Research Statement

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Introduction

My current research involves the development of the discontinuous Petrov-Galerkin (DPG) finite element method for space-time simulations of compressible and incompressible fluid dynamics. DPG represents the generalization and systemization of several ideas in stabilized finite element methods and provides a rich methodology for solving partial differential equations.

Scientific Importance

DPG – a robust framework for computational mechanics. The primary strength of the method lies in its suitability to any well-posed variational problem. DPG offers a fundamental framework for developing robust residual-minimizing finite element methods, even for equations that usually cause problems for standard techniques, such as convection-dominated diffusion and Stokes flow. DPG methods have provably optimal convergence rates and often come very close to the best solution possible in the discrete space.

In contrast to most other numerical methods, the discontinuous Petrov-Galerkin finite element method retains exceptional stability on extremely coarse meshes. DPG is also inherently very adaptive. It is possible to compute the residual error without knowledge of the exact solution, which can be used to robustly drive adaptivity. This results in a very automated technology, as the user can initialize a computation on the coarsest mesh which adequately represents the geometry then step back and let the program solve and adapt iteratively until it resolves the solution features.

DPG has been successfully applied to a wide range of physical applications. Theoretical groundwork for DPG applied to the Poisson equation was laid in [1]. The time-harmonic Helmholtz equation was the focus of [2, 3] and [4]. Linear elasticity and plate problems were addressed in [5], [6], and [7], and Maxwell was addressed in [8, 9]. Linear fluid dynamics problems include convection-diffusion [10, 11, 12, 13, 14] and stationary Stokes flow[15, 14]. The robust stability properties of DPG appear to carry over into the nonlinear regime as well; Moro, Peraire and Nguyen observed [16, 17] that on a single element, the HDPG method (referring to DPG applied to a hybridized Discontinuous Galerkin method) converges, whereas HDG on its own does not. Moreover, HDPG required an order of magnitude less artificial diffusion to converge to a nonlinear solution of the compressible Navier-Stokes equations. Chan *et al.* [18] showed that for both the viscous Burgers' equation and the compressible Navier-Stokes equations at high Mach/Reynolds number, DPG converges on an extremely

coarse mesh, allowing the use of an adaptive scheme to capture shock and boundary layer phenomena starting from an initial mesh of $O(1)$ elements. Roberts reports similar results boasting similar stability for high Reynolds numbers for the incompressible Navier-Stokes equations [19].

Current Research

DPG for fluid dynamics applications. Local conservation is considered by many fluid dynamics practitioners to be an extremely important feature in a CFD code. Thus, my initial work on DPG included the development of a variant formulation that explicitly enforced conservation element-by-element via Lagrange multipliers [14].

Past explorations of the DPG method focused exclusively on steady state problems. Most simulations of realistic engineering applications require highly adaptive meshes for efficient computation, but traditional time stepping algorithms are horribly inefficient in such cases as the entire simulation needs to move forward at the pace of the most restrictive element, which may be orders of magnitude smaller than other elements in the domain. A space-time DPG formulation presents an attractive alternative as we will be able to preserve our natural stability and adaptivity from the steady problems while extending it in time. Thus we achieve an adaptive solution technique for transient problems in a unified framework.

More recently, I've been using the framework we've developed to study a classical open question in compressible flow problems: whether primitive, conservation, or entropy variables are ideal for fluid simulations. A related capability that we have been developing is the ability to use entropy to develop a physically relevant measure of our residual.

Future Research

DPG for multiphysics and magnetohydrodynamics. The field of magnetohydrodynamics (MHD) appears to be a promising target for space-time DPG. Initial investigations applying DPG the Maxwell's equations have been encouraging. Coupling Maxwell with my work on Navier-Stokes will not be trivial, but we expect this approach to be quite fruitful. Typically the techniques used to solve fluid dynamics and electromagnetics are very different, but within the DPG framework these can both be solved with the same technology. Depending on the level of interest and collaborations I am able to foster at Sandia, other research directions could include transient elastodynamics, wave propagation, heat transfer, or turbulence, but I believe the MHD option holds the most promise. From my experience at Lawrence Livermore, I understand that multiphase flows are an important aspect of simulations at the DOE labs, thus I would also like to incorporate Ju Liu's recent work (in collaboration with Tom Hughes) on thermodynamically consistent multiphase flow models into our DPG framework.

I would also like to further develop the marriage of DPG and high performance computing. Many of the features inherent to the DPG method appear promising in the context of massively parallel simulations. DPG is very compute intensive compared to the associated communication and memory costs. Most of the work is spent in embarrassingly parallel

local solves for the optimal test functions and local stiffness matrix assembly. Additionally, the stability properties of DPG make high order stability a triviality, and in general, high order methods tend to have a more attractive compute/communication profile than low order methods. In our codes, we use QR factorization for optimal test function solves, but this factorization is recyclable as we essentially have many right hand sides. The division of degrees of freedom into internal vs element interface unknowns produces a global system which can be statically condensed into a solve purely in terms of the element interface degrees of freedom. In addition to significantly cutting down on the size of the global solve, this produces a embarrassingly parallel post-processing solve for the internal degrees of freedom. This property was one of the motivations behind the development of the hybridized discontinuous Galerkin (HDG) [20] method. No matter what system of equations is being considered, DPG always produces a Hermitian positive definite stiffness matrix for the global solve. This property has not really been leveraged in our simulations so far, since we have focused on direct rather than iterative solvers, but we anticipate it might be an attractive feature in the future. Multiphysics simulations are becoming increasingly accessible and desirable as compute resources scale up. Since the only requirement for a well-defined discrete DPG method is a well-defined continuous problem, it is certainly possible that each different part of the multiphysics simulation could be discretized with DPG – no need to develop many different methods for each part of the simulation.

Wider Impact

Benefits to Sandia. In terms of computational technology, I am developing a new finite element method with significant promise for multiphysics simulations. In particular, the space-time approach caries substantial benefits over time stepping when dealing with adaptivity and solution features on multiple scales. The robustness of DPG on coarse meshes with automatic adaptivity promises an easier mesh design process for computational scientists. Scalability of the method is currently under very active development, but inherent features of DPG and early results are very encouraging. This research will advance development of the Camellia [21] DPG library which was initiated at Sandia and is built exclusively on top of Trilinos [22]. Camellia supports rapid application development and is much simpler to use than most general finite element libraries available, with an interface inspired by the FEniCS project. In the next year, Camellia is expected to be released as an open source project, possibly as a module within Trilinos. This project should ultimately make it easier for other Sandia researchers to leverage HPC resources to solve their own computational problems, as DPG and Camellia provide a framework for scientific computation rather than simply a driver to solve a single class of problems.

Based on our previous experience with DPG for fluid flow and new results for DPG for electromagnetism, we are very confident that magnetohydrodynamics and multiphase flows are a reasonable objective for the von Neumann Fellowship. There are some difficult computing challenges to overcome, but they are by no means insurmountable. By the end of my postdoctoral experience, I believe that we will have a user friendly DPG library that we can present to the greater computational community for straightforward computations of realistic scientific and engineering problems on high performance computing systems.

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