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14. ABSTRACT
Report developed under STTR contract for topic AF08-T023: High-Order Modeling of Applied Multi-Physics Phenomena. This objective of this Phase 1 work was to establish the feasibility of constructing a simulation approach for multi-physics phenomena based on Discontinuous Galerkin (DG) discretizations using high-order accurate approximations (up to 6th order accurate). Techniques were developed, implemented and demonstrated for efficiently and accurately discretizing the full Navier-Stokes equations, for robustly capturing shocks at high order, for extending DG methods to problems with moving meshes, and for incorporating adjoint-based techniques for robust adaptive error control and for design optimization. Furthermore, these techniques were applied to both fluid flow problems, as well as electromagnetic scattering problems, and benchmarked alongside an existing production simulation tool for fluid dynamics problems. The results obtained in this work have demonstrated key capabilities with high-order DG discretizations which are instrumental for extending these methods to complex three-dimensional multi-physics production simulation capabilities with complex geometries.

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High-Order Modeling of Applied Multi-Physics Phenomena

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GLOSSARY

ALE : Arbitrary Lagrangian Eulerian
BR2: Bassi Rebay second method
DG: Discontinuous Galerkin
GCL: Geometric Conservation Law
GMRES: Generalized Minimum Residual
HIARMS: HPC Institute for Advanced Rotorcraft Modeling and Simulation
IP : Interior Penalty
IRK : Implicit Runge-Kutta
NSU2D: Navier-Stokes Unstructured Two-Dimensional Solver
SVN: Subversion
UW: Univerity of Wyoming

1. INTRODUCTION

This report covers progress made over the entire nine month period of the Phase 1 STTR project entitled *High-Order Modeling of Applied Multi-Physics Phenomena*, awarded to Scientific Simulations LLC and performed in collaboration with the University of Wyoming.

The objective of this project has been to demonstrate the potential of a novel simulation capability based on high-order discretizations in both space and time for application to practical engineering problems involving complex physical phenomena and complicated geometries. The long-term goal is to develop a tool which can accurately handle multiphysics simulations, both in analysis mode, and for design optimization purposes.

The general approach used relies on high-order (up to 6th order) Discontinuous Galerkin discretizations in space, and backwards difference as well as higher-order implicit Runge-Kutta temporal discretizations (up to 5th order). The work performed in this project is intended to show how the favorable asymptotic properties of these high-order methods, combined with the geometrical flexibility afforded by the use of DG methods on unstructured meshes, can lead to revolutionary advances in simulation capability, enabling the accurate simulation of complex phenomena with a wide range of scales from first principles, while reducing discretization errors to acceptable levels. Furthermore, adjoint-based sensitivity analysis techniques were also included and investigated in order to demonstrate the possibility of performing simulations with quantifiable error bounds, the enhancement of the reliability of h-p adaptive methods, and enabling the solution of design optimization problems using high-order methods.

The Phase I portion of this project has sought to develop and demonstrate the key technologies and capabilities which will be required to construct a production level simulation tool. The productionalization of these capabilities in the Phase 2 work will be facilitated by making extensive use of the three-dimensional unstructured mesh simulation software infrastructure already developed by Scientific Simulations LLC for second-order accurate finite-volume methods. The outcome of a successful combined Phase 1 and 2 award will be a revolutionary high-order simulation capability which will be marketed to government and commercial clients as a replacement tool to current second-order accurate simulation codes.

2. WORK PERFORMED

The original Phase 1 STTR proposal concentrated on several specific key techniques which are required to be demonstrated in order to justify the feasibility of the overall approach for constructing a production level solver in subsequent Phase 2 work. Seven individual tasks were outlined in the Phase 1 proposal. All tasks have been performed during the course of this project and results obtained for each specific task are reported in the following section. The seven tasks consist of:

- **Task 1:** Demonstrate and document performance of Interior Penalty method for the simulation of diffusion phenomena and viscous flows.
- **Task 2:** Investigate and compare the effectiveness of shock capturing using DG methods with limiters versus high-order sub-cell shock capturing with artificial dissipation terms.

- **Task 3:** Extend high-order geometric conservation law for DG methods to high-order implicit Runge-Kutta time-stepping schemes.
- **Task 4:** Demonstrate adjoint-based shape optimization for aerodynamic problems based on high-order DG discretizations with curved boundaries.
- **Task 5:** Demonstrate goal-oriented h-p adaptivity using adjoint-based error estimation for aerodynamic problems using DG discretizations.
- **Task 6:** Extend current DG solver to multi-physics formulation and demonstrate by solving electromagnetics problem.
- **Task 7:** Validate and benchmark current DG discretization approach with existing mature second-order accurate finite-volume unstructured mesh solver.

Additional work was also performed on other tasks which were considered critical to the demonstration of the feasibility of this approach for large scale three-dimensional simulations. This additional work included devising a technique for creating curved mesh elements in boundary layer regions, and extending the Navier-Stokes Interior Penalty (IP) discretization to three dimensions.

3. RESULTS

3.1 Task 1: Interior Penalty Method for Diffusion

The original discontinuous Galerkin discretization developed for inviscid flows in previous work [1] has been extended to the full Navier-Stokes equations using the interior penalty (IP) method [2] with an explicit expression developed for the penalty parameter which removes the previously heuristic nature of this approach [3]. This approach is appealing since it constitutes one of the simplest DG approaches to diffusion terms, retains a nearest-neighbor stencil, and provides equivalent performance compared to more complex discretizations. This is illustrated in Figure 1 (reproduced from Reference [4]) where the accuracy achieved for the solution of a Poisson equation using the IP method is compared with the more commonly used BR2 DG discretization [5], showing equivalent accuracy for discretization orders of accuracy ranging from p=1 to p=4. The discretization of the Navier-Stokes equations using the IP method has been implemented for both triangular and quadrilateral elements, while the efficiency of the h-p multigrid solver previously developed for inviscid flows has been enhanced by adding a line-implicit solver in boundary layer regions and using the entire line-solver driven h-p multigrid algorithm as a preconditioner for a GMRES krylov method. Figure 2 illustrates the solution of laminar viscous flow (Re = 5000) over a slotted airfoil configuration on a hybrid mesh including triangular and quadrilateral elements, using a fourth-order accurate DG discretization and making use of the IP method for the discretization of the viscous terms. Figure 2(c) shows the convergence rate achieved for this test case using the baseline h-p multigrid solver with an element-implicit (Jacobi) smoother on each multigrid level, a line-implicit smoother, and using the latter approach as a preconditioner for GMRES. The inclusion of a line-implicit smoother is seen to be crucial for obtaining efficient convergence rates in the presence of anisotropic meshes, while the addition of GMRES provides further modest speedup.

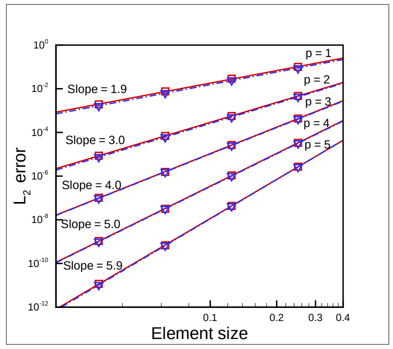
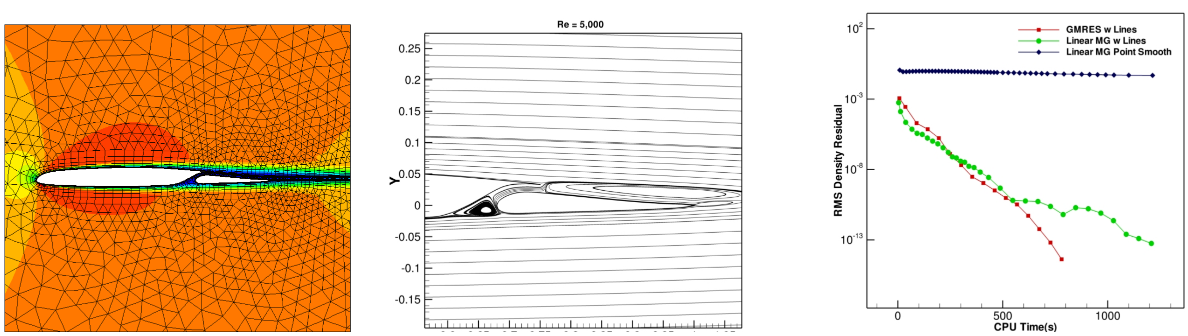
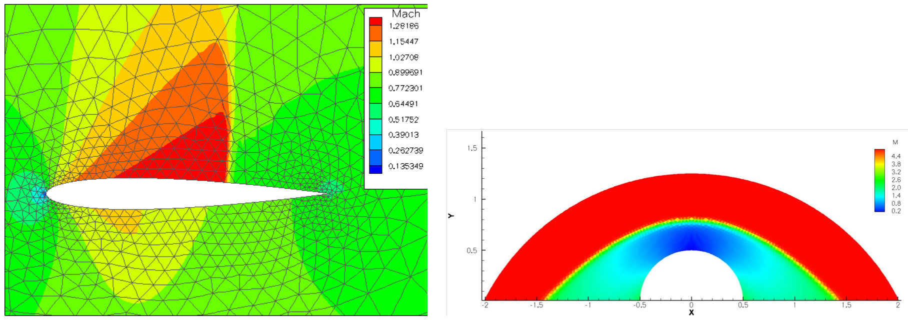


Figure 1: Comparison of accuracy achieved with IP discretization and BR2 discretization for Poisson equation problem in two-dimensions for various discretization orders of accuracy.



(a) (b) (c)

Figure 2: (a) Computed Mach contours for viscous flow over slotted airfoil configuration at Mach = 0.2 and Reynolds number of 5000 using fourth-order (p=3) discretization on mixed-element unstructured mesh. (b) Details of separation pattern obtained for this test case. (c) Convergence of h-p multigrid for this test case with element-implicit solver, line-implicit solver, and used as a preconditioner for GMRES.



(a) (b)

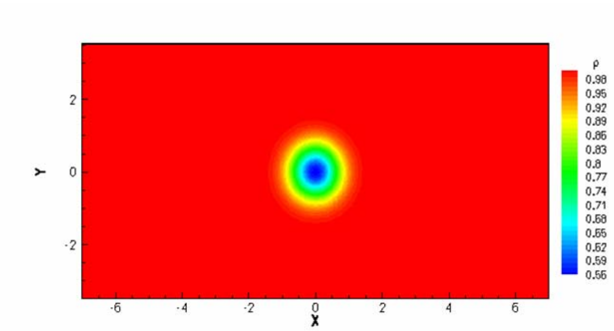
Figure 3: (a) Simulation of transonic flow over NACA 0012 airfoil at Mach=0.8 and 1.25 degrees incidence using artificial dissipation approach illustrating sub-cell shock capturing resolution with fourth-order (p=3) DG discretization. (b) Simulation of hypersonic inviscid flow over cylinder at Mach = 6 using third-order (p=2) DG discretization with limiting procedure for robustly capturing strong shock wave.

3.2 Task 2: Shock Capturing

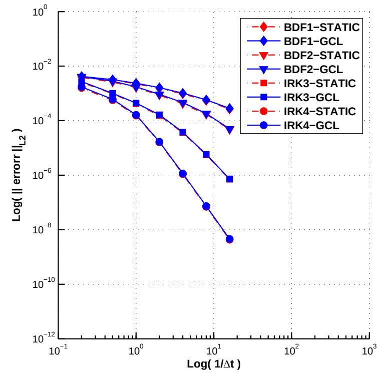
Two approaches have been investigated for shock capturing with high-order DG discretizations. The first approach is based on the use of artificial dissipation terms, discretized using the IP method, to smooth out and capture shocks. A captured shock for an inviscid transonic NACA0012 test case is shown in Figure 3(a), showing good sub-cell resolution of the shock wave. While this approach works well for relatively weak transonic shocks, it has been found to be problematic for strong shocks encountered in hypersonic flows. Therefore, a non-linear limiting or filtering technique has been developed for capturing strong shocks. The approach is based on filtering techniques originally derived for image reconstruction problems [6]. The idea is to use this approach as a filter on oscillatory solutions produced near under-resolved or discontinuous phenomena to restore monotone profiles. Figure 3(b) illustrates the solution of Mach 6 flow over a cylinder calculated using the non-linear filtering approach, showing a crisp nearly monotone shock structure. Results similar to those displayed in Figure 3(a) have also been obtained for transonic flow problems. These two approaches will be further investigated and the most promising strategy will be used in the three-dimensional solver in the Phase 2 project.

3.3 Task 3: Arbitrary-Lagrangian-Eulerian Formulations

An arbitrary Langrangian-Eulerian formulation for DG discretizations suited for solutions on dynamically deforming meshes which guarantees discrete conservation as embodied in the Geometric Conservation Law (GCL) has previously been derived for first and second-order time discretizations [7]. In the current work, this has been extended to higher-order implicit Runge-Kutta time discretization schemes. For a first-order backwards difference scheme, the basic idea consists of formulating the problem as a space-time DG discretization with constant basis functions in the time direction. The extension to higher-order IRK schemes is then obtained by applying this formulation at each individual stage in the IRK scheme. This formulation has been validated by first verifying that uniform flow remains an exact solution in the presence of prescribed mesh deformations, including the deformation of curved high-order elements. Subsequently, it was verified that



(a)



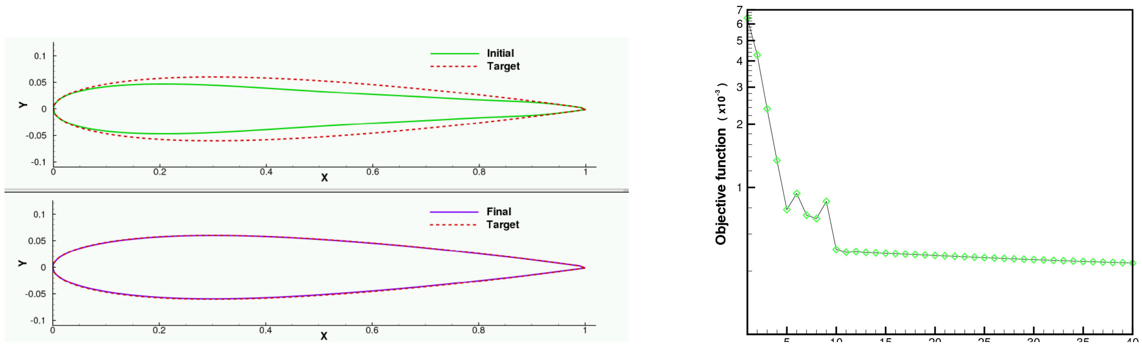
(b)

Figure 4: (a) Simulation of vortex convection problem on dynamically deforming mesh for testing accuracy of ALE formulation. (b)Temporal accuracy observed for static and moving mesh cases with various temporal discretizations for GCL compliant ALE DG scheme.

the order properties of third- and fourth-order implicit Runge-Kutta schemes are preserved in the presence of moving curved-element meshes for the test case of a convecting inviscid vortex in a uniform flow. These results are summarized in Figure 4, where the temporal error as a function of time step size is compared for static and dynamic mesh cases.

3.4 Task 4 : Adjoint-Based Shape Optimization

The Phase 1 work has also investigated the use of a DG adjoint capability for driving shape optimization problems. In order to enable the computation of shape sensitivities, the adjoint problem must be first formulated and solved. The adjoint operator is formulated by first forming the complete Jacobian of the discretized flow equations and then taking the transpose of this matrix. This constitutes the discrete adjoint approach, and is easily implemented since the Jacobian is available from the linear multigrid solver as a set of diagonal block sub-matrices, which are easily transposed, and a set of off-diagonal block sub-matrices, which are transposed and swapped to form the complete transpose operator. Solution of the adjoint problem is then performed using the same h-p multigrid scheme as employed for the flow problem, albeit in linear form. The computed adjoint field must then be multiplied by the sensitivity of the residual with respect to changes in the geometric element mappings, which may include the effect of changes in element curvature. These terms have been derived and demonstrated for an inviscid subsonic airfoil shape optimization problem, as depicted in Figure 5. Using an objective based on the difference in prescribed and calculated airfoil surface pressure, the target surface pressure distribution and airfoil shape were recovered in 40 design cycles, using a simple steepest descent optimization strategy with 145 design variables (Hicks-Henne bump functions) used to define the airfoil. The target airfoil was defined as a perturbation of the initial airfoil which ensured the realizability of this optimization problem. Although this represents a relatively simple optimization problem, it serves to demonstrate the ability to perform shape optimization with DG discretizations in the presence of curved mesh elements. This demonstration will serve as the basis for the incorporation of a shape optimization capability in the three-dimensional solver in Phase 2, where the principal task will consist of deriving the linearizations of the residual with respect to the element mappings.



(a)

(b)

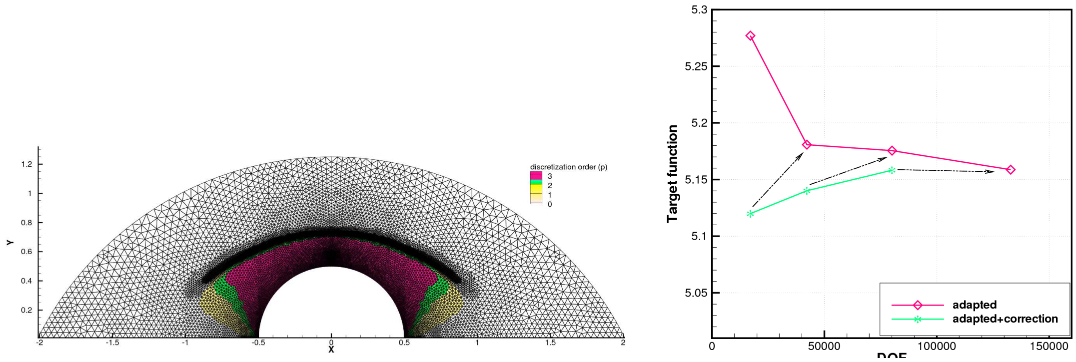
Figure 5: (a) Evolution of designed airfoil from initial shape to final shape compared with target airfoil for shape optimization using high-order DG discretization of the Euler equations on mesh with curved surface elements. (b) Convergence of optimization problem as measured by decrease in objective function versus number of design cycles using steepest descent optimization procedure.

3.5 Task 5 : Goal-Oriented h-p Adaptivity

Adjoint-based error-estimation techniques have been the subject of considerable interest recently for both spatial and temporal error estimation [8–11]. The UW group has investigated adjoint formulations for both finite-volume and DG discretizations over the last several years [10–14]. The use of adjoint methods for driving h-p refinement strategies with DG discretizations has been pursued in the Phase 1 project. Although the adjoint error-estimation strategy remains essentially unchanged from previous implementations, the key ingredient for enabling h-p refinement is a smoothness indicator, which is used to make the choice between h or p refinement in regions of large error. We have implemented two smoothness indicators, one based on the relative size of the highest solution modes versus the lower solution modes [15], and another based on the size of the discontinuous jumps between neighboring elements [16]. While both methods give satisfactory results, the second approach has been found to be more reliable for flows with strong shocks. Figure 6(a) illustrates the solution obtained for hypersonic flow over a circular cylinder using h-p adaptivity with the jump-based smoothness indicator for the adjoint-estimated error in the surface integrated temperature on the cylinder. In this case, extensive h-refinement occurs in the shock region where the solution is non-smooth, and p refinement occurs in the region between the shock and the cylinder surface. Note that no refinement (h or p) occurs in areas lateral to the cylinder, since these areas have little influence on the objective of interest (surface temperature). Figure 6(b) illustrates the convergence of the simulation objective with each successive refinement step, showing the increasingly accurate error prediction provided by the adjoint procedure at each successive refinement level.

3.6 Task 6: Multi-Physics Formulations

One of the consequences of the local compact stencil of Discontinuous Galerkin discretizations is that a simple data structure consisting of elements and faces can be used to support the discretization of various types of equations. In the Phase 1 work we have demonstrated this by extending our



(a) (b)

Figure 6: (a) h-p adaptive refinement pattern for hypersonic flow (Mach 6) over cylinder based on error in surface integrated temperature;(b) Convergence of integrated temperature functional with refinement levels and error prediction provided by adjoint.

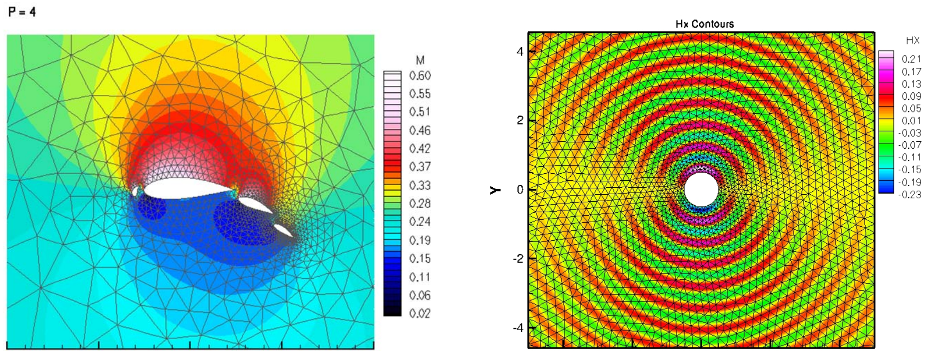
existing two-dimensional DG Euler equation solver to solve the governing equations for electromagnetics. Figure 7(a) illustrates an inviscid flow solution obtained over an idealized four-element airfoil geometry, while Figure 7(b) illustrates the solution of electromagnetic scattering over a cylinder using the same code modified to discretize the linear Maxwell's equations. A further extension of this code to include linear aeroacoustic problems is currently under development. In this case, the discretization is closely related to the electromagnetic problem, with the exception that 4 instead of 3 field variables are required, and the linear equation coefficients depend on the background mean flow field which must be read in at run time.

3.7 Task 7: Efficiency Benchmarks

The performance of the two-dimensional Discontinuous Galerkin Navier-Stokes solver has been compared to that of a production level two-dimensional unstructured mesh finite volume code (NSU2D [17]). For these comparisons, the line-implicit h-p multigrid GMRES solver was used for the high-order Discontinuous Galerkin code, using discretization orders ranging from first-order to fourth-order, while the NSU2D code relies on a second-order accurate finite-volume vertex-based discretization, and makes use of an agglomeration multigrid technique for convergence acceleration. The two codes were found to require roughly equivalent computational resources for cases involving the same number of degrees of freedom, thus favoring the DG scheme due to the higher accuracy achieved for this scheme using the same number of unknowns.

3.8 Additional Results

An additional objective addressed during this project relates to the ability to generate curved mesh elements which conform to the surface geometry. This was partly motivated by comments in the debriefing of the original STTR proposal review, but also became necessary upon the introduction of stretched meshes near the surface. In our approach, additional surface points within each surface element are obtained by accessing the original spline definition of the geometry. The displacements between these new points and their projection onto the linear surface edge of the surface elements is then used to define the curvature of the surface elements. For highly stretched meshes, this may lead to cross-over with neighboring linear elements, and therefore the curvature is propagated to

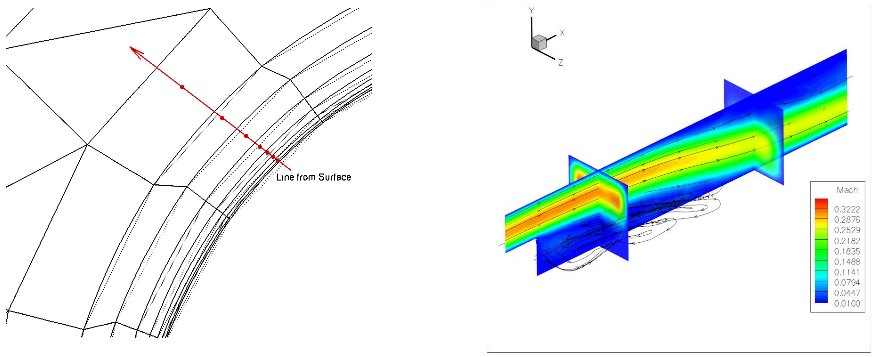


(a) (b)

Figure 7: (a) Inviscid flow solution over idealized four element airfoil configuration using p=4 (fifth-order) accurate DG discretization. Mach = 0.2, Incidence = 0 degrees. (b) Instantaneous x-component magnetic scattering field computed for incident radiation over circular cylinder using p=4 (fifth-order) accurate DG discretization.

neighboring elements by marching along lines normal to the boundary layer direction, specifying the same displacements on each subsequently encountered mesh edge, until isotropic elements at the edge of the boundary layer are encountered. The validity of the resulting curved element mesh is then confirmed by verifying that the Jacobian values are positive at all quadrature points in each element. Note that it is not sufficient to calculate the volume of these elements, as this corresponds to an average Jacobian value at all quadrature points. Figure 8(a) illustrates the curved elements for the stretched mesh used in the viscous airfoil flow simulation obtained using this procedure. Extensions to three-dimensions are currently underway, using the VGRID grid generation program with a facility for projecting new surface points onto the patched geometry description used by VGRID.

The previously developed three-dimensional DG Euler solver [18] is being continuously upgraded to incorporate the advances demonstrated in the two-dimensional setting described above. Since this will ultimately become a deliverable production code, it is important that rigorous software engineering practices be adopted from the outset for the development of this code. To this end, the three-dimensional DG solver has been placed under the SVN software version control system [19] and the Hudson [20] regression testing system, which are the same systems used in the HIARMS project underway in the University of Wyoming research group. Individual regression tests are being implemented and added to the test suite on a continual basis. The planned three-dimensional implementations include extension to the Navier-Stokes equations using the IP method, support for mixed element meshes, and the generation of curved surface and interior elements for consistent high-order three-dimensional meshes. At present, a three-dimensional DG Navier-Stokes discretization using the analogous IP method has been implemented in three-dimensions for tetrahedral meshes with straight (non-curved) elements and faces. Figure 8(b) illustrates the solution of flow over a backwards facing step at a Reynolds number of 500 computed with the element-implicit solver in the absence of multigrid.



(a) (b)

Figure 8: (a) Illustration of generation of curved surface and interior boundary layer elements obtained by propagating curvature information from boundary along lines normal to boundary layer. (b) Three-dimensional viscous flow computed over backwards facing step using fourth-order (p=3) DG discretization with IP method used for viscous terms on fully tetrahedral mesh for subsonic flow at Reynolds number of 500.

4. ESTIMATE OF TECHNICAL FEASIBILITY

The Phase 1 project has been designed to establish the technical feasibility of constructing a robust high-order accurate Discontinuous Galerkin solver for complex three-dimensional configurations suitable for production use. The specific tasks described in the proposal for the Phase 1 project were chosen to demonstrate specific capabilities which will be required for the construction of a successful three-dimensional production simulation capability.

The Phase 1 project has successfully achieved all of the objectives set out at the beginning of the project, and all seven technical tasks specified in the proposed work plan have been completed. The Phase 1 work has demonstrated the feasibility of using the IP method for discretizing the Navier-Stokes equations in two and three dimensions. Two shock capturing schemes have been implemented in two dimensions and used successfully to capture transonic and hypersonic shocks. A consistent approach for formulating high-order DG discretizations in the presence of dynamically deforming meshes has also been derived and demonstrated, thus making feasible the application of this simulation approach to more complex problems with moving or deforming bodies. An adjoint solution technique has been developed and used to demonstrate the potential for shape optimization in the presence of curved surface elements with high-order accuracy, as well as for predicting error in specific functional objectives and for driving h-p adaptive schemes, which hold great promise for delivering highly accurate and certifiably correct solutions. Using the same software framework and data-structures, the two-dimensional DG code was extended to electromagnetic problems, illustrating the potential for solving multi-physics problems within a single software framework based on DG discretizations. A technique for handling stretched meshes in the presence of curved surface geometries has also been devised, and strategies for extending this approach to three dimensions have been developed. Finally, the two-dimensional DG Navier-Stokes solver was benchmarked against a production finite-volume Navier-Stokes solver and found to be competitive in terms of required computational resources.

These findings validate a set of important capabilities which will be instrumental in the construction of a three-dimensional production solver based on DG discretizations. At present, a three-dimensional Navier-Stokes solver based on high-order DG discretizations and using the efficient h-p multigrid solver originally developed in two dimensions has been developed and has been validated on simple geometries. The successful demonstration of these tasks in the Phase 1 project, along with the current operational status of our three-dimensional solver, and currently planned extensions, present a strong case for the feasibility of achieving the goals set out in the Phase 1 proposal, namely the construction of a high-order accurate simulation tool, suitable for complex geometries, usable in the presence of dynamically deforming geometries, and capable of incorporating the latest advances in numerical simulation technology, such as adaptive refinement and design optimization.

5. CONCLUSION AND FURTHER WORK

The tasks completed in the Phase 1 project were mostly carried out in the two-dimensional setting. Work is currently underway to extend these capabilities into the three-dimensional Navier-Stokes DG code which has been developed in the project and described above. In order to incorporate all the capabilities demonstrated in the Phase 1 project, a re-engineering of the original three-dimensional code is required. The three-dimensional code must be capable of solving multiphysics problems, handling cases with dynamically deforming meshes, where individual mesh elements may have different orders of geometric mappings (i.e. straight-faced elements employing linear mappings, curved elements employing higher-order mappings). Individual mesh elements may also have different solution accuracies (p orders) in order to enable h-p adaptive refinement schemes. Thus, a new data-structure has been devised where mesh elements may have different shapes (mixed element meshes), may have individually specifiable solution order, individually specifiable geometric mapping orders, and where all ALE terms are incorporated and high enough quadrature rules are implemented in order to guarantee conservation in the presence of moving meshes. This data structure is currently being implemented in a linked list fashion, and will enable all the capabilities demonstrated in the Phase 1 project to be integrated into the three-dimensional solver.

Based on the demonstrated results from the Phase 1 project, it is anticipated that continued development of this technology and extension into the three-dimensional setting following the path described above, will revolutionize our ability to simulate complex engineering problems with high fidelity in the near future.

6. PERSONNEL INVOLVED IN PROJECT

- Dimitri Mavriplis. Professor, Department of Mechanical Engineering, University of Wyoming; Technical specialist, Scientific Simulations LLC.
- Michael Long. Software Engineer and Application Specialist. Scientific Simulations LLC.
- Li Wang. PhD Student, Department of Mechanical Engineering, University of Wyoming. (PhD awarded May 2009).
- Nick Burgess. PhD Student, Department of Mechanical Engineering, University of Wyoming.

7. PUBLICATIONS RESULTING WHOLLY OR IN PART FROM PROJECT

- *Techniques for High-Order Adaptive Discontinuous Galerkin Discretizations in Fluid Dynamics.*, Li Wang, PhD Thesis, Department of Mechanical Engineering, University of Wyoming, May 2009.
- *Progress in High-Order Discontinuous Galerkin Methods for Aerospace Applications.* D. J. Mavriplis, C. Nastase, L. Wang, K. Shahbazi, N. Burgess, AIAA Paper 2009-0601, AIAA Aerospace Sciences Meeting, Orlando FL, January 5-8, 2009.
- *Adjoint Based h-p Adaptive Discontinuous Galerkin Methods for Aerospace Applications.* L. Wang and D. J. Mavriplis AIAA Paper 2009-0952, AIAA Aerospace Sciences Meeting, Orlando FL, January 5-8, 2009.
- *On the Geometric Conservation Law for High-Order Discontinuous Galerkin Discretizations on Dynamically Deforming Meshes.* D. J. Mavriplis and C. Nastase, paper to be submitted to Journal of Computational Physics, 2009.

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