Research Proposal

Truman E. Ellis

Scientific Importance

DPG – a robust framework for computational mechanics. The discontinuous Petrov-Galerkin (DPG) finite element methodology was first proposed by Demkowicz and Gopalakrishnan [1, 2] in 2009 and has since gained significant interest from computational mechanics researchers. The primary strength of the method lies in its suitability to a very broad class of well-posed problems. 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.

Mesh design for computational mechanics can be a time-consuming and expensive process. The stability properties and nonlinear convergence of most numerical methods rely on a minimum level of mesh resolution. This means that unless the initial computational mesh is fine enough, convergence can not be guaranteed. Any meshes below this minimum resolution level are termed to be in the "pre-asymptotic regime." This condition implies that meshes need to in some way anticipate the solution before it is known. On top of the minimum requirement that the surface meshes must adequately represent the geometry of the problem under consideration, resolution requirements on the volume mesh make the computational mechanics practitioner's job significantly more time consuming. Thus, mesh design and simulation become an iterative trial and error process. A common process is for an engineer to study the problem at hand and attempt to predict regions that require extra resolution. Then they will spend hours coaxing the mesher to produce an adequate mesh before importing the mesh into the solver. Too often, the solver will fail to converge on the given mesh due to some unforeseen mesh inadequacy on part of the solution domain. The engineer then needs to descend back into the mesher to fix the problem elements. This process is repeated until the solver is satisfied and convergence can be reached. This iterative trial and error is undesirable while working on personal computers or modestly sized compute clusters, but becomes increasing costly as the problem is scaled up to the tens or hundreds of thousands of processors common in high performance computing environments.

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 and HPC. Many of the features inherent in the DPG method appear promising in the context of high performance computing. 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 skeleton unknowns produces a global system which can be statically condensed into a solve purely in terms of the skeleton 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) [3] method. No matter what system of equations is being considered, DPG always produces a Hermitian (symmetric if real) 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. As compute resources scale up, many more HPC simulations are increasingly becoming coupled in multiphysics simulations. 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.

In the context of linear problems, DPG has been successfully applied to a wide range of physical applications. Theoretical groundwork for DPG applied to the Poisson equation was laid in [4]. The time-harmonic Helmholtz equation was the focus of [5, 6] and [7]. Linear elasticity and plate problems were addressed in [8], [9], and [10], and Maxwell was addressed in [11, 12]. Linear fluid dynamics problems include convection-diffusion [13, 14, 15, 16, 17] and stationary Stokes flow[18, 17]. The robust stability properties of DPG appear to carry over into the nonlinear regime as well; Moro, Peraire and Nguyen observed [19, 20] 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.

Chan *et al.* [21] 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 [22]. The issue of local conservation within the DPG framework was addressed by Ellis *et al.* [17].

Space-time DPG for transient problems. Previous explorations of the DPG method focused exclusively on steady state problems. The easiest extension of steady DPG to transient problems would be to do an implicit time stepping technique in time and use DPG for only the spatial solve at each time step. We did indeed explore this approach, but it didn't seem to be a natural fit with the adaptive features of DPG. Clearly the Courant-Friedrichs-Lewy (CFL) condition is not binding since we were interested in implicit time integration schemes, but it can be a guiding principle for temporal accuracy in this case. So if we are interested in temporally accurate solutions, we are limited by the fact that our smallest mesh elements (which may be orders of magnitude smaller than the largest elements) are constrained to proceed at a much smaller time step than the mesh as a whole. We can either restrict the whole mesh to the smallest time step, or we can attempt some sort of local time stepping. A space-time DPG formulation presents an attractive choice as we will be able to preserve our natural adaptivity from the steady problems while extending it in time. Thus we achieve an adaptive solution technique for transient problems in a unified framework. Space-time methods have also been found superior in their satisfaction of geometric conservation laws for problems with moving boundaries [23]. Van der Vegt and van der Ven [24] note that that "The space-time DG method provides optimal efficiency for adapting and deforming the mesh while maintaining a conservative scheme which does not require interpolation of data after mesh refinement or deformation."

Research Plan

Research directions. The ultimate objective for this research is to refine and extend my work on space-time DPG for transient fluid dynamics. My dissertation research will be limited to 2D incompressible and compressible Navier-Stokes, but from our experience with DPG's stability properties, we expect straightforward application of these ideas to problems outside of fluid dynamics. In particular, 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 method. Depending on the level of interest and collaborations I am able to foster at Sandia, I could also see this research going in the direction of transient elastodynamics, wave propagation, heat transfer, or turbulence, but I am most interested in the MHD option. From my experience at Lawrence Livermore, I understand that multiphase flows are an important aspect of fluid simulations at the DOE labs, thus I would also like to incorporate Ju Liu's (in collaboration with Tom Hughes) recent work on thermodynamically consistent multiphase flow models into our DPG framework.

Benefits to Sandia. I am an active contributor to the *Camellia* [25] DPG code which was started at Sandia and makes heavy use of *Trilinos* [26]. The primary developer, Nathan Roberts, whom I will be collaborating with on this research, works full time at Argonne National Lab on further developments of *Camellia*. In the next year, he plans on releasing *Camellia* as an open source project, possibly as another module in *Trilinos*. Additionally, I will be making inroads developing a numerical technology which has the potential to contribute to Sandia's greater computational science efforts. Usage of Sandia's high performance computing systems will be critical to the success of this project, but this project should ultimately allow other Sandia researchers to leverage those compute resources to solve their own problems.

Expected schedule. Predicting the pace of research is obviously an inexact science, but by my rough estimates, my work would progress as follows. Most of the interesting electromagnetics problems take place in 3D, so the priority for the first year will be improving the performance and scaling of *Camellia* for 3D problems and exploring iterative solvers and preconditioners. Scaling and performance improvements are likely to continue through the duration of the research as new bottlenecks and improvements come to light. I will also be working on adding support for complex values. The Helmholtz equation will serve as a model problem during this development. The second year will be devoted to solving Maxwell's equations in 3D starting with the steady state version and moving to space-time transient simulations. I will probably also begin initial 2D magnetohydrodynamics simulations at this point. In the third year, I will begin working on increasingly complex 3D magnetohydrodynamics problems and multiphase flows. Throughout this process, I intend to build collaborations with Sandia researchers who are already working on these problems so I can learn from their expertise and pursue problems in alignment with Sandia's greater goals.

Expected results. The theory behind the DPG method has matured significantly over the last few years, and numerical experiments have confirmed it over and over. Thus, we expect that solving a new class of problems will not pose a problem. The challenges then lie on the computing side of things. Making our code efficient and scalable for 3D problems will not be trivial, but we expect it to be doable.

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