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Development of an Advanced Computational Fluid Dynamics Technology for the Next-Generation Nuclear Reactor System Analysis and Safety Margin Characterization Code

Reactor Concepts

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1. Summary

This report describes the research activities we have conducted at NCSU for our NEUP project. The work toward achieving the objectives of the project is reported. The significant achievements and accomplishments are presented. A number of numerical experiments are conducted to demonstrate that the goal of the proposed work has been successfully achieved. Issues, recommendations, and future work are discussed.

2. Introduction

The accuracy of many finite-volume and finite-element methods currently used in computational fluid dynamics is at best second order. These well established and fairly mature research and production CFD methods are able to provide orders of improvements in comparison to 1^{st} order methods. In spite of an exhaustive effort on all possible refinements and improvements on their efficiency and robustness, the second-order CFD methods can hardly achieve the designed second-order accuracy in practice on unstructured tetrahedral grids, and therefore cannot deliver engineering-required accuracy in time for a variety of applications. Furthermore, Uncertainty Quantification (UQ) for a requested simulation using a second-order method can only be provided by a higher-order (>2nd) method.

Over the last several years, it has become clear that orders of magnitude improvements in both accuracy and efficiency can be achieved by replacing second-order methods with higher-order methods in CFD. This recognition has opened previously unimaginable opportunities to tackle a variety of complex flow problems in science and engineering. However, the promise of these methods has remained, to a great extent, unrealized because of the several difficulties raised by the application of these methods to flow problems of practical interests.

As the leader of higher-order methods in CFD applications, the discontinuous Galerkin (DG) methods[1-28] have received many attentions recently. The discontinuous Galerkin methods (DGM) combine two advantageous features commonly associated with finite element and finite volume methods (FVM). As in classical finite element methods, accuracy is obtained by means of high-order polynomial approximation within an element rather than by wide stencils as in the case of FVM. The physics of wave propagation is, however, accounted for by solving the Riemann problems that arise from the discontinuous representation of the solution at element interfaces. In this respect, the methods are therefore similar to FVM. What is known so far about these methods offers a tantalizing glimpse of their full potential. Indeed, what set these methods apart from the crowd are many distinct, attractive features they possess: 1) They have several useful mathematical properties with respect to conservation, stability, and convergence; 2) The methods can be easily extended for higher-order (>2nd) approximation; 3) The methods are well suited for complex geometries since they can be applied on arbitrary grids. In addition, the methods can also handle non-conforming elements, where the grids are allowed to have hanging nodes; 4) The methods are highly parallelizable, as they are compact and each element is independent. Since the elements are discontinuous, and the inter-element communications are minimal, domain decomposition can be efficiently employed. The compactness also allows for structured and simplified coding for the methods; 5) They can easily handle adaptive strategies, since refining or coarsening a grid can be achieved without considering the continuity restriction commonly associated with the conforming elements. The methods allow easy implementation of *hp*-refinement, for example, the order of accuracy, or shape, can vary from element to element. 6) They have the ability to compute low Mach number flow problems without recourse to the time-preconditioning techniques normally required for the finite volume methods. In contrast to the enormous advances in the theoretical and numerical analysis of the DGM, the development of a viable, attractive, competitive, and ultimately superior DG method over the more mature and well-established second order methods is relatively an untouched area. This is mainly due to the fact that the DGM have a number of weaknesses that have yet to be addressed, before they can be robustly used for flow problems of practical interest in a complex configuration environment. In particular, there are three most challenging and unresolved issues in the DGM: a) how to efficiently discretize diffusion terms required for the Navier-Stokes equations, b) how to effectively control spurious oscillations in the presence of strong discontinuities, and c) how to develop efficient time integration schemes for time accurate and steady-state solutions. Indeed, compared to the finite element methods and finite volume methods, the DG methods require solutions of systems of equations with more unknowns for the same grids. Consequently, these methods have been recognized as expensive in terms of both computational costs and storage requirements.

Our research effort has been to bridge this gap between potential and reality by developing a higher-order reconstructed discontinuous Galerkin (rDG) method[18-28] that can provide significant improvements in accuracy and efficiency for solving a variety of complex flow problems compared to today's state-of-the-art second order methods. In reconstructed DG methods, termed rDG(PnPm), Pn indicates that a piecewise polynomial of degree of n is used to represent a DG solution, and Pm represents a reconstructed polynomial solution of degree of m ($m \geq n$) that is used to compute the fluxes. The rDG(PnPm) schemes are designed to enhance the accuracy of the discontinuous Galerkin method by increasing the order of the underlying polynomial solution. The beauty of the rDG(PnPm) schemes is that they provide a unified formulation for both finite volume and DG methods, and contain both classical finite volume and standard DG methods as two special cases of rDG(PnPm) schemes, and thus allow for a direct efficiency comparison. When $n=0$, i.e. a piecewise constant polynomial is used to represent a numerical solution, rDG(P0Pm) is nothing but classical high order finite volume schemes, where a polynomial solution of degree m ($m \geq 1$) is reconstructed from a piecewise constant solution. When $m=n$, the reconstruction reduces to the identity operator, and rDG(PnPn) scheme yields a standard DG method. Our lately developed reconstructed discontinuous Galerkin method based on a hierarchical WENO reconstruction[36,37] is designed not only to reduce the high computing costs for the DG methods, but also to avoid spurious oscillations in the vicinity of strong discontinuities, thus effectively overcoming the two shortcomings of the DG methods. Our numerical experiments for a variety of flow problems indicate that the rDG(P1P2) method is able to capture shock waves within one cell without any spurious oscillations, achieve the designed third-order of accuracy: one order accuracy higher than the underlying DG method, and thus significantly increase its accuracy without significant increase in computing costs and memory requirements.

3. Research Activities

The main objective of the research effort in this project is to develop, apply, and implement an advanced Computational Fluid Dynamics (CFD) technology that can be used in a next generation simulation code for design and safety analysis of advanced nuclear energy systems. The main research efforts involved in this project can be divided into three tasks: 1) Development and assessment of a third order spatial discretization method based on a reconstructed discontinuous Galerkin for the compressible Navier-Stokes equations on unstructured hybrid grids; 2) Development and implementation of a third-order implicit temporal discretization method for the rDG ; and 3) Verification and Validation of. The work performed in these three areas for this project is detailed below.

3.1 Development of a class of reconstructed DG methods on arbitrary grids

The objective of this task is to develop and assess a class of reconstructed discontinuous Galerkin methods for solving compressible flow problems on arbitrary grids. The reconstructed DG (rDG) methods, termed PnPm schemes and were introduced by Dumber et al.[18-20], where Pn indicates that a piecewise polynomial of degree of n is used to represent a DG solution, and Pm represents a reconstructed polynomial solution of degree of m ($m \geq n$) that is used to compute the fluxes. The beauty of PnPm schemes is that they provide a unified formulation for both finite volume and DG methods, and contain both classical finite volume and standard DG methods as two special cases of PnPm schemes, and thus allow for a direct efficiency comparison. When n=0, i.e. a piecewise constant polynomial is used to represent a numerical solution, P0Pm is nothing but classical high order finite volume schemes, where a polynomial solution of degree m ($m \geq 1$) is reconstructed from a piecewise constant solution. When m=n, the reconstruction reduces to the identity operator, and PnPn scheme yields a standard DG method.

Obviously, the construction of an accurate and efficient reconstruction operator is crucial to the success of the PnPm schemes. In Dumbser's work, this is achieved using a so-called in-cell recovery, where recovered equations are obtained using a L2 projection, i.e., the recovered polynomial solution is uniquely determined by making it indistinguishable from the underlying DG solutions in the contributing cells in the weak sense. The resultant over-determined system is then solved using a least-squares method that guarantees exact conservation, not only of the cell averages but also of all higher order moments in the reconstructed cell itself, such as slopes and curvatures. However, this conservative least-squares recovery approach is computationally expensive, as it involves both recovery of a polynomial solution of higher order and least-squares solution of the resulting over-determined system. Furthermore, the recovery might be problematic for a boundary cell, where the number of the face-neighboring cells might be not enough to provide the necessary information to recover a polynomial solution of a desired order.

Fortunately, recovery is not the only way to obtain a polynomial solution of higher order from the underlying discontinuous Galerkin solutions. Rather, reconstruction widely used in the finite volume methods provides an alternative, probably a better choice to obtain a higher-order polynomial representation. Luo et al.[26-28] develop a reconstructed discontinuous Galerkin method using a Taylor basis[13] for the solution of the compressible Euler and Navier-Stokes equations on arbitrary grids, where a higher order polynomial solution is reconstructed by use of a strong interpolation, requiring point values and derivatives to be interpolated on the face-neighboring cells. The resulting over-determined linear system of equations is then solved in the least-squares sense. This reconstruction scheme only involves the von Neumann neighborhood, and thus is compact, simple, robust, and flexible. Furthermore, the reconstruction scheme guarantees exact conservation, not only of the cell averages but also of their slopes due to a judicious choice of our Taylor basis.

More recently, Zhang et al.[29,30] presented a class of hybrid DG/FV methods for the conservation laws, where the second derivatives in a cell are obtained from the first derivatives in the cell itself and its neighboring cells using a Green-Gauss reconstruction widely used in the finite volume methods. This provides a fast, simple, and robust way to obtain a higher-order polynomial solutions. The numerical experiments indicate that this efficient reconstruction scheme is able to achieve a third-order accuracy: one order accuracy higher than the underlying second order DG method.

A comparative study has been conducted to assess the performance of these three reconstruction methods[31-32]. The numerical experiments indicate that all three reconstructed discontinuous Galerkin methods can deliver the desired third order of accuracy and significantly improve the accuracy of the underlying second-order DG method, although the least-squares reconstruction method provides the best performance in terms of both accuracy and robustness.

Unfortunately, the attempt to extend this rDG method to solve 3D Euler equations on tetrahedral grids was not successful. Like the second order cell-centered finite volume methods rDG(P0P1)[33], the resultant rDG(P1P2) method is unstable. Although rDG(P0P1) methods are in general stable in 2D and on Cartesian or structured grids in 3D, they suffer from the so-called linear instability on unstructured tetrahedral grids, when the reconstruction stencils only involve von Neumann neighborhood, i.e., adjacent face-neighboring cells[33]. The rDG(P1P2) method exhibits the same linear instability, which can be overcome by using extended stencils. However, this is achieved at the expense of sacrificing the compactness of the underlying DG methods. Furthermore, these linear reconstruction-based DG methods will suffer from non-physical oscillations in the vicinity of strong discontinuities for the compressible Euler equations. Alternatively, ENO, WENO, and HWENO can be used to reconstruct a higher-order polynomial solution, thereby not only enhancing the order of accuracy of the underlying DG method but also achieving both linear and non-linear stability. This type of hybrid HWENO+DG schemes has been presented on 1D and 2D structured grids by Balsara et al.[34], where the HWENO reconstruction is relatively simple and straightforward.

Our effort has been focused on developing a Reconstructed Discontinuous Galerkin method, rDG(P1P2), based on a WENO reconstruction using a Taylor basis[13] for solving compressible flow problems on hybrid grids. This rDG(P1P2) method is designed not only to reduce the high computing costs of the DGM, but also to avoid spurious oscillations in the vicinity of strong discontinuities, thus effectively addressing the two shortcomings of the DGM. In this rDG(P1P2) method, a quadratic solution is first reconstructed to enhance the accuracy of the underlying DG method in two steps: (1) all second derivatives on each cell are first reconstructed using the solution variables and their first derivatives from adjacent face-neighboring cells via a strong interpolation; (2) the final second derivatives on each cell are then obtained using a WENO strategy based on the reconstructed second derivatives on the cell itself and its adjacent face-neighboring cells. This reconstruction scheme, by taking advantage of handily available and yet valuable information namely the gradients in the context of the DG methods, only involves von Neumann neighborhood and thus is compact, simple, robust, and flexible. As the underlying DG method is second-order, and the basis functions are at most linear functions, fewer quadrature points are then required for both domain and face integrals, and the number of unknowns (the number of degrees of freedom) remains the same as for the DG(P1). Consequently, this rDG method is more efficient than its third order DG(P2) counterpart. The gradients of the quadratic polynomial solutions are then modified using a WENO reconstruction in order to eliminate non-physical oscillations in the vicinity of strong discontinuities, thus ensuring the non-linear stability of the RDG method. The developed rDG(P1P2) method is used to compute a variety of flow problems ranging from nearly incompressible flows to supersonic flows on hybrid grids to demonstrate its accuracy, robustness, versatility, and essentially non-oscillatory property. The presented numerical results indicate that this rDG(P1P2) method is able to 1) capture shock waves sharply essentially without any spurious oscillations, 2) provide the accurate simulations for a wide range of flow regimes from nearly incompressible flows to supersonic flows without using time-derivatives preconditioning methods, without modifying the Riemann flux functions, and without adjusting any parameters, and 3) achieve the designed third-order of accuracy for smooth flows: one order accuracy higher than the underlying DG(P1) method, and thus significantly increase its accuracy without significant increase in computing costs and memory requirements.

Our work on the development of this rDG method has been published in a number of papers. Two papers published in journal of computational physics are attached in appendix 1 of this report for the sake of completeness.

3.2. Development of an accurate, efficient higher-order method for temporal discretization

Our ultimate objective is to develop an overall third-order accurate numerical method in both space and time for the solution of the compressible Navier-Stokes equations on 3D hybrid grids. The focus of this task is placed on the development of a robust high-order fully-implicit temporal discretization for the rDG methods. This research work is strongly motivated by the need to develop an accurate and fast arbitrary high-order implicit method for solving time-accurate flow problems in order to keep the overall higher-accuracy of the higher-order reconstructed discontinuous Galerkin methods. It has been conclusively demonstrated in the literature that the use of higher order methods in space alone does not ensure a more accurate solution in that the error deduced by the time-stepping methods can be dominant. Explicit methods such as multi-stage Runge-Kutta schemes may be the only choice for certain unsteady applications such as shock wave and transition simulations, when the time scales of interest are small, or more precisely, when they are comparable to the spatial scales. However, when dealing with many low reduced frequency phenomena with disparate temporal and spatial scales, explicit methods are notoriously time-consuming, since the allowable time step is much more restrictive than that needed for an acceptable level of time accuracy. Therefore, it is desirable to develop a fully implicit method, where the time step is solely determined by the temporal accuracy consideration for the flow physics and is not limited by the numerical stability consideration. Implicit methods, such as the first-order accurate backward Euler scheme, the Crank-Nicholson method, and the second-order backward differentiation formula, can be used for these types of problems. These time integration schemes are relatively efficient because they solve only one implicit set of equations per time step. However, they require a fixed time step, thus rendering them less efficient. They are not A-stable, thus rendering them less robust. They only provide a second-order temporal accuracy, thus rendering them less accurate. The development of accurate and fast arbitrary high-order implicit methods is needed in order to keep the overall higher-accuracy and higher-efficiency of the higher-order discontinuous Galerkin methods. Recently, a diagonally implicit Runge-Kutta (IRK) method, originally developed by Bijl et al[38] for the finite volume solutions of the Navier-Stokes equations is extended by Wang et al.[39] to solve the compressible Euler equations using higher-order discontinuous Galerkin methods. They conclude that the diagonally implicit Runge-Kutta method is more efficient than the second-order time integration schemes. We have extended and implemented IRK method for the time accurate solutions of the compressible Navier-Stokes equations on arbitrary grids using the reconstructed discontinuous Galerkin method[40,41]. A system of nonlinear equations arising from a diagonally implicit Runge-Kutta temporal discretization of the unsteady Euler and Navier-Stokes equations is solved at each time step using a pseudo-time marching approach. The resulting systems of linear algebraic equations are solved using the GMRES+LU-SGS method. Three approaches: analytical derivation, divided differencing, and automatic differentiation (AD) are presented, developed, and compared to construct the Jacobian matrix. The developed implicit rDG method is used to compute a variety of unsteady flow problems on 3D hybrid grids. The numerical results obtained indicate that the use of the present implicit methods lead to orders of improvements in performance over its explicit counterpart, while without significant increase in memory requirements and that the implicit method where the construction of Jacobian matrix is based on the AD approach performs the best in terms of robustness and efficiency.

Our work on the development of implicit methods for the rDG method has been published in a number of papers. Two papers published in journal of Computers & Fluids are attached in appendix 2 of this report for the sake of completeness.

4. Conclusions and Recommendations

A reconstructed discontinuous Galerkin method has been developed for the compressible flows at all speeds. The developed rDG has been used to compute a variety of flow problems to assess its accuracy and test its robustness for a variety of compressible flows. The numerical experiments clearly demonstrate that the developed rDG(P_1P_2) method is able to achieve the designed third-order accuracy: one order accuracy higher than the underlying DG method, and obtain the accurate solutions for a wide range of flow regimes from nearly incompressible flows to supersonic flows without adjustment of any parameters and without recourse to the time-derivative preconditioning methods.

Although the execution of this project meets or exceeds our initial expectations, there are so many topics that can be pursued as a follow-up of this project. In particular, 1) implementation of this rDG method in RELAP-7 for hydraulics in the framework of MOOSE and 2) development of a two-phase flow capability using the rDG method in the framework of MOOSE, are two projects on which we are ready to collaborate with our colleagues at INL.

5. Accomplishments

The most significant accomplishment in this project is probably that we are able to demonstrate the accuracy, efficiency, robustness, and non-oscillatory property of our rDG method. The developed rDG(P1P2) method not only enhances the accuracy of discontinuous Galerkin method but also avoids spurious oscillation in the vicinity of discontinuities, which is crucial for the simulation of the two phase flow problems. This rDG method truly signifies a giant leap towards development of higher-order CFD code for application of complex flow problems in nuclear engineering.

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Refereed Conference Papers

1. Yidong Xia, Hong Luo, Chuanjin Wang, and Robert Nourgalev, An implicit, reconstructed discontinuous Galerkin method for the unsteady compressible Navier-Stokes equations on 3D hybrid grids, AIAA-2014-3220, 7th AIAA Theoretical Fluid Mechanics Conference, Atlanta, GA, June16-20, 2014

2. Yidong Xia, Hong Luo, Chuanjin Wang, and Robert Nourgalev, Implicit Large Eddy Simulation of Turbulent Flows Using a Reconstructed Discontinuous Galerkin Method, AIAA-2014-0224, 52nd Aerospace Sciences Meeting, National Harbor, MD, Jan. 13-17, 2014.

3. Yidong Xia, Hong Luo, Seth C. Spiegel, Megan Frisbey, and Robert Nourgaliev, A Parallel, Implicit Reconstructed Discontinuous Galerkin Method for the Compressible Flows on 3D Arbitrary Grids, AIAA-2013-3062, 21st AIAA Computational Fluid Dynamics Conference, San Diego, CA, 24-27 June, 2013.

4. Yidong Xia, Megan Frisbey, and Hong Luo, A Reconstructed Discontinuous Galerkin Method Based on a Hierarchical WENO Reconstruction for Computing Shock Waves on Hybrid Grids, AIAA-2013-3063, 21st AIAA Computational Fluid Dynamics Conference, San Diego, CA, 24-27 June, 2013.

5. Luo, H., Xia Y, Frisbey, F., and Nourgaliev, R. A WENO Reconstruction-Based Discontinuous Galerkin Method for Compressible Flows on Hybrid Grids, AIAA-2013-0516, 51st AIAA Aerospace Sciences Meeting, Grapevine, Texas, Jan. 7-10, 2013.

6. Xia Y, Luo, H., and Nourgaliev, R. An Implicit Reconstructed Discontinuous Galerkin Method Based on Automatic Differentiation for the Navier-Stokes Equations on Tetrahedron Grids, AIAA-2013-0687, 51st AIAA Aerospace Sciences Meeting, Grapevine, Texas, Jan. 7-10, 2013.

7. Xia Y, Luo H., and Nourgaliev, R., An Implicit Reconstructed Discontinuous Galerkin Method on Tetrahedral Grids, *Seventh International Conference on Computational Fluid Dynamics*, Hawaii, USA, July 9-13, 2012.

8. Luo, H., Xia Y., and Nourgaliev, R., A Hermit WENO Reconstruction-Based Discontinuous Galerkin Method for Compressible Flows on Tetrahedral Grids; *Seventh International Conference on Computational Fluid Dynamics*, Hawaii, USA, July 9-13, 2012.

9. Luo, H., Xia Y, Nourgaliev, R. A Hierarchical Hermit WENO Reconstruction-Based Discontinuous Galerkin Method for the Compressible Flows on Tetrahedral Grids, AIAA-2012-2838, 42nd AIAA Fluid Dynamics Conference and Exhibit, 25-28 June 2012, New Orleans, LA.

10. Xia Y, Luo H., and Nourgaliev, R., An Implicit Method for a Reconstructed Discontinuous Galerkin Method on Tetrahedral Grids, AIAA-2012-2834, 42nd AIAA Fluid Dynamics Conference and Exhibit, 25-28 June 2012, New Orleans, LA.

11. Luo, H., Li, SJ, Xia Y, Nourgaliev, R., and Cai C., A Hermit WENO Reconstruction-based Discontinuous Galerkin Method for the Euler Equations on Tetrahedral Grids, AIAA-2012-0461, 50th AIAA Aerospace Sciences Meeting including the New Horizons Forum and Aerospace Exposition, Nashville, Tennessee, Jan. 9-12, 2012.

Note:

Appendices 1 and 2 have been removed, as the example journal articles were copyrighted.