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Extended Summary

1. Motivation

Multidimensional, higher-order (2nd and higher) numerical methods have come to the forefront in recent years due to significant advances of computer technology and numerical algorithms, and have shown great potential as viable design tools for realistic applications. To achieve this goal, *implicit high-order* accurate coupling of the multiphysics simulations is a critical component. One of the issues that arise from multiphysics simulations is the necessity to resolve multiple time scales. For example, the dynamical time scales of neutron kinetics, fluid dynamics and heat conduction significantly differ (typically $>10^{10}$ magnitude), with the dominant (fastest) physical mode also changing during the course of transient [Pope and Mousseau, 2007]. This leads to the severe time step restriction for stability in traditional multiphysics (i.e. operator split, semi-implicit discretization) simulations. The lower order methods suffer from an undesirable numerical dissipation. Thus implicit, higher order accurate scheme is necessary to perform seamlessly-coupled multiphysics simulations that can be used to analyze the "what-if" regulatory accident scenarios, or to design and optimize engineering systems.

The high-temperature gas-cooled nuclear reactor concepts will have fundamental differences from the conventional light water reactors (LWR), and the nominal operational conditions are expected to be at higher thermal loadings. Under high heat flux conditions, density variations in the coolant become significant. In these regimes, the "traditional approaches" (i.e. incompressible flow simulations with the Boussinesq approximation for buoyancy) may cease to be valid. An example of this effect was reported by the work of Darbandi and Hosseinizadeh [Darbandi and Hosseinzadeh, 2007], where greater than 10% difference in the local Nusselt number has been observed. Therefore, development of more appropriate numerical methods based on the fully compressible formulation is necessary to eliminate deficiencies of the "traditional approaches".

In this work, the Discontinuous Galerkin (DG) method for compressible fluid flow is incorporated into the Jacobian-Free Newton-Krylov (JFNK) framework [Knoll and Keys, 2003]. Advantages of combining the DG with the JFNK are two-fold: *a)* enabling *robust and efficient high-order-accurate modeling of all-speed flows on unstructured grids*, thus opening the possibility for high-fidelity simulation of nuclear-power-industry-relevant flows; and *b)* the ability to *tightly, robustly and high-order-accurately couple with other relevant physics* (neutronics, thermal-structural response of solids, etc.). In the present study, we focus on the physics-based preconditioning (PBP) of the Krylov method (GMRES), used as the linear solver in our implicit time discretization scheme; exploiting the compactness of the spatial discretization of the DG family.

2. JFNK-DG framework

The *Discontinuous Galerkin (DG) method* can be thought as a higher order extension of the *finite volume method (FVM)* that utilizes the Galerkin finite element framework. The FVM has long been a popular choice for solving the hyperbolic conservation laws. Its (relatively) simple formulation can be easily extended to multi-dimension; however, the higher order accurate FVM requires wide stencils, which may become very cumbersome for the multidimensional unstructured grids as well as the treatment of the boundary conditions, parallelization and adaptive mesh refinement [Cockburn and Shu, 1998]. The DG, on the other hand, makes use of the orthogonal polynomials (such as the Legendre polynomial), to construct the higher-order accurate solution within an element, which alleviates above-mentioned difficulties of the FVM. Thus, an arbitrary higher-order scheme can be derived by utilizing only the von Neumann neighborhood elements. For simplicity of the presentation, we consider the one-dimensional[1] scalar hyperbolic conservation law of the form:

$$\frac{\partial U(x,t)}{\partial t} + \frac{\partial F(x,t)}{\partial x} = 0 \tag{1}$$

where, $U(x,t)$ and $F(x,t)$ are the vectors of conservative variables and the fluxes, respectively. The weak form of the DG method can be obtained multiplying Eq.(1) on the l-th order discontinuous basis function $w_l(x)$ and integrating over the element:

$$\int_{x_{i-1/2}}^{x_{i+1/2}} w_l(x) \left[\frac{\partial U(x,t)}{\partial t} + \frac{\partial F(x,t)}{\partial x} \right] =$$

$$\int_{x_{i-1/2}}^{x_{i+1/2}} w_l(x) \frac{\partial U(x,t)}{\partial t} + w_l(x)\hat{F}(x,t)\Big|_{x_{i+1/2}} - w_l(x)\hat{F}(x,t)\Big|_{x_{i-1/2}} - \int_{x_{i-1/2}}^{x_{i+1/2}} F(x,t)\frac{\partial w_l(x)}{\partial x} = 0 \tag{2}$$

where $\hat{F}$ is the numerical flux. The hierarchical (orthogonal) basis functions are commonly used in order to produce the diagonal mass matrix. For example, if the (scaled) Legendre polynomial $P_l(x)$ is chosen, then Eq. (2) becomes:

$$\frac{dU_l(t)}{dt} + \frac{2l+1}{\Delta x}\left[P_l(x)\hat{F}(x,t)\Big|_{x_{i+1/2}} - P_l(x)\hat{F}(x,t)\Big|_{x_{i-1/2}} - \int_{x_{i-1/2}}^{x_{i+1/2}} F(x,t)\frac{\partial P_l(x)}{\partial x} \right] = 0 \tag{3}$$

Eq.(3) is integrated over the time interval $[t_n, t_{n+1}]$ to yield discretized nonlinear residual functions:

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[1] Extension to 3D is straightforward [Cockburn et al., 1990].

$$\text{Res}(U^{n+1}) = U_l^{n+1} - U_l^n + \frac{(2l+1)\Delta t}{\Delta x}\left[P_l(x)\hat{F}^{n+\alpha}(x,t)\Big|_{x_{i+1/2}} - P_l(x)\hat{F}^{n+\alpha}(x,t)\Big|_{x_{i-1/2}} - \int_{x_{i-1/2}}^{x_{i+1/2}} F^{n+\alpha}(x,t)\frac{\partial P_l(x)}{\partial x} \right] \quad (4)$$

The Newton-Krylov (NK) method is a synergetic combination of the Newton method and Krylov Subspace–Iteration methods. At the each step of the Newton iteration, we must solve the linear system of equations of the form:

$$J^k \delta U^k = -\text{Res}(U^k) \quad (5)$$

where J^k is the Jacobian matrix of the kth Newton step, using a Krylov method (commonly, GMRES), and the solution is updated as

$$U^{k+1} = U^k + \delta U^k \quad (6)$$

The JFNK takes advantage of the fact that the Krylov methods involve only simple matrix-vector product operations and do not require computation of the Jacobian matrix directly. The matrix-vector product Jv can be approximated by the forward finite difference [Brown and Saad, 1990]:

$$Jv \approx \frac{\text{Res}(U+\varepsilon v) - \text{Res}(U)}{\varepsilon} \quad (7)$$

Thus, only nonlinear residual function (4) evaluations are required in order to solve the discrete system.

The Newton method allows to employ fully implicit time discretization schemes (i.e., 2nd-order Crank-Nicholson and high-order Runge-Kutta [Kanevsky et al., 2007]); therefore the stability issues are avoided.

3. Physics-based preconditioning

The key to success of the JFNK is an efficient preconditioning of the GMRES. The right-preconditioned system can be expressed as

$$J^k M^{-1}(M\delta U^k) = -\text{Res}(U^k) \quad (8)$$

where M is the preconditioning matrix. The matrix-vector operation for the above system can be approximated by

$$JM^{-1}v \approx \frac{\text{Res}(U+\varepsilon M^{-1}v) - \text{Res}(U)}{\varepsilon} \quad (9)$$

Physics-based preconditioning (PBP) techniques are widely used for solving the non-linear system [Knoll et al., 2005], [Mousseau et al., 2000], [Mousseau and Knoll, 2004], [Reisner et al., 2005]. The preconditioning step can be thought as the equivalent procedure to approximating the new time step solution by a simpler (and less expensive) method. Here, a classical operator-splitting, or semi-implicit discretization can be utilized as the PBP for the JFNK. An effective selection of the PBP can substantially reduce the number of Krylov vectors, which consequently reduces both the memory requirement and computational effort. Here, we use the *Implicit Continuous fluid Eulerian (ICE)* method [Harlow and Amsden, 1971] as PBP of our JFNK-DG.

4. Preliminary results

In this section, we utilize our JFNK-DG framework to solve one and two-dimensional compressible Euler equations. In the first example, we demonstrate the high-order convergence rate of the JFNK-DGM using the method of manufactured solutions [Knupp et al., 2003]. The following solution is manufactured:

$$\rho(x,t) = \rho_{\min} + (\rho_{\max} - \rho_{\min})\operatorname{sech}\left(\frac{x - \omega t}{\delta}\right)$$

$$E(x,t) = E_{\min} + (E_{\max} - E_{\min})\tanh\left(\frac{x - \omega t}{\delta}\right) \qquad (10)$$

$$m(x,t) = \left[\rho_{\min} + (\rho_{\max} - \rho_{\min})\operatorname{sech}\left(\frac{x - \omega t}{\delta}\right)\right]\left[U_{\min} + (U_{\max} - U_{\min})\operatorname{sech}\left(\frac{x - \omega t}{\delta}\right)\right]$$

Figure 1(a) shows the result of the convergence tests using the 1st (DG-0) to 4th (DG-4) order DGMs with Crank-Nicholson time discretization. Consistency of the computed and theoretical convergence rates is evident for all the cases. Note that in the x-axis of the Figure 1(a) we show the total number of degrees of freedom (DOFs), and it clearly shows that the higher-order methods can obtain much more accurate result with fewer DOFs. Figure 1(b) shows the eigenvalues of the Jacobian matrices for DGMs of different order. Since the Jacobian is non-symmetric, the eigenvalues are in general complex. The higher-order discretization results in a wider spread of eigenvalues, which indicates poor conditioning of the Jacobian. Setting the stability and dynamic CFL numbers to be 25 and 1, respectively, the condition numbers (estimated as ratios of the absolute values for maximum and minimum singular values) are computed to be 650, 2476, 2547 and 4016 for DG-0, DG-1, DG-2 and DG-3, correspondingly. Figures 1(c)(d) demonstrate clustering of eigenvalues by applying the *ICE-* and the *Block-Diagonal* physics-based preconditionings, for DG-1 and DG-2. As expected, both the block-diagonal and the ICE preconditionings result in significant improvement of the conditioning of the Jacobian matrix. Moreover, the ICE preconditioning collapses all eigenvalues to the real axis, which implies that the complex components of the eigenvalues are related to acoustic waves.
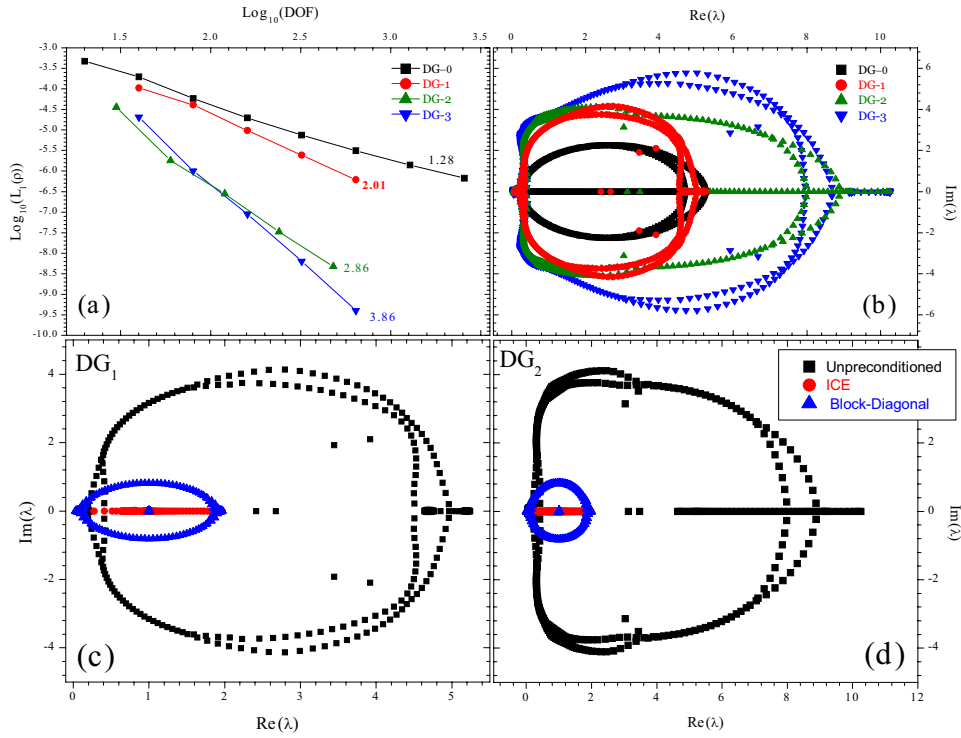
Figure 1. (a) Demonstration of the high-order convergence of the DGM; (b) GMRES-Jacobian's eigenvalue structures for DGMs with different spatial discretization order; (c)(d) Effect of the Physics-Based preconditioning on eigenvalues of the Jacobian matrices of the linear and quadratic DGMs (CFL$_{stb/dyn}$ = 25/1; M=0.04).

As a second example, we solved the two dimensional "Traveling wave" problem. The velocity and pressure profiles are given by

$$
\begin{aligned}
u(x,y,t) &= 1 + 2\cos(2\pi(x-t))\sin(2\pi(y-t)) \\
v(x,y,t) &= 1 - 2\sin(2\pi(x-t))\cos(2\pi(y-t)) \\
P(x,y,t) &= P_0 - (\cos(4\pi(x-t)) + \cos(4\pi(y-t)))
\end{aligned}
\tag{11}
$$

P_0 and the constant initial density are set to 70.25 and 0.1, respectively, corresponding to Mach number of 0.1. Figure 2(a) shows the convergence rate for total energy using the linear and quadratic DGM. Again, the consistent convergence rates are observed. Figure 2 (b),(c),and (d) show dynamics of the velocity and vorticity fields for times 0.0, 0.2 and 0.4, respectively.
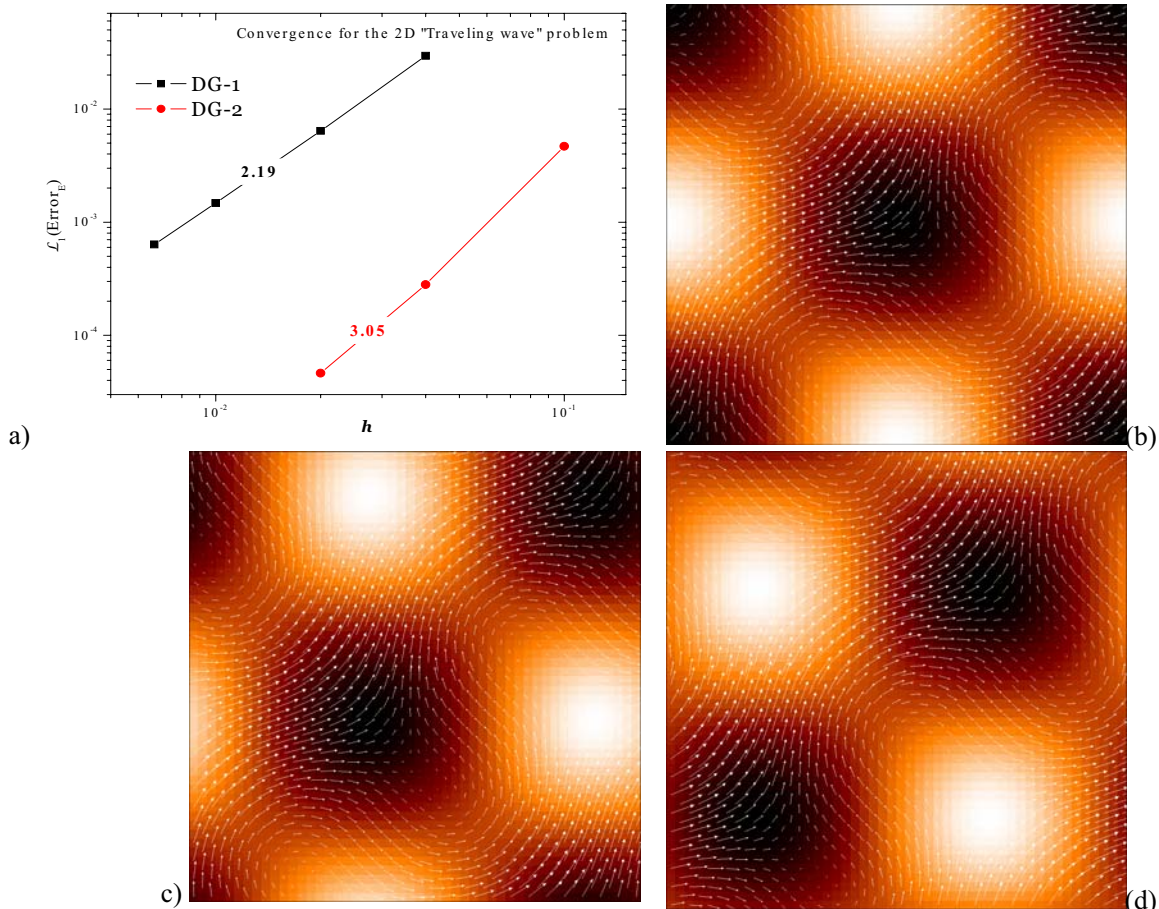
Figure 2. "Traveling wave" problem: (a) convergence plot for DG-1 and DG-2; b), c), d) vorticity and velocity fields at t = 0.0, 0.2 and 0.4.

5. Summary

In this work, we have developed a fully implicit higher-order discontinuous Galerkin method (JFNK-DG) with demonstration of the high-order convergence and the efficiency of the physics-based preconditioning. The preliminary results for test-problems show that the consistent convergence rates are achieved, and the effective clustering of the eigenvalues due to Physics-based preconditionings (ICE and Block-Diagonal) produces a significant acceleration of the GMRES convergence. Work is ongoing to test our all-speed DG-JFNK methodology on more complex problems, such as high-heat flux natural convection, relevant to the new generation of nuclear reactors. This will be included in the full paper.

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