean flow-velocity and Nusselt number across multiple overlapping domains. We demonstrate use of these methods for solving incompressible flow problems in various complex domains.

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References

[1] Michel O. Deville, Paul F. Fischer, and Ernest H. Mund. *High-order methods for incompressible fluid flow*. Vol. 9. Cambridge University Press, 2002.

[2] Paul F. Fischer, Katherine Heisey, and Misun Min. "Scaling limits for PDE-based simulation." In: *22nd AIAA Computational Fluid Dynamics Conference*. American Institute of Aeronautics and Astronautics, June 2015. DOI: 10.2514/6.2015-3049.

[3] Brandon E. Merrill, Yulia T. Peet, Paul F. Fischer, and James W. Lottes. "A spectrally accurate method for overlapping grid solution of incompressible Navier–Stokes equations." In: *Journal of Computational Physics* 307 (2016), pp. 60–93.

[4] Ketan Mittal, Som Dutta, and Paul Fischer. "Nonconforming Schwarz-spectral element methods for incompressible flow." In: *arXiv preprint arXiv:1811.04891* (2018).

[5] Anthony T Patera. "A spectral element method for fluid dynamics: Laminar flow in a channel expansion." In: *Journal of Computational Physics* 54.3 (1984), pp. 468–488. ISSN: 0021-9991. DOI: 10.1016/0021-9991(84)90128-1.

Designing CFD algorithms for bandwidth

Philip Roe*

In many applications, extreme accuracy is not possible because of uncertainties in geometry, material properties or environment. High-order methods are then used to extend the range of wavenumbers over which the needed accuracy can be maintained. That is to say, they enable the use of coarse grids.

Accuracy can be achieved by matching Taylor series, and so can bandwidth, as evidenced by so-called Dispersion-Relationship-Preserving schemes. These DRP schemes do successfully make the point that on a given mesh, a high-order scheme can be outperformed by a lower-order scheme. However, I wish for physical principles that promote high bandwidth, together with robustness. It may be noted that these are high-frequency properties, whereas accuracy is a low frequency property. I would like to propose that a good principle is to match the stencil of the discrete problem with the domain of dependence of the continuum problem. We already know that there is a rough connection; too small a stencil cannot be stable and too large a stencil admits spurious solutions. Ideally we would like a stencil that consists only of points that strongly influence the required solution.

In one dimension the best methods are characteristic-based. The evolution of a particular wave mode proceeds almost independently from the others, on its own stencil that is biased in the "upwind" direction. And, trivially, all domains of dependence are confined to the single line. It is easy to choose good stencils, and the methods that result are highly effective.

In more than one dimension the different modes may have dissimilar domains of dependence. I will focus here on the ideal gas Euler equations, which have both advective and acoustic modes. Sufficiently similar systems can be treated in the same way. Each mode is "driven" by a different set of terms[1] in the governing equations.

$$\begin{aligned} \partial_t \rho + \mathbf{v}\cdot\nabla\rho + \rho\nabla\cdot\mathbf{v} &= 0 \\ \partial_t \mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{v} + \frac{1}{\rho}\nabla p &= 0 \\ \partial_t p + \mathbf{v}\cdot\nabla p + \gamma p\nabla\cdot\mathbf{v} &= 0 \end{aligned} \tag{1}$$

If we discard the two highlighted terms, the pressure becomes a passive scalar, and the first two equations form what are known as the "pressureless Euler equations" used, for example to model dust clouds.

$$\begin{aligned} \partial_t \rho + \mathbf{v}\cdot\nabla\rho + \rho\nabla\cdot\mathbf{v} &= 0 \\ \partial_t \mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{v} &= 0 \end{aligned} \tag{2}$$

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[1]It is not possible to define separate acoustic and advective variables in the flux without losing the correct eigenstructure. Here we are breaking the Euler equations into two nonconservative parts.We are instead dividing the evolution operator into two different processses.

These equations decouple. The velocity satisfies the generalized (nonconservative) Burgers equation

$$\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} = 0 \tag{3}$$

whose exact (but implicit) solution in any number of dimensions is

$$\mathbf{v}(\mathbf{x}, t) = \mathbf{v}(\mathbf{x} - t\mathbf{v}) \tag{4}$$

The density then follows from a continuity argument.

If we retain only the highlighted terms we have

$$\begin{aligned} \partial_t \mathbf{v} + \frac{1}{\rho} \mathbf{v} \cdot \nabla p = 0 \\ \partial_t p + \gamma p \nabla \cdot \mathbf{v} = 0 \end{aligned} \tag{5}$$

which is a nonlinear wave equation. In the linear case, the operations (5) and (2) commute[2] so the linearized Euler equations can be solved numerically by alternating the operations and this will carry no penalty. The different operators can use different stencils. For the advection operator, streamline interpolation is used, and for the acoustic operator an extension of Poisson's spherical mean formula to the acoustic system. It turns out that the nonlinear operators also commute, to second order, if special forms of local linearization are employed.

There are several possible ways to implement these ideas. One is to store primitive variables at the nodes of Lagrange quadratic elements and update them by a finite difference procedure. From a combination of the old and new values an average flux over the timestep is computed. By integrating this around an element a third-order estimate is found for the new conserved quantities in each element, and the primitive variables are adjusted to be consistent with this. Results will be presented for the full Euler equations (translating vortex) that require much less run time than the third-order DG1 method, and significantly less than the theoretically fifth-order DG2 method.

A numerical framework for high-fidelity simulations of vaporizing aluminum droplets in shocked flows

Pratik Das* H. S. Udaykumar*

Shock-induced vaporization of Aluminum droplets plays a crucial role in the combustion process inside solid rocket motors and heterogenous explosives. The reaction of the evaporated aluminum with combustion products increases the rate of energy deposition in such systems. In this work, we present a numerical framework for high-fidelity simulations of shock-induced vaporization of aluminum droplets. The current framework couples high-order explicit numerical-schemes with levelset based sharp-interface method to simulate vaporizing droplets in high-speed flows. The calculations include the effects of viscosity, surface tension and evaporation of the liquid into the surrounding gaseous phase while treating the liquid-vapor interface in a sharp manner. The interaction of the characteristic waves with the gas-liquid interface is accurately captured using a Riemann solver-based ghost fluid method. The ghost fluid method is further modified to account for the interfacial jump conditions due to the effects of surface tension, Marangoni stresses, and evaporation. The high-order flow solver in conjunction with the current sharp-interface method and the ghost fluid method provides a numerical tool to study vaporization of aluminum droplets for a wide range of shock Mach numbers and Reynolds numbers.

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High-order modal discontinuous Galerkin method with applications for quantum Boltzmann transport equation*

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The present work deals with the development of the numerical method for solving Quantum Boltzmann transport equation in the context of electron transport at nanoscales under strongly out-of-equilibrium conditions. Quantum Boltzmann transport equation describes the incoherent time evolution of a quantum system consisting of a large number of quasiparticles (for instance electrons, phonons, excitons) and their interactions. Due to the high number of dimensions (six dimensions in phase space and one dimension in time) and their intrinsic physical properties (in particular the non-parabolicity of the momentum-energy dispersion), the construction of numerical method represents a challenge and requires a careful balance between accuracy and computational complexity.

Among traditional high-order methods, the discontinuous Galerkin methods have received increasing attention as a numerical technique for predicting the flow behavior of gas dynamics problems. In this present work, we proposed a multi-dimensional explicit modal discontinuous Galerkin method based on structured meshes for solving the Quantum-Boltzmann transport equation. The transport equations are discretized in space, momentum and time for one- dimensional systems and applied to the description of electron and exciton transport in single- walled carbon nanotubes. The method presented herein is generalizable to higher dimensions, and heterogeneous devices.

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A high-order perturbation of surfaces method for vector electromagnetic scattering by doubly layered periodic crossed gratings

Youngjoon Hong*

The accurate simulation of scattering of electromagnetic waves in three dimensions by a diffraction grating is crucial in many applications of engineering and scientific interest. In this contribution we present a novel High-Order Perturbation of Surfaces method for the numerical approximation of vector electromagnetic scattering by a periodic layered medium. For this we apply the method of Transformed Field Expansions which delivers a Fourier collocation, Legendre-Galerkin, Boundary Perturbation approach to solve the problem in transformed coordinates. A sequence of numerical simulations demonstrate the efficient and robust spectral convergence which can be achieved with the proposed algorithm.

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Tuesday, June 4, Afternoon Session I (Room: Aztlan)

Full waveform seismic inversion with SW4

N. Anders Petersson* Bjorn Sjogreen † Ke Chen‡

We report on recent efforts to generalize the parallel seismic wave propagation code SW4 to improve seismic material models by using full waveform inversion (FWI). FWI was relatively recently introduced in the field of seismology as a nonlinear inverse problem, in which an objective functional is minimized through gradient optimization, under the constraints imposed by the seismic wave equation. Here the objective functional measures the distance between observed and synthetic ground motions, typically from small to medium-sized earthquakes (e.g. magnitude 2-4 events). If the earthquake source function and material models in the computational simulation model were exact, the synthetic motions would agree with the observations, at least down to the fundamental limitations of the linear seismic wave equation.

To perform the optimization, SW4 uses a quasi-Newton algorithm (e.g. BFGS), where the gradient of the objective functional is calculated by solving the adjoint elastic wave equation and convolving the adjoint and forward wave fields in time. Because SW4 uses a summation-by-parts (SBP) finite difference discretization and an energy conserving time integration method, the discretization is self-adjoint. With minor modifications, SW4 can therefore be used to also solve the adjoint wave equation.

In practice the convergence of the quasi-Newton algorithm is often hampered by poor initial material models, sparse observational data of questionable quality, and imprecise source models. We discuss how the convergence properties can be improved by modifying the objective functional, windowing and filtering of the data, using a hierarchical parameterization of the material model, and by imposing algebraic relations between the density, compressional, and shear wave speeds of an isotropic elastic material.

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Weight-adjusted Bernstein-Bezier DG methods for wave propagation in heterogeneous media*

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High order time-domain discontinuous Galerkin (DG) methods yield efficient and accurate simulations of wave propagation through complex geometries due to their low numerical dispersion and dissipation. However, the computational cost of DG methods on tetrahedral meshes grows rapidly with the order of approximation. This issue can be addressed using properties of Bernstein polynomial bases; however, this approach is limited to piecewise constant approximations of heterogeneous media. In this work, we propose a Bernstein-Bezier weight-adjusted DG method, which extends the Bernstein-Bezier DG method to heterogeneous media with sub-element variations by combining it with the weight-adjusted DG method. This approach reduces the computational complexity from $O(N^6)$ to $O(N^4)$ in three dimensions, where N is the polynomial degree. Numerical examples demonstrate speedups achieved by this approach on Graphics Processing Units (GPUs).

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Dispersion analysis of different basis functions applied to high-order discontinuous Galerkin method for the acoustic wave equation*

João A. Isler† Alexandre F. G. Olender† Bruno S. Carmo†

Wave propagation in the earth's interior involves three-dimensional domains with heterogeneous materials, discontinuities between interfaces and complex geometries. As a consequence from these challenging physical obstacles, a wide variety of numerical methods for seismology problems have been extensively studied in the last four decades. Many methods have been employed to solve the acoustic wave equation in heterogeneous media, however high-order discontinuous Galerkin methods arose as one of the main solutions, since high-order finite element methods have a number of benefits associated to very low numerical error and high geometric flexibility [1], and discontinuous Galerking methods can accommodate discontinuities in sharp interfaces and wavefields. In addition, it is ideally suited for parallel computers [3].

Discontinuous Galerkin methods applied in wave problems suffer from numerical dispersion and dissipation which can affect their accuracy. Considering dispersive properties, there are only few papers which evaluate their effects for different basis functions, although they seriously influence the performance of discontinuous Galerkin methods. In this work, we study dispersive properties of high-order discontinuous Galerkin method. Different basis functions used in approximating the exact solution were chosen to assess their effects in the numerical dispersion. Among the basis functions employed here, the Legendre and Lagrange polynomials are the most commonly used in high-order methods [1], so that modal and nodal expansions were explored. The finite element framework adopted to develop the numerical analysis was Firedrake [2], which is a software designed to provide a modern environment, being a tool for automating the numerical solution of partial differential equations, which allows easy code implementation involving complex problems in science and engineering.

References

[1] G. E. Karniadakis and S. J. Sherwin. *Spectral/hp Element Methods for Computational Fluid Dynamics*. 2nd edn. Oxford University Press, 2005.

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[2] F. Rathgeber, D. A. Ham, L. Mitchell, M. Lange, F. Luporini, A. T. T. McRae, G.-T. Bercea, G. R. Markall, and P. H. J. Kelly. "Firedrake: automating the finite element method by composing abstractions." In: *ACM Transactions on Mathematical Software* 43.3 (2016). Article 24.

[3] Z. J. Wang. "High-order methods for the euler and navier–stokes equations on unstructured grids." In: *Progress in Aerospace Sciences* 43 (2007), pp. 1–41.

Computational and convergence analysis of different high-order discontinuous Galerkin implementations for the acoustic wave equation*

A. F. G. Olender† J. A. Isler † B. S. Carmo †

Different approaches to the Discontinuous Galerkin method are investigated for the solution of the acoustic wave equation using the Firedrake software. The Firedrake project is an open source software that enables automatic generation of solutions to partial differential equations using a variety of finite element methods. Because of its use of a Domain Specific Language, aimed at replicating mathematical notation, called the Unified Form Language, equations in the variational form are quickly implemented in a python interface. We use this software for modelling the bidimensional acoustic wave equation using different high-order Discontinuous Galerkin formulations. The first method used is a high-order Nodal Discontinuous Galerkin method and it is compared with a weight-adjusted Discontinuous Galerkin (WADG) method presented by J. Chan and Warburton [1]. The Nodal DG method uses Lagrangian basis functions and WADG is based on matrix-valued weights. Both methods are applied to the same mesh, with a Perfectly Matched Layer boundary condition. The Perfectly Matched Layer boundary reduces reflection at the surface boundary allowing us to limit the area of computation and create a more accurate model of a wide space. The wave equation is of interest in the field of seismic modelling. Its use is mainly aimed at a computationally demanding inverse problem, whose forward counterpart is the focus of this work. The forward problem is solved by both high-order methods and they are analyzed by comparing the computational efficiency, measured by number of floating point operations per second, and convergence rates between both. By evaluating different high-order DG schemes on the forward problem we found that the WADG is suitable for a future implementation of the inverse problem.

References

[1] R. J. Hewett J. Chan and T. Warburton. “Weight-adjusted discontinuous galerkin meth- ods: wave propagation in heterogeneous media.” In: *SIAM Journal on Scientific Computing* 39.6 (2017), A2935–A2961. DOI: 10.1137/16M1089186.

*This document has been approved for public release; its distribution is unlimited.

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Efficient high-order discrete geometric model from CAD

François Guibault* Houman Borouchaki† Patrick Laug‡

In the area of geometric modeling, major challenges are linked to the efficient visualization of CAD surfaces and to the generation of meshes well suited for numerical simulations. In this context, the elaboration and implementation of a discrete geometric model provide a simple and universal representation model, without the need for CAD. Such a model is a geometrically accurate representation of the model by means of a triangulation composed of polynomial elements. A first study aiming to build a discrete universal model has been carried for a model using degree 1 (one) elements, a "triangulation" composed of quadrilaterals and triangles. The advantage of this model of degree 1 lies in its geometric simplicity. However, in the case of complex surfaces, it may require a very large number of elements, in particular to represent some essential model characteristics such as high geometric curvatures. The discrete model is essentially used for visualization purpose and can also be considered for meshing. In this latter context, this discrete model is a universal representation regardless of the original analytical model which enables geometric queries (position, first and second derivatives, ...) to be formulated without reference to the CAD model. In addition, another benefit of the discrete model is to isolate meshing operations from curve and surface parameterization.

This paper presents an extension of the degree 1 approach allowing to efficiently reconstruct a high order discrete geometric model (using quadric, cubic, ..., elements). The reconstruction is made up of several steps. It first proceeds by discretizing and approximating patch boundary curves using polynomials of a user-specified order. Next, for each parametric domain, a grid conforming to this discretization is built. This grid is geometrically adapted through refinement in order to obtain an accurate geometric model. The resulting discrete network of curve and surface elements is then dynamically refined so that it conforms to the original CAD data within a user-specified tolerance, while minimizing the overall model size. By construction, the model is essentially composed of quadrilateral curved elements, possibly with some triangular elements in the vicinity of the boundary. Edges of quadrilaterals are aligned with parametric directions of the original surfaces and are geometrically conformal. Several numerical operations required by this reconstruction process are computationally intensive. These operations have been carefully designed to minimize computational and memory resources. Some illustrative examples will demonstrate the efficiency of the proposed approach.

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Tuesday, June 4, Afternoon Session II (Room: Templo Mayor)

Frame approximations with square matrices

Rodrigo B. Platte* Tony Liu*

Frame expansions are often used to approximate functions and solve PDEs in complex domains. Fourier extension or embedding, for example, are commonly used to compute solutions of problems in general regions with spectral rates of convergence. Another instance of frame approximation arises when singular functions are used to augment smooth bases to capture singularities in the solution. Traditionally, these approximations are computed by discrete least-squares. In this talk, we show that an appropriate choice of approximation points and bases functions can be found that allows these computations to be performed using interpolation, or square collocation in the case of PDE solvers.

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Direct high-order propagation algorithms for hyperbolic problems

Thomas Hagstrom* Daniel Appelö†

Local domain-of-dependence is a fundamental feature of hyperbolic pdes. Mathematically, this means that updates of the solution at a point or in a cell over a time step can be expressed as the action of some integral operator applied to data at neighboring points. In this talk we examine three direct high order propagation algorithms which exploit this fact. First, we consider methods based on Hermite interpolation on structured staggered grids, including both the original dissipative methods and our more recently-developed leap-frog formulations. Second, we consider applications to DG methods on unstructured grids, where we either directly approximate the integral update formulas or pursue a fully discrete approach where we impose a localized truncation of the discrete solution operator. Third, we consider the reduced order modeling of the discrete solution operator in highly heterogeneous media as an approach to deriving computationally-based hyperbolic homogenization algorithms.

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Near-optimal points for constrained approximation and solution of PDEs on complex geometries

Tony Liu* Rodrigo Platte†

We explore strategies for computing near-optimal sampling points for the approximation of functions with constraints. One approach is to find nodes that minimize the Lebesgue constant on a given domain. This can be done by using a greedy algorithm that adds one point per iteration. Alternatively, one can compute near-optimal Fekete points by constraining a rank-revealing algorithm on the approximation matrix consisting of the basis functions evaluated at the candidate points. We demonstrate that these points, when adequately computed, can be effectively used to solve differential equations on complex geometries using high degree polynomials. Numerical examples are shown to illustrate the accuracy of the proposed methods.

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High-order, dispersionless, spatio-temporally parallel "fast-hybrid" wave equation solver at $\mathcal{O}(1)$ sampling cost

Thomas G. Anderson* Oscar P. Bruno * Mark Lyon †

We propose [1] and demonstrate a frequency/time hybrid integral-equation method for the time dependent wave equation in two and three-dimensional spatial domains (Figure 1 displays results of some representative simulations produced with the techniques discussed). Relying on Fourier Transformation in time, the method utilizes a fixed (time-independent) number of frequency-domain integral-equation solutions to evaluate, with superalgebraically-small errors, time domain solutions for arbitrarily long times. The approach relies on two main elements, namely, 1) A smooth time-windowing methodology that enables accurate band-limited representations for arbitrary long time signals, and 2) A novel Fourier transform approach which, without causing spurious periodicity effects, delivers dispersionless spectrally accurate solutions. The algorithm can handle dispersive media, complex physical structures, it enables parallelization in time in a straightforward manner, and it allows for time leaping–that is, solution sampling at any given time T at $\mathcal{O}(1)$-bounded sampling cost, for arbitrarily large values of T, and without requirement of evaluation of the solution at intermediate times. The proposed frequency/time hybridization strategy, which generalizes to any linear partial differential equation in the time domain for which frequency-domain solutions can be obtained (including e.g. the time-domain Maxwell's equations), provides significant advantages over other available alternatives such as volumetric discretization and convolution-quadrature approaches.

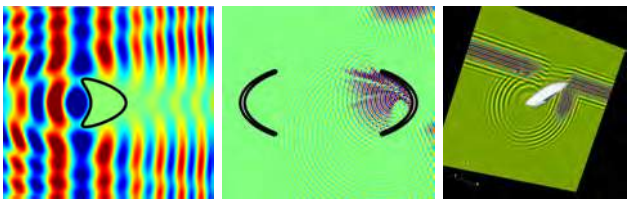

Figure 1: Screenshots from simulations utilizing the proposed "Fast-Hybrid" algorithms.

References

[1] Thomas G. Anderson, Oscar P. Bruno, and Mark Lyon. *High-order, dispersionless "fast-hybrid" wave equation solver. Part I: $\mathcal{O}(1)$ sampling cost via incident-field windowing and recentering.* 2018. eprint: `arXiv:1807.02718`.

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Seismic simulations with SW4*

Bjorn Sjogreen† Anders Petersson†

SW4 is a seismic simulation code that solves the elastic wave equations to compute the waves emanating from earthquakes. SW4 uses a fourth order accurate finite difference discretization with summation by parts (SBP) boundary operators. Various material models and source mechanism are supported. We discuss recent progress on numerical techniques implemented in SW4. Improvements and additions to the code are:

a) Development of coupling conditions to other solvers using stable boundary closure. This is possible to do by using SBP boundary operators at the interface. However, because the interface is often the interior of a subcube of the logically rectangular domain, the SBP technique becomes complicated due to boundary edges and internal corners. Using the centered five point wide operator up to the boundary requires two layers of data points, which leads to increased memory usage. To overcome this, we develop a stable coupling condition that uses only one layer of data points, and that does not require SBP boundary operators.

b) Inclusion of viscoelastic wave attenuation into the fourth order accurate framework. Wave attenuation is modeled by a added memory variables that satisfy a system of ordinary differential equations (ODEs). The memory variables are coupled to the elastic wave equation. For our older second order accurate solver, WPP, we proved energy norm stability for a second order accurate discretization of the auxiliary system of ODEs. We will describe the fourth order accurate discretization of the attenuation model that is used in SW4.

c) Support for GPU computing. We will demonstrate some recent highly resolved earthquake simulations using GPUs and briefly discuss the coding effort that enabled high performance computing with SW4 on GPUs.

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Wednesday, June 5, Morning Session I (Room: Aztlan)

Efficient matrix-free iterative solvers for very high-order finite element discretizations*

Will Pazner†

Modern computer architectures favor the use of high-order discretizations for many problems. These methods feature high accuracy per degree of freedom and high arithmetic intensity, both of which are attractive properties for modern architectures such as GPUs. However, the cost of assembling or even storing the matrix associated with these discretizations can be prohibitively expensive, thus necessitating the use of matrix-free methods and solvers. Sum-factorization and related techniques allow for efficient operator evaluation, however solving the resulting large linear systems remains challenging. Furthermore, common preconditioners such as those arising from domain decomposition methods require dense blockwise factorizations, which are not possible without an explicit representation of the matrix.

In this talk I will describe recent work on the development of matrix-free preconditioners and solvers for very high-order finite element discretizations. These solvers and preconditioners are based on the ideas of tensor-product approximation, sparsification and spectrally-equivalent low-order discretizations. We apply these solvers to both discontinuous Galerkin and continuous Galerkin discretizations, with applications to relevant problems in computational fluid dynamics.

For discontinuous Galerkin methods, we approximate the elemental local problems using a tensor-product form that is amenable to efficient solution via a Schur technique that is similar to fast diagonalization. These approximations are generated using a construction known as the Kronecker product singular value decomposition, which is computed using a matrix-free Lanczos procedure. The resulting preconditioners can be used to solve time-dependent problems on highly stretched or anisotropic meshes, for which explicit time integration would give rise to an overly restrictive CFL condition.

We also consider sparsification-based approaches, whereby a low-order sparse operator is constructed in order to precondition the original high-order operator. Because of its increased sparsity, it is affordable to explicitly assemble this low-order operator, which can then be solved using traditional techniques such as multigrid. In order for this operator to effectively precondition the high-order operator, effective smoothers and transfer operators must be designed. The matrix-free construction of such smoothers will be discussed.

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A time-implicit static condensation scheme for high-order discontinuous Galerkin spectral element methods with Gauss-Lobatto points

Andrés M. Rueda-Ramírez* David A. Kopriva† Esteban Ferrer*
Gonzalo Rubio* Eusebio Valero*

Traditionally, high-order Discontinuous Galerkin (DG) methods have been implemented using explicit time-integration methods. These time-integration schemes perform well when the spatial and temporal scales are similar, but are very inefficient for solving steady-state problems and very stiff equations because they become unstable when the time step size is large. Although important advances have been made, it is still a challenge to develop efficient time-implicit DG solvers able to overcome the severe time step restriction of explicit schemes.

Static condensation is an efficient solution technique that was originally developed for solving linear systems that arise from time-implicit discretizations of the high-order Continuous Galerkin (CG) method. However, in traditional DG methods it cannot be used directly. Certain techniques have been developed to make modal DG methods suitable for static-condensation, but they imply the use of specially tailored basis functions with elementally non-orthogonal expansions.

In this work, we present a nodal (collocation) time-implicit Discontinuous Galerkin Spectral Element Method (DGSEM) with Gauss-Lobatto (GL) points, and show that it can be formulated as a Schur complement problem and solved using static condensation, while keeping elementally orthogonal expansions. By doing this, the linear system size is reduced, specially for high orders of accuracy, maintaining the advantageous properties of orthogonal basis expansions.

The proposed method is tested for solving the compressible Euler and Navier-Stokes equations in several test cases, where we investigate the performance of direct and iterative (Krylov subspace) linear solvers for solving the global and condensed systems. Furthermore, we report the condition number of the obtained system matrices when different discretizations are used and provide a thorough study of the conditions where the static condensation algorithm is useful. In those conditions, significant speed-ups are obtained as compared to previous explicit and implicit implementations.

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Uniform substructuring preconditioners for high order FEM on triangles and the influence of nodal basis functions*

Shuai Jiang† Mark Ainsworth†

The importance of preconditioners to the p-version of the finite element method was recognized even in the earliest days. Implicit time stepping schemes and singularly perturbed elliptic problems give rise to matrices in which the mass matrix dominates and preconditioners are needed which are robust in the time-step or the singular perturbation parameter in addition to the polynomial order and the mesh-size.

A *robust* substructuring type preconditioner is developed for high order approximation of problem for which the element matrix takes the form $(1-\kappa)\mathbf{L}+\kappa\mathbf{M}$ where $\kappa \in (0,1)$ and $\mathbf{M}, \mathbf{L}$ are the mass and stiffness matrices respectively. A standard preconditioner for the pure stiffness matrix results in a condition number bounded by $C_\kappa(1+\log^2 p)$ where C_κ blows up as $\kappa \to 1$. It is shown that the the best uniform bound in κ that one can hope for is $O(p^2)$. More precisely, we show that the upper envelope of the bound $C_\kappa(1+\log^2 p)$ is Cp^2.

What, then, can be done to obtain a preconditioner that is robust for all $\kappa \in [0,1]$? The solution turns out to be a relatively minor modification of the basic substructuring algorithm: one simply augments the preconditioner with a suitable Jacobi smoothener over the coarse grid degrees of freedom. This is shown to result in a condition number bounded by $O(1+\log^2 p)$ where *the constant is independent of* $\kappa \in [0,1]$. Numerical results are given which shows that the simple expedient of augmentation with nodal smoothening reduces the condition number by a factor of up to two orders of magnitude.

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Taming the CFL number for discontinuous Galerkin methods by local exponentiation: numerical examples

Mingyu Hu* Daniel Appelö†

High-order discontinuous Galerkin (DG) methods are spectrally accurate and thus are especially beneficial for solving wave propagation problems. However, a drawback with DG methods is that the Courant-Friedrichs-Lewy (CFL) number decreases rapidly with increasing basis polynomial order. In this talk, the speaker will propose a local low-rank approximation to the exponential integrator for time-stepping to tame the CFL condition for stiff hyperbolic partial differential equations (PDEs). The construction of the novel time-stepper is motivated by the nature of wave propagation. The accuracy of this time stepping method is inherited from the exponential integrator and the local property of it allows lower costs and parallel implementation. The method is therefore expected to be useful in design and inverse problem where many solves of the PDE are required. Potential applications include (1) design of meta-material from unit cell response to the propagation of electromagnetic waves, (2) inner-cavity geometry update, and (3) extension to implementation of helmholtz solvers by exact controllability method. In this talk, we demonstrate the stability and error convergence of the method in 1D Maxwell's equation on uniform grids. In 2D scalar wave equation, we demonstrate the asymptotic error convergence property on an annulus with quadrilateral grid. Moreover, the speaker will demonstrate the performance the time-stepper in full-waveform inversion (FWI). Results in source inversion for 1D Maxwell's equation and in cavity geometry inversion for 2D wave equation will be presented.

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Boundary condition strategies for collision-based hybrid methods for linear kinetic models *†

Zheng Chen‡ Cory D. Hauck§

Numerical simulations for linear kinetic models defined over position-velocity phase-space are computationally costly. Especially when the collision frequencies vary much over the domain, and multiscale phenomena exhibit. A collision-based hybrid method introduced by Hauck and McClarren [3] is proposed to save computational cost for collisional models but keep the accuracy in the meantime. The method separates the kinetic equation into a system of two equations for collided and uncollided components of the distribution function. The collided equation is simulated with a low-resolution angular discretization, and the uncollided equation is simulated with a high-resolution angular discretization. Proper mapping between the two components is required after each time stepping. One of the interesting questions about this hybrid method is how to assign the boundary condition to the two components to keep it accurate. Numerical results show putting all boundary data on the uncollided component leads to non-physical solutions. In this project, the splitting methods for boundary data are investigated. Inspired by the boundary layer problem for linear kinetic models discussed in Bensoussan, Lions, and Papanicolaou [1] and Golse, Jin, and Levermore [2], an interior-boundary splitting strategy is proposed and analyzed. Numerical results will be shown to validate the analysis. An adaptive splitting method is also discussed for the multiscale setting.

References

[1] Alain Bensoussan, Jacques L Lions, and George C Papanicolaou. "Boundary layers and homogenization of transport processes." In: *Publications of the Research Institute for Mathematical Sciences* 15.1 (1979), pp. 53–157.

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[2] François Golse, Shi Jin, and C David Levermore. "The convergence of numerical transfer schemes in diffusive regimes i: discrete-ordinate method." In: *SIAM journal on numerical analysis* 36.5 (1999), pp. 1333–1369.

[3] Cory D Hauck and Ryan G McClarren. "A collision-based hybrid method for time-dependent, linear, kinetic transport equations." In: *Multiscale Modeling & Simulation* 11.4 (2013), pp. 1197–1227.

Wednesday, June 5, Morning Session II (Room: Templo Mayor)

Designing time filters using a general linear method approach

Victor P. DeCaria* Sigal Gottlieb† Zachary J. Grant‡ William J. Layton*

Time filtering has been used to enhance the order of accuracy of given methods. This is particularly useful in the context of legacy codes, in which the time-stepping module is given and difficult to change. However, modifying the inputs and outputs is simple and allows for higher order. In this talk, we show how time filtering approaches can be seen as equivalent to generating a general linear methods. We use this GLM approach to develop an optimization routine that allows us to find new time-filtering methods with high order and efficient linear stability properties. We will present our new methods and show their performance when tested on sample problems.

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Diagonally-implicit Runge-Kutta schemes devoid of order reduction *

David Ketcheson † Rodolfo Ruben Rosales ‡ Benjamin Seibold §
David Shirokoff ¶ Dong Zhou‖

Order reduction is a generic phenomenon that arises for stiff ODEs, as well as for PDE initial boundary value problems. For Runge-Kutta schemes, one existing approach to avoid order reduction is to construct schemes with high stage order. Unfortunately, high stage order (above two) is incompatible with diagonally implicit Runge-Kutta (DIRK) schemes. In this talk, we present a relaxed property, called weak stage order, that can recover up to fourth order convergence with DIRK schemes.

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Implicit and explicit parallel across method error inhibiting schemes

Zachary J. Grant* Adi Ditkowski † Sigal Gottlieb‡

It is well known that classic time stepping methods globally lose one order of accuracy in comparison to its local truncation error due to an accumulation of the errors over time. However it was shown in the work by Gottlieb and Ditkowski that by using a block multi-step approach with carefully chosen coefficients it is possible to impact the interaction between the local truncation errors of the varying schemes and so inhibit the growth of the global error. These methods are known as Error Inhibiting Schemes (EIS). This strategy allows one to achieve higher orders of accuracy than one would originally expect, and suggests a new approach to create high order methods. An additional characteristic of these schemes is the ability to compute the components of the block approximations in parallel allowing one to drastically reduce the overall runtime in comparison to their serial multi-stage counterparts. This particular structure is known in the time stepping community as parallel across method approach. In this work we extend the parallel EIS formulation to explicit and implicit methods which have global errors two orders of accuracy higher than their local truncation errors. We then use this theoretical understanding to construct new methods of varying orders that also enjoy many desirable properties such as A-stability, L-stability, low cost error estimators, and adaptive step-sizes.

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High-order continuous triangular finite element explicit time stepping via a twisted mass-matrix inversion scheme

Jay M. Appleton* Brian T. Helenbrook†

In this work we present a novel high order accurate, continuous, triangular finite element, explicit time stepping scheme. The explicit time stepping of finite elements offers an efficient approach to advancing the approximate solution of a partial differential equation in time. However, it typically requires the inversion of a large mass matrix at each time step. This difficulty is avoided with the nodal Gauss-Lobatto-Legendre (GLL) quadrilateral finite element method by an approximate diagonal mass matrix evaluated under numerical integration. For the GLL quadrilateral method using a p degree polynomial basis, the approximate mass matrix is capable of exactly projecting any polynomial of degree (p-1). We say that this approach is (p-1)-exact and we define a pseudo-mass matrix to be any other matrix acting in place of the standard mass matrix.

There are many advantages to working with triangular finite elements when using unstructured meshes. And, in previous works we showed that no (p-1)-exact diagonal pseudo-mass matrix exists, and developed an alternative (p-1)-exact lower-triangular pseudo-mass matrix approach that avoids the need to work with the full mass matrix but only exists for p from 2 to 5. In that work, we created a change of basis and pseudo-mass matrix pair by constraining an underlying orthogonality to the new basis functions. Now, we use this approach to develop a mass matrix inversion scheme that works with the popular modified Dubiner basis. To do this we change the orthogonality constraints as we develop the pseudo-mass matrix and change of basis which creates a twisted mass matrix. The result is a high order continuous triangular finite element that is appropriate for computationally inexpensive (p-1)-exact explicit time stepping. We will present the necessary concepts and the desired accuracy constraints, discuss the construction of the twisted mass matrix, illustrate the resultant inversion scheme, and then present some computational results.

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Regionally implicit discontinuous Galerkin schemes

Pierson Guthrey* James Rossmanith†

The Regionally Implicit Discontinous Galerkin methods are a novel numerical method for nonlinear hyperbolic conservation laws which is able to take a timestep restriction number (CFL) of at least 0.6 independent of problem dimensions (1D to 3D problems) and the method order (1st order to 10th order methods), while maintaining a nearest-neighbor stencil. It achieves this using a nonlinear system solve to form an implicit prediction for a cell and its neighbors (thus the system is small), followed by an explicit corrector step which provides high order accuracy. This moderate CFL restriction combined with the small method stencil makes this method an ideal candidate for parallelization, as the communication overhead is minimized.

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Wednesday, June 5, Morning Session III (Room: Tehuanco)

High order multiderivative time integrators

David C. Seal*

Runge-Kutta and Taylor methods are both subsets of a larger class of methods called multistage multiderivative methods. This class of methods increases the order of a solver by introducing additional stages and/or derivatives to the solver. This provides greater flexibility to Taylor type methods as the additional stages can be used to increase the order of accuracy and modify the regions of absolute stability. In addition, it reduces the total number of stages (and communications) that a Runge-Kutta method would otherwise require in order to increase the order of the solver. In this talk, we present recent results where we leverage techniques found in the spectral deferred correction literature to extend these solvers to arbitrary order. Moreover, we point to parallel in time implementations of these methods, and we discuss how the higher derivative terms can be efficiently computed for sample partial differential equations.

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Error boundedness of discontinuous Galerkin methods with variable coefficients

Philipp Öffner* Hendrik Ranocha†

The study of the long time error behaviour of numerical methods for time dependent partial differential equations is important in practical applications. In this talk, we focus on this topic in the context of hyperbolic conservation laws and discontinuous Galerkin methods. It is well-known in the literature that for linear problems with constant coefficients the selection of the numerical flux (e.g. central or upwind) [1] and the choice of the polynomial basis (e.g. Gauß-Lobatto-Legendre or Gauß-Legendre) [2] affect both the growth rate and the asymptotic values of the errors.

Here, we extend these investigation allowing variable coefficients in our model problem [3]. Both, chosen bases and fluxes have still an big influence on the error behaviours, but now also the properties of the coefficients have to be taken into account. We derive conditions guaranteeing that the errors remain bounded in time and behave similar to the case of constant coefficients. If these conditions are violated, the errors can show a completely different behaviours. We analyse and give an explanation for this phenomenon which confirms our analytical investigation. Finally, we extend our investigation to linear systems with variable coefficients and proclaim the problems that occur there.

References

[1] David A Kopriva, Jan Nordström, and Gregor J Gassner. "Error boundedness of discontinuous Galerkin spectral element approximations of hyperbolic problems." In: *Journal of Scientific Computing* 72.1 (2017), pp. 314–330.

[2] Philipp Öffner. "Error boundedness of correction procedure via reconstruction/flux reconstruction." In: *arXiv preprint arXiv:1806.01575* (2018).

[3] Philipp Öffner and Hendrik Ranocha. "Error boundedness of discontinuous Galerkin methods with variable coefficients." In: *Journal of Scientific Computing* (2019), pp. 1–36.

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WaveHoltz: iterative solution of the Helmholtz equation via the wave equation

Daniel Appelö* Fortino Garcia† Olof Runborg ‡

Designing efficient iterative solvers for the Helmholtz equation is notoriously difficult and has been the subject of much research. The main two difficulties in solving the Helmholtz equation are the resolution requirements and the highly indefinite character of the discretized system of equations. Following the work considered in the late 1990's by Bristeau, Glowinski, and Périaux [1] on so called exact controllability methods, we introduce a novel idea that enables the use of time domain methods for wave equations to design frequency domain Helmholtz type solvers. Our approach yields an underlying linear operator corresponding to a symmetric positive definite matrix allowing us to both solve a nice coercive problem and accelerate convergence via methods such as conjugate gradient (CG). Numerical examples with high order discretization techniques are presented. Additionally, we propose a method to achieve the solution to multiple Helmholtz problems (of varying frequencies) for the small added cost of a forward wave equation solve.

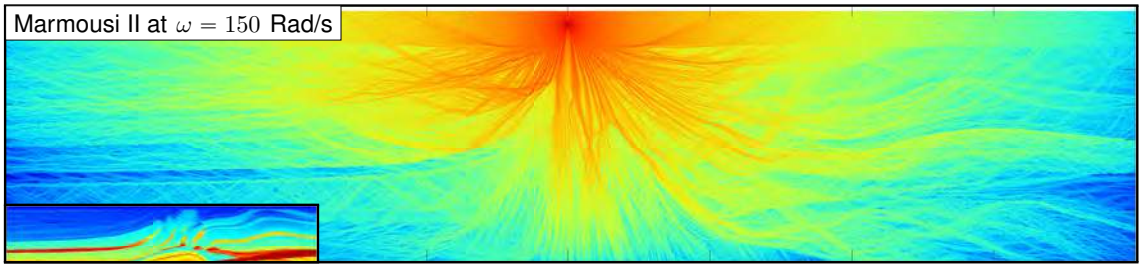

Figure 1: Magnitude of the solution to the Helmholtz equation due to a point source at 150Rad/s. The color scale is logarithmic. The inlay displays the velocity (compressional) structure with regions ranging from 1km/s to $\sim$ 4.6km/s.

References

[1] Marie-Odile Bristeau, Roland Glowinski, and Jacques Périaux. "Controllability methods for the computation of time-periodic solutions; application to scattering." In: *Journal of Computational Physics* 147.2 (1998), pp. 265–292.

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Order adaptive methods for polymer self-consistent field theory

Hector Ceniceros*

An high order and memory-efficient method for the solution of polymer self-consistent field theory (SCFT) will be presented. This new approach combines spectral integration in the polymer chain contour variable with a spectral deferred correction technique to solve the SCFT Fokker-Planck equations with arbitrarily high order of accuracy. The result is a robust method that achieves high accuracy with a minimal number of discrete contour nodes, which translates into vastly reduced memory requirements and increased computational efficiency. In particular, this spectral deferred correction method enables the computation of strongly segregated systems with unprecedented accuracy. Moreover, the framework of deferred corrections allows us to adaptively increase the order of accuracy during the outer saddle point iteration to drastically reduce the cost of a SCFT computation.

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Spurious pressure in Scott-Vogelius elements

Chunjae Park*

We will analyze the characteristics of Scott-Vogelius finite elements on singular vertices, which spoil the inf-sup condition and cause spurious pressures on solving Stokes equations. A simple postprocessing will be suggested to remove those spurious pressures.

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Wednesday, June 5, Afternoon Session I (Room: Aztlan)

Adaptive moving mesh central-upwind schemes

Alexander Kurganov*

We introduce adaptive moving mesh central-upwind schemes for 1-D and 2-D hyperbolic systems of conservation and balance laws. The proposed methods consist of three steps. First, the solution is evolved by solving the studied system by the second-order semi-discrete central-upwind scheme on either the 1-D nonuniform grid or 2-D structured quadrilateral mesh. When the evolution step is complete, the grid points are redistributed according to the moving mesh differential equation. Finally, the evolved solution is projected onto the new mesh in a conservative manner.

The resulting adaptive moving mesh methods are applied to the 1-D and 2-D Euler equations of gas dynamics, granular hydrodynamics systems and Saint-Venant systems of shallow water equations. Our numerical results demonstrate that in both cases, the adaptive moving mesh central-upwind schemes outperform their uniform mesh counterparts.

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High order mimetic methods on curvilinear grids

Jose E. Castillo*

High Order Mimetic methods, based on Castillo Grone Discrete Mimetic Divergence and Gradient operators, have been used successfully on several applications. These operators satisfy in the discrete sense the same properties that the continuum divergence and gradients operators do so they are more faithful to the physics. In this paper we investigate the extension of these operators to general curvilinear grids. In particular, we investigate the discrete conservation of mass, momentum and energy for some wave models for complex underlying physical space domains.

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Accuracy and stability of windowed Fourier methods for computations on the sphere

Genesis Islas* Rodrigo Platte†

Windowed Fourier transforms have long been used to study local features of signals and are often called short-time Fourier transforms. They are commonly used to determine frequency and phase content of local sections of a signal as it changes over time. They are, however, rarely used in the solution and analysis of differential equations because regions near the boundaries of the domain are difficult to handle. Smooth manifolds, on the other hand, are boundary-free, and windowed Fourier transforms provide an excellent framework for approximation and numerical solution of PDEs on these surfaces.

In this talk, a spectral method based on windowed Fourier approximations will be presented. It relies on domain decomposition and is suitable for adaptive and parallel implementation. One of the advantages of this approach is that computations can be carried out using fast Fourier transforms on a nearly uniform grid. Approximations are obtained on overlapping domains, and a global solution is obtained using the partition of unity. Algorithms for computations on spherical geometries will be presented in detail.

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High-order explicit stochastic semi-Lagrangian spectral method to solve transport equations

Hareshram Natarajan* Gustaaf Jacobs†

A local, explicit high order accurate semi-Lagrangian spectral element method is developed for the solution of stochastic transport equations which model reactive turbulent flows.

The subgrid scale quantities of the LES simulation are represented using a multi-variate probability density function (PDF). The high-dimensional PDF that depends on the number of species is generally solved using a Monte-Carlo approach for a stochastic differential equation. Hence reducing the computational cost as compared to solving the Fokker-Planck type of equations for the PDF.

The semi-Lagrangian method developed solves for the stochastic different equation. We perform this by seeding Lagrangian particles at the Gauss quadrature collocation nodes within each element. The particle is advected by integrating the stochastic differential equation in time. A new interpolant is constructed from the advected nodes with a least squares method constrained by boundary conditions and mass conversation. The interpolant maps the function back to the Gauss quadrature nodes. With the stable explicit time restrictions particles cannot leave the element's bounds. The method is explicit, local and hence can be easily parallelized. It is therefore consistent with discontinuous Galerkin spectral element LES solver that provides the velocity field.

Numerical tests with one and two dimensional advection, diffusion and advection-diffusion equations are carried out. The method is shown to have spectral convergence.

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Pseudo-spectral simulation of shock turbulence interaction using observable Navier-Stokes equations

Majid Allayari*

Shocks and turbulence give rise to flow singularities and irregularities that are significant computational challenges. Specifically, the nonlinear convective terms in the Euler and Navier-Stokes (NS) equations are the source of these irregularities and discontinuities. In this study, we present the numerical results of canonical shock-turbulence interaction problems based on an inviscid regularization of the Navier-Stokes equations; namely the observable Navier-Stokes equations (ONS). In ONS equations the regularization is implemented at the level of derivation of the governing equation and not at the discretization level. The performance of the ONS and observable Euler equations (OE) were initially tested for 1D Shu-Osher and Burgers equations. We also performed 3D simulation of the pseudo-spectral discretization of the ONS equations for Mach number of $M = 1.5$ and Taylor Reynolds number of $Re_\lambda = 40$. The performance of the pseudo-spectral NS solver was verified by comparison with available Direct Numerical Simulations (DNS) and Large Eddy Simulations (LES) of the same problem. It is observed that the ONS equations accurately capture the large scales of the flow using grid sizes competitive with the state-of-the-art LES methods and significantly coarser grid sizes than available DNS.

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Wednesday, June 5, Afternoon Session II (Room: Templo Mayor)

A high order finite difference method for the elastic wave equation on curvilinear staggered grids

Ossian O'Reilly* Daniel Roten† Kim Olsen‡

We develop a high order finite difference method to solve the elastic wave equation on staggered curvilinear grids. The development of this method is motivated by earthquake science and engineering design for seismic applications involving topography. Unlike other schemes that only stagger velocity and stress at the positions per grid cell, this scheme staggers all components at eight positions per grid cell in 3D. In this way, it overcomes a factor of four increase in computation and memory costs. However, since not all of the additional terms that arise from the coordinate transform can be directly discretized, interpolation is needed. To obtain a provably stable method, the governing equations are expressed in Cartesian components. A skew-symmetric splitting of the governing equations is used and it is discretized by summation-by-parts interpolation and differentiation operators on staggered grids. The free surface boundary condition is imposed by a penalty term. The use of interpolation results in widened stencils, which can increase the halo size in MPI implementations. To avoid increased memory and MPI communication costs, we adopt a 1D coordinate transform in the vertical direction, and only perform MPI decomposition in the horizontal plane. Numerical tests demonstrate the method's capability for resolving surface waves in the presence of topography.

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Towards a multi-element-shape extension for the spectral difference method

A. Veilleux* H. Deniau† G. Daviller‡ G. Puigt§

The Spectral Difference method was introduced in 1996 by Kopriva and Kolias [6] as the staggered-grid Chebyshev multidomain method and applied to structured quadrilateral grids using a tensor product framework by Kopriva [5]. The scheme stability was demonstrated by Jameson [4] for tensor product cells but foundations of a stable formulation on simplex cells were not established until the pioneering work of May, Balan and Schöberl [1, 2]. They proposed a Spectral Difference method based on the Raviart-Thomas polynomial approximation (SDRT) for triangles which was shown to be stable up to the 4th order of accuracy. We are interested in the definition of a stable formulation of the spectral difference method on simplex cells for orders of accuracy higher than 4th. The present study focuses on the stability analysis of SDRT schemes using the Matrix Power method, following the procedure proposed by Vanharen et al. [7], which is suitable to properly describe the behavior of polynomial discontinuous methods. Stable SDRT schemes up to the 6th order are found, which overcomes the referenced results. Two-dimensional Euler equations are then discretized with SDRT schemes up to the 6th order for the 'fast vortex' test case (VI1) from the High Order Workshop [3] on unstructured triangular grids (Fig. 1) with periodic boundary conditions. Results after 10 periods show a good accuracy for SDRT schemes for orders higher than 3 (Fig. 2).

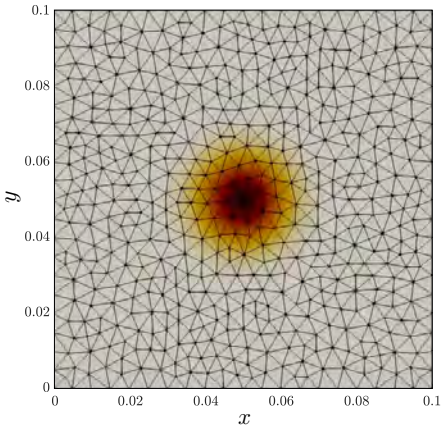

Figure 1: Initialisation of the VI1 test case [3] on unstructured triangular mesh

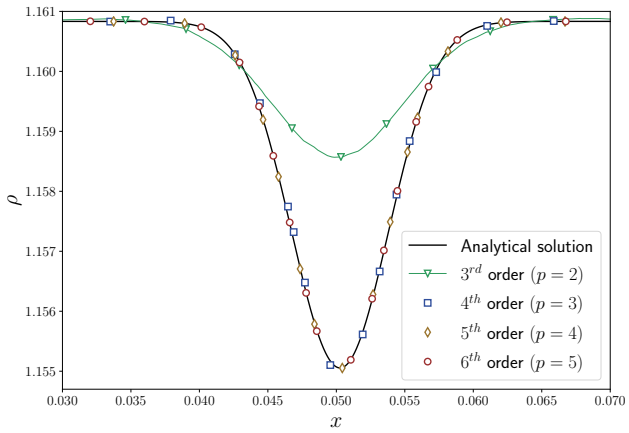

Figure 2: Cross-section of the density at $y = 0.05$ after 10 periods for several orders of accuracy

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References

[1] Aravind Balan, Georg May, and Joachim Schöberl. "A stable spectral difference method for triangles." In: *49th AIAA aerospace sciences meeting including the new horizons forum and aerospace exposition*. 2011, p. 47.

[2] Aravind Balan, Georg May, and Joachim Schöberl. "A stable high-order spectral difference method for hyperbolic conservation laws on triangular elements." In: *Journal of Computational Physics* 231.5 (2012), pp. 2359–2375.

[3] *HiOCFD5*. URL: `https://how5.cenaero.be/`.

[4] Antony Jameson. "A proof of the stability of the spectral difference method for all orders of accuracy." In: *Journal of Scientific Computing* 45.1-3 (2010), pp. 348–358.

[5] David A. Kopriva. "A conservative staggered-grid chebyshev multidomain method for compressible flows. ii. a semi-structured method." In: *Journal of Computational Physics* 128.2 (1996), pp. 475–488.

[6] David A. Kopriva and John H. Kolias. "A conservative staggered-grid chebyshev multidomain method for compressible flows." In: *Journal of Computational Physics* 125.1 (1996), pp. 244–261.

[7] Julien Vanharen, Guillaume Puigt, Xavier Vasseur, Jean-François Boussuge, and Pierre Sagaut. "Revisiting the spectral analysis for high-order spectral discontinuous methods." In: *Journal of Computational Physics* 337 (2017), pp. 379–402.

A numerical framework of high order well-balanced finite difference schemes based on the weighted compact nonlinear scheme and alternative WENO scheme for the shallow water equations

Peng Li* Wai-Sun Don† Zhen Gao‡

In this talk, a numerical framework of the high order well-balanced finite difference schemes based on the weighted compact nonlinear scheme (WCNS) [1] and alternative WENO scheme [2] are proposed for the shallow water equations. We employ a special splitting technique for the source term proposed in [3] and the reconstruct methods for the conservative variables in [4] to maintain the exact C-property, which can be proved theoretically. In the meantime, the genuine high order accuracy of the numerical schemes can be observed successfully, and small perturbation of the stationary state can be resolved and evolved well. In order to capture the strong discontinuities and large gradients, the fifth-order upwind weighted nonlinear interpolations together with the $6th$-order cell-centered compact scheme or high order approximation for the second and fourth derivatives of the flux are used to construct WCNS and alternative WENO schemes respectively. In addition, the local characteristic projections are considered to further restrain the potential numerical oscillations. A variety of representative one- and two-dimensional examples are tested to demonstrate the good performance of the proposed schemes.

References

[1] Xiaogang Deng and Hanxin Zhang. "Developing high-order weighted compact nonlinear schemes." In: *Journal of Computational Physics* 165.1 (2000), pp. 22–44.

[2] Yan Jiang, Chi-Wang Shu, and Mengping Zhang. "An alternative formulation of finite difference weighted eno schemes with lax–wendroff time discretization for conservation laws." In: *SIAM Journal on Scientific Computing* 35.2 (2013), A1137–A1160.

[3] Yulong Xing and Chi-Wang Shu. "High order finite difference weno schemes with the exact conservation property for the shallow water equations." In: *Journal of Computational Physics* 208.1 (2005), pp. 206–227.

[4] Yulong Xing and Chi-Wang Shu. "High order well-balanced finite volume weno schemes and discontinuous galerkin methods for a class of hyperbolic systems with source terms." In: *Journal of Computational Physics* 214.2 (2006), pp. 567–598.

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High order mimetic finite difference modeling of anisotropic flow *

Angel Armando Boada Velazco † Jose Castillo †

The flow in porous or fractured heterogeneous media is usually assumed to be described by a full tensor. However, due to complexities in the formulation, implementations often assume a diagonal tensor (flow directions are aligned with the coordinate axis) which may cause that their solutions do not correspond with the physics. High Order Mimetic Finite Differences are discrete analogs of the continuous differential operators and have been used broadly in many applications. In this paper, we examine the viability of High Order Mimetic Finite Differences on flow through anisotropic and heterogeneous media (full tensor) by way of the Mimetic Flux operator. Numerical examples will be provided.

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A fast high-order Poisson solver for 2/3D complex geometries via an integral equation method

Xiaoyu Wei* Andreas Klöckner*

A novel Poisson solver is presented in two and three dimensions for complex geometries. It employs an integral equation approach that is based on the decomposition of the solution into two parts: one being a volume potential and the other consists of layer potentials over the domain boundary. The volume potential part is evaluated with efficient box fast multipole method (FMM) over a semi-structured volume mesh encompassing the physical domain. Then the remaining part is solved from a second-kind integral equation (SKIE) via generalized minimal residual method (GMRES), where the matrix-vector product is implemented using the quadrature-by-expansion (QBX) method. The overall asymptotic computational complexity of our Poisson solver is O(N), which is the same as multigrid (MG) methods. The main advantage of our method lies in the fact that it only requires solving for unknowns at the boundary and the linear system is typically well-conditioned as it is a discretization of a compact perturbation of the identity.

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Wednesday, June 5, Afternoon Session III (Room: Tehuanco)

FFT-based high order central difference schemes for the three-dimensional Poisson equation with various types of boundary conditions

Hongsong Feng * Shan Zhao*

In this work, we propose a matched high-order finite difference method (MHFD) for solving Poisson's equation via fast Fourier transform (FFT) with ease in dealing with various boundary conditions. The popular high order fast methods in the literature including compact differences and spectral methods face difficulty in dealing with different combination of boundary conditions. Besides, standard high order central finite differences require artificial nodes information near the boundary, which poses a challenge to integrating boundary conditions in fast Fourier transform. To avoid this issue from fictitious points, anti-symmetricity property of solution across the boundary is desired to facilitate utilization of fast Sine transform. But this strong requirement is not true for general problems subject to different boundary conditions that are not even homgeneous. Therefore, given Cartisian grids on a rectangular domain of interest, we can extend the domain by introducing several layers of exterior grid lines to give an immersed boundary problem such that zero solutions beyond the original rectangular domain makes anti-symmetricity naturally true across the enlarged rectangular domain boundary. Then the introduced problem can be efficiently solved by augmented matched interface and boundary method (AMIB) with incorporation of FFT. In this way, a systematic method is constructed with accuracy of high order finite difference and the efficiency of FFT both achieved. Various numerical experiments are carried out to verify the validity and effectiveness of the method in 2D and 3D.

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A hybrid high order Hermite WENO scheme for hyperbolic conservation laws

Jianxian Qiu*

In this presentation, we propose a class of hybrid high order finite volume Hermite weighted essentially non-oscillatory (HWENO) scheme, with Total Variation Diminishing Runge-Kutta time discretization for solving hyperbolic conservation laws. The zeroth-order and the first-order moments are used in the spatial reconstructions. The main idea of the hybrid HWENO scheme is that we first use a shock detection technique to identify the discontinuous, then, if the cell is identified as a troubled-cell, then we modify the first order moment in the troubled-cell and employ HWENO reconstruction in spatial discretization, otherwise, we directly use high order linear reconstruction. Compared with other HWENO schemes, the one advantage is its simpleness as we only use one set of stencil for spatial discretization, and the second advantage is its higher efficiency for using linear approximation straightforwardly in smooth regions. Meanwhile, the hybrid HWENO scheme still keeps the compactness. A collection of benchmark numerical tests for one and two dimensional cases are performed to demonstrate the numerical accuracy, high resolution and robustness of the proposed scheme.

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High-order blended compact difference schemes for the three dimensional elliptic partial differential equation with mixed derivatives and variable coefficients

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A new sixth-order blended compact difference (BCD) scheme is proposed for approximating the three dimensional elliptic partial differential equation with mixed derivatives and variable coefficients. The scheme takes transport variable, its first- and second-order derivatives as unknowns, in which, the sixth-order combined compact difference (CCD) schemes are employed for the computation of the first-order and second-order pure derivatives as well as the nine-point sixth-order compact difference schemes are used for the computation of the second-order mixed derivatives. Furthermore, new sixth-order accuracy schemes are proposed to compute the values of the first- and second-order derivatives on boundaries. The distinguishing feature of the present schemes is that methodologies of explicit compact difference and implicit compact difference are blended together and the derivation of the schemes, the algorithm design and programming are simple and easy to operate. The truncation error of the present BCD scheme for the interior gird points is analyzed. Finally, some numerical examples are given to demonstrate good resolution and high accuracy of the present method.

In order to effectively and conveniently solve some problems with the BCD scheme, we introduce a new software named PHOEBE Solver and illustrate how to use it. We note that this software can also be used to efficiently solve various other kinds of partial differential equations with various schemes/algorithms existing in the literature. The motivation for us to develop this software, functions and distinguishing features of this software are also introduced.

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Assessing standard and kinetic energy conserving discontinuous Galerkin formulations for marginally resolved two dimensional Navier-Stokes flows

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Results of marginally resolved discontinuous Galerkin spectral element computations are presented using the standard formulation and a kinetic energy conserving split form of the non-linear advective volume fluxes. The schemes are assessed for the flow over a square cylinder, an airfoil and of a plane jet. For these flows, the robustness, accuracy and computational efficiency of the formulations are compared and discussed. It is shown that the kinetic energy conserving formulation is significantly more robust than the standard scheme for under-resolved simulations. A disadvantage of the split form is the restriction to Gauss-Lobatto nodes with the inherent underintegration and lower accuracy as compared to Gauss quadrature used with the standard scheme. The results indicate a higher accuracy for the standard Gauss form at the cost of increased stiffness with smaller time steps as compared to the Gauss-Lobatto nodes. In addition, spurious oscillations are present in some cases when using the standard form, giving the advantage to the kinetic energy conserving scheme for marginally resolved numerical simulations.

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Boundary condition strategies for collision-based hybrid methods for linear kinetic models *†

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Numerical simulations for linear kinetic models defined over position-velocity phase-space are computationally costly. Especially when the collision frequencies vary much over the domain, and multiscale phenomena exhibit. A collision-based hybrid method introduced by Hauck and McClarren [3] is proposed to save computational cost for collisional models but keep the accuracy in the meantime. The method separates the kinetic equation into a system of two equations for collided and uncollided components of the distribution function. The collided equation is simulated with a low-resolution angular discretization, and the uncollided equation is simulated with a high-resolution angular discretization. Proper mapping between the two components is required after each time stepping. One of the interesting questions about this hybrid method is how to assign the boundary condition to the two components to keep it accurate. Numerical results show putting all boundary data on the uncollided component leads to non-physical solutions. In this project, the splitting methods for boundary data are investigated. Inspired by the boundary layer problem for linear kinetic models discussed in Bensoussan, Lions, and Papanicolaou [1] and Golse, Jin, and Levermore [2], an interior-boundary splitting strategy is proposed and analyzed. Numerical results will be shown to validate the analysis. An adaptive splitting method is also discussed for the multiscale setting.

References

[1] Alain Bensoussan, Jacques L Lions, and George C Papanicolaou. "Boundary layers and homogenization of transport processes." In: *Publications of the Research Institute for Mathematical Sciences* 15.1 (1979), pp. 53–157.

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[2] François Golse, Shi Jin, and C David Levermore. "The convergence of numerical transfer schemes in diffusive regimes i: discrete-ordinate method." In: *SIAM journal on numerical analysis* 36.5 (1999), pp. 1333–1369.

[3] Cory D Hauck and Ryan G McClarren. "A collision-based hybrid method for time-dependent, linear, kinetic transport equations." In: *Multiscale Modeling & Simulation* 11.4 (2013), pp. 1197–1227.

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