MODAL DISCONTINUOUS GALERKIN METHOD FOR SHOCK WAVE STRUCTURES

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Abstract: The discontinuous Galerkin (DG) finite element method has been popular as a numerical technique for solving the conservation laws. In the present study, in order to investigate the shock wave structures in highly thermal nonequilibrium, an explicit modal cell-based DG scheme is developed for solving the conservation laws in conjunction with nonlinear coupled constitutive relations (NCCR). Convergent iterative methods for solving algebraic constitutive relations are also implemented in the DG scheme. It is shown that the new scheme works well for all Mach numbers, for example, $Ma = 15$.

Key words: discontinuous Galerkin (DG); shock structure; nonlinear coupled constitutive relations

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INTRODUCTION

The finite volume method has been commonly used in computational fluid dynamics (CFD). However, the accuracy of the finite volume method is limited to the second order in most cases. The accuracy can be improved by high resolution schemes that usually involve high computational effort. The discontinuous Galerkin(DG) method is regarded as an alternative approach for CFD based on the finite volume framework. The DG finite element method has been popular as a numerical technique for solving the conservation laws[1-6] and has been successfully applied to a variety of problems, such as fluid dynamics, acoustics and magnetohydrodynamics.

Depending on the basis function applied to the scheme, the DG scheme may be divided into modal[1-4] or nodal[5-6]. It has also been developed for the Burgers equation[1,2,4], which is a simplified model equation of the hyperbolic conservation laws, and the compressible Navier-Stokes-Fourier (NSF) equations[4-6]. This method combines key features of the finite element and finite volume methods. In the DG method, field variables are considered discontinuous across elemental boundary, which circumvents the need of assembling computationally demanding global matrix and leads to a less in-core memory required in computation. The DG method easily handles complicated geometry and boundary conditions by utilizing unstructured grids and multi-grids. Moreover, the DG method can be parallelized and thus suits well for parallel computer platforms. The DG method has several useful mathematical properties with respect to conservation, stability, and convergence[3]. These advantages are the motivations to select the DG method for numerical solutions of the conservation laws in the present work. The aim of the present study is to develop an explicit modal DG scheme for the conservation laws in conjunction with nonlinear coupled constitutive relation (NCCR) models in order to investigate the structure of shock waves in thermal

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nonequilibrium. The theoretical breakthrough of the proposed scheme is that a DG scheme for rarefied gases is developed by introducing an auxiliary unknown of the stress and by solving the non-Newtonian constitution relation in algebraic way.

1 DG SCHEME FOR NSF EQUATIONS

Non-dimensional vector form of the NSF equations can be expressed as[7-8]

$$\partial_t \boldsymbol{U} + \nabla \boldsymbol{F}_{\text{inv}}(\boldsymbol{U}) + \nabla \boldsymbol{F}_{\text{vis}}(\boldsymbol{U}, \nabla \boldsymbol{U}) = 0$$

$$\boldsymbol{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho E \end{pmatrix}, \quad \boldsymbol{F}_{\text{inv}} = \begin{pmatrix} \rho u \\ \rho u^2 + \dfrac{1}{N_\delta Re} p \\ \rho E u + \dfrac{1}{N_\delta Re} p u \end{pmatrix}$$

$$\boldsymbol{F}_{\text{vis}} = \frac{1}{Re} \begin{pmatrix} 0 \\ \Pi \\ \Pi u + \dfrac{1}{EcPr} Q \end{pmatrix}$$

where one-dimensional variables are defined: ρ is the mass density, u the fluid velocity in x-direction, p the pressure, E the total energy density, Π the shear stress in x-direction, and Q the heat flux. If the spatial coordinate is reduced by the mean free path λ, the dimensionless parameters are $N_\delta = \sqrt{2\gamma/\pi}\, Ma$, Reynolds number $Re = \sqrt{\gamma\pi/2}\, Ma$, and $Ec = (\gamma - 1) Ma^2$[7]. The parameter γ is the specific heat ratio of gas, Pr the Prandtl number, and Ma the reference Mach number. For classical NSF model, the shear stress Π and the heat flux Q are computed as follows: $\Pi = -(4/3)\, \mu(\partial u/\partial x)$, $Q = -K(\partial T/\partial x)$, where K is the thermal conductivity $K = T^s$, T the gas temperature and s a constant, $T = p/\rho$, and μ the viscosity, $\mu = T^s$. The relation, $p = \gamma Ma^2(\gamma - 1)(\rho E - 0.5\rho u^2)$, is also used in the formulation.

The mixed DG formulation proposed in Ref. [4] is employed in spatial discretization of the NSF equations. This formulation will solve the second-order derivatives in viscous terms by adding auxiliary unknown $\boldsymbol{S}$, because the second-order derivative cannot be accommodated directly in a weak formulation using a discontinuous function space. In this work, $\boldsymbol{S}$ is chosen to be derivatives of the conserved variables $\boldsymbol{U}$, setting $\boldsymbol{S}(\boldsymbol{U}) = T^s \nabla \boldsymbol{U}$. Then a coupled system for $\boldsymbol{S}$ and $\boldsymbol{U}$ can be derived as

$$\begin{cases} \boldsymbol{S} - T^s \nabla \boldsymbol{U} = 0 \\ \partial_t \boldsymbol{U} + \nabla \boldsymbol{F}_{\text{inv}}(\boldsymbol{U}) + \nabla \boldsymbol{F}_{\text{vis}}(\boldsymbol{U}, \boldsymbol{S}) = 0 \end{cases}$$

The spatial derivatives of primitive variables such as u_x are then computed by expanding the derivatives of the conservable variables, for example $T^s u_x = (1/\rho)(T^s(\rho u)_x - T^s \rho_x u)$. Constitutive relations for two models are expressed as follows: For the NSF model $(\Pi, Q)_{\text{NSF}} = f_{\text{linear}}(\boldsymbol{S}(\boldsymbol{U}))$, and for the NCCR model $(\Pi, Q)_{\text{NCCR}} = f_{\text{non-linear}}(\boldsymbol{S}(\boldsymbol{U}), p, T)$. In order to discrete the coupled system (1), the numerical solutions of $\boldsymbol{U}$ and $\boldsymbol{S}$ are approximated by $\boldsymbol{U}_{\text{h}}$ and $\boldsymbol{S}_{\text{h}}$, respectively, shown as

$$\boldsymbol{U}_{\text{h}}(x,t) = \sum_{i=0}^{k} U_j^i(t)\, \varphi^i(x)$$

$$\boldsymbol{S}_{\text{h}}(x,t) = \sum_{i=0}^{k} S_j^i(t)\, \varphi^i(x)$$

where φ is the basis function. Computational domain contains N elements (cells) that are equally spaced. In this study, orthogonal Legendre basis function is adopted for the function φ. The coupled system (1) is multiplied with the basis function φ, and then integrated by parts for derivative terms over element I, so the weak formulation of the coupled system can be derived to find $\boldsymbol{U}_{\text{h}}$ and $\boldsymbol{S}_{\text{h}}$

$$\begin{cases} \displaystyle\int_I \boldsymbol{S}\varphi \,\mathrm{d}x + \int_I T^s \nabla \varphi\, \boldsymbol{U}\mathrm{d}x - \int_{\partial I} T^s \varphi\, \boldsymbol{U}\mathrm{d}x = 0 \\ \displaystyle\frac{\partial}{\partial t}\int_I \boldsymbol{U}\varphi \,\mathrm{d}x - \int_I \nabla \varphi\, \boldsymbol{F}_{\text{inv}}\mathrm{d}x + \int_{\partial I} \varphi\, \boldsymbol{F}_{\text{inv}}\mathrm{d}x - \\ \qquad \displaystyle\int_I \nabla \varphi\, \boldsymbol{F}_{\text{vis}}\mathrm{d}x + \int_{\partial I} \varphi\, \boldsymbol{F}_{\text{vis}}\mathrm{d}x = 0 \end{cases}$$

where ∂I denotes the boundaries of the element I. The equations of auxiliary unknowns are resolved first to compute the derivatives of conservative variables, in which the variable $T(x,t)$ is updated at each time step. The boundary integrals of each element are replaced by a numerical flux function $\boldsymbol{h}$ as follows.

$$\boldsymbol{h}_{\text{inv}}(\boldsymbol{U}^-, \boldsymbol{U}^+, \boldsymbol{n}) = 0.5[\boldsymbol{F}_{\text{inv}}(\boldsymbol{U}^-) + \boldsymbol{F}_{\text{inv}}(\boldsymbol{U}^+) - C(\boldsymbol{U}^+ - \boldsymbol{U}^-)]$$

where $C = \max(|u^-| + a^-/Ma, |u^+| + a^+/Ma)$.

For inviscid terms, the local Lax-Friedrichs

(LxF) flux, $\boldsymbol{h}_{\text{inv}}$, is applied. The Mach number a/Ma, instead of the speed of sound $a(=T^{1/2})$, appears in formulation of the coefficient C from the characteristic speed in dimensionless form. The central flux is applied to the remaining boundary integrals

$$\boldsymbol{h}_{\text{vis}}(\boldsymbol{U}^-,\boldsymbol{S}^-,\boldsymbol{U}^+,\boldsymbol{S}^+;\boldsymbol{n}) \cong$$
$$0.5[\boldsymbol{F}_{\text{vis}}(\boldsymbol{U}^-,\boldsymbol{S}^-)+\boldsymbol{F}_{\text{vis}}(\boldsymbol{U}^+,\boldsymbol{S}^+)]$$
$$\boldsymbol{h}_{\text{aux}}(\boldsymbol{U}^-,\boldsymbol{U}^+;\boldsymbol{n}) \cong$$
$$0.5[T^{s-}\boldsymbol{U}^-+T^{s+}\boldsymbol{U}^+]$$

The volume integrals within the element I are resolved by the Gaussian quadrature with the $(2k+1)$ Gaussian points[1]. The slope limiter and shock detection proposed in Ref. [2] are adopted for this DG scheme. At the upstream boundary, all Euler characteristics are incoming for supersonic flow and therefore their initial values can be pre-determined. Otherwise, at the subsonic downstream boundary, only one characteristic is incoming and thus one physical condition must be imposed[8]. In the present study, the downstream velocity specified by the Rankine-Hugoniot condition is retained to maintain the shock stationary. Other variables are extrapolated by using the interior adjacent values. Finally, the coupled system (1) can be written in semi-discrete form $\boldsymbol{L}(\partial\boldsymbol{U}/\partial t)=\boldsymbol{R}(\boldsymbol{U})$, which is resolved by the Runge-Kutta time integration. The time step Δt is computed as[6]

$$\Delta t=\frac{1}{(k+1)^2}\frac{\Delta x\text{CFL}}{|u|+a/Ma+\mu/\Delta x}$$

where CFL is Courrant-Friedrichs-Lewycondition (CFL$\leqslant$1).

2 BURGERS EQUATION

An explicit modal DG scheme is first developed for the Burgers equation

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}=\mu\frac{\partial^2 u}{\partial^2 x}$$

with exact solution

$$u(x,t)=u_{\text{r}}+\frac{(u_{\text{l}}-u_{\text{r}})}{1+\exp((u_{\text{l}}-u_{\text{r}})(x-st))/(2\mu)}$$
$$s=\frac{u_{\text{l}}+u_{\text{r}}}{2}$$

where u_{l} and u_{r} are the fixed boundary values. In this model equation, the auxiliary unknown $S=\Pi=-\mu\partial u/\partial x$ only is set to resolve second-order derivative, and μ is assumed constant. The variables u and S are numerically approximated as $\boldsymbol{U}_{\text{h}}$ and $\boldsymbol{S}_{\text{h}}$. The LxF flux is selected for solving the boundary integral of nonlinear term $(u^2/2)$ with the coefficient $C=\max(u^-,u^+)$. The central flux is applied for the remaining boundary integral to find $\boldsymbol{U}_{\text{h}}$ and $\boldsymbol{S}_{\text{h}}$ in weak formulation. The limiter proposed in Ref. [2] and orthogonal Legendre basis functions are used for calculations. The linear element and first-order Runge-Kutta time integration are used to resolve $\boldsymbol{L}(\partial u/\partial t)=\boldsymbol{R}(u)$. Elements are equally spaced in computational domain. The NCCR model for the Burgers equation is also implemented into the DG scheme via an iterative method. The values Π at elemental interfaces are obtained via the iterative method. For positive and negative $\hat{\Pi}$

$$\hat{\Pi}_{n+1}=\text{arcsinh}(\hat{\Pi}_n(1+\hat{\Pi}_n))$$
$$\hat{\Pi}_{n+1}=\frac{\hat{\Pi}_n}{q(\hat{\Pi}_n)-\hat{\Pi}_n},\quad q(\hat{\Pi}_n)=\frac{\sinh(\hat{\Pi}_n)}{\hat{\Pi}_n}$$

where the caret "$\hat{}$" over a symbol represents a dimensionless quantity in the ratio of the stress to the pressure.

Figs. 1—2 show computational results of the Burgers equation with $N=200$, $\Delta x=0.04$, CFL=0.25, and $\mu=0.1$. In Fig. 1, the DG NS results give good agreement with exact analytic solution, and show the effect of the NCCR model in computational results. Fig. 2 presents the normal stress Π between the NS and NCCR models.

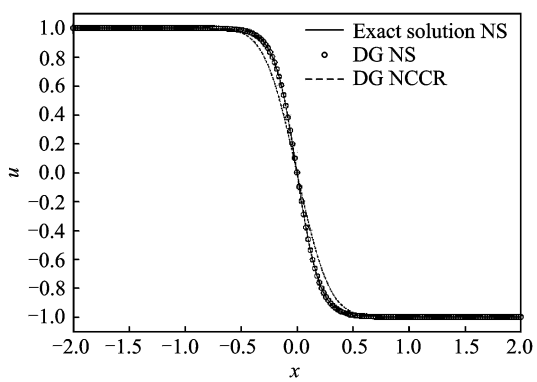

Fig. 1 Shock structure profiles of velocity with NS and NCCR models

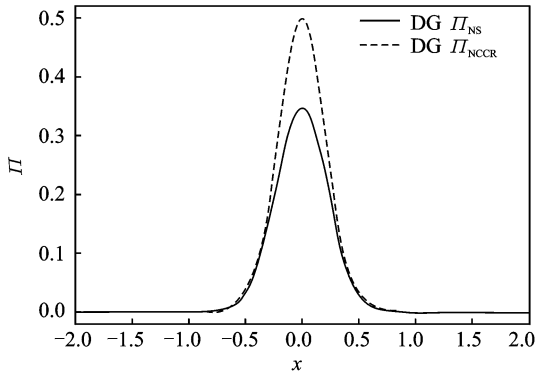

Fig. 2 Values of shear stress Π with NS and NCCR models

3 EXTENSION TO NSF AND CONSERVATION LAWS WITH NCCR

The NCCR model for the conservation laws developed on the basis of the moment method proposed in Refs. [7-8] is implemented into the DG scheme. Initial shear stress and heat flux in the NCCR model are computed by the values Π and Q at elemental interfaces from the NSF model

$$\hat{\Pi}_0 = \frac{N_\delta}{p}\Pi = \frac{N_\delta}{p} f_{\text{linear}}(S(U))$$

$$\hat{Q}_0 = \frac{N_\delta}{p}\frac{Q}{\sqrt{T/(2\varepsilon)}} = \frac{N_\delta}{p}\frac{f_{\text{linear}}(S(U))}{\sqrt{T/(2\varepsilon)}}$$

where $\varepsilon \equiv \dfrac{1}{PrEcT/\Delta T}$, $\hat{R}^2 = 1.5\hat{\Pi}^2 + \hat{Q}^2$.

The NCCR model is expressed as

$$\hat{\Pi} q(c\hat{R}) = (\hat{\Pi} + 1)\hat{\Pi}_0$$

$$\hat{Q} q(c\hat{R}) = (\hat{\Pi} + 1)\hat{Q}_0$$

$$\hat{R}_{n+1} = \frac{1}{c}\operatorname{arcsinh}[c(\hat{\Pi}_n + 1)\hat{R}_0]$$

For positive and negative $\hat{\Pi}$ and $\hat{Q}$, we have

$$\frac{\hat{Q}_{n+1}}{\hat{\Pi}_{n+1}} = \frac{\hat{Q}_n}{\hat{\Pi}_n} = \frac{\hat{Q}_0}{\hat{\Pi}_0}, \quad \hat{\Pi}_{n+1} = \frac{\hat{\Pi}_0}{q(c\hat{R}_n) - \hat{\Pi}_0}$$

$$\hat{Q}_{n+1} = \frac{(\hat{\Pi}_n + 1)\hat{Q}_0}{q(c\hat{Q}_n)}$$

In these expressions, $\hat{\Pi}_1$ and $\hat{Q}_1$ are given by the equations

$$\hat{\Pi}_1 = \frac{\operatorname{arcsinh}(c\hat{R}_0)\hat{\Pi}_0}{c\hat{R}_0}, \quad \hat{Q}_1 = \frac{\operatorname{arcsinh}(c\hat{R}_0)\hat{Q}_0}{c\hat{R}_0}$$

Solution of iterative method for NCCR equations is considered converged when $|\hat{R}_{n+1} - \hat{R}_n| \leqslant 10^{-5}$. The converged values at the iteration $(n+1)$ are then embedded back into the DG scheme via the following calculations

$$\Pi = \frac{p}{N_\delta}\hat{\Pi}_{n+1}, \quad Q = \frac{p\sqrt{T/(2\varepsilon)}}{N_\delta}\hat{Q}_{n+1}$$

4 COMPUTATIONAL RESULTS

Upstream boundary values are set with $p = u = \rho = T = 1$ at initial condition, and are maintained in whole computed procedure. The Rankine-Hugoniot conditions are used to compute downstream boundary values. A computational domain 60λ is used in all cases, covering the entire shock structure. The Maxwellian monatomic gas with $s = 1.0$, $c = 1.0138$, $Pr = 0.75$, CFL $= 0.5$, and $\Delta x = 0.2$ are used for all simulations. Steady state solution is reached when the RMS norm of the density is below 10^{-9}. The linear element and first Runge-Kutta method are selected for all simulations. Computational results are normalized based on quantity such as in case of the density $\bar{\rho} = (\rho - \rho_{\text{upstream}})/(\rho_{\text{downstream}} - \rho_{\text{upstream}})$.

The simulation results of the cases $Ma = 5$ and 8 are presented in Figs. 3 – 5. For the NSF model, the results agree well with the exact ana-

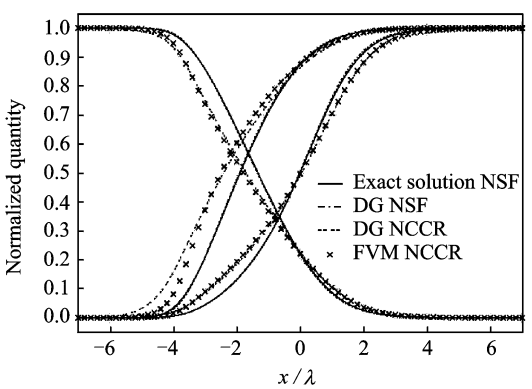

Fig. 3 Shock structure profiles at $Ma = 5$ with NSF and NCCR models

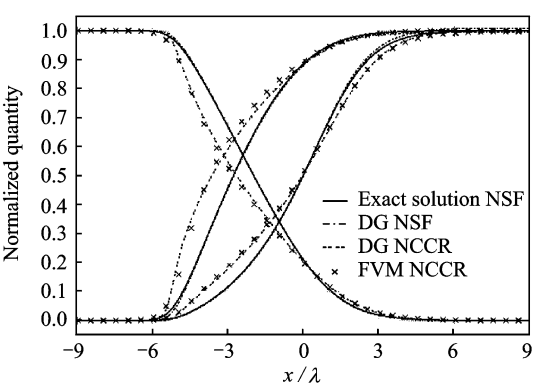

Fig. 4 Shock structure profiles at $Ma = 8$ with NSF and NCCR models

lytic solution. The difference between numerical results of the NSF and NCCR models is shown in Figs. 3—4, and the DG NCCR results give good agreement to the finite volume method (FVM) NCCR results in a previous work[7-8]. Fig. 5 shows numerical results of heat fluxes and shear stresses between the NSF and NCCR models. Fig. 6 presents the normalized density profiles at various Mach numbers with the NCCR model.

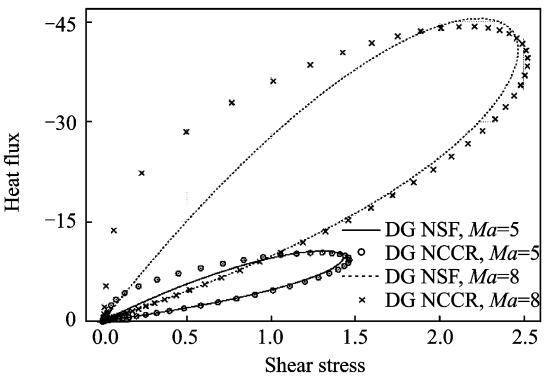

Fig. 5 Computational heat flux and shear stress at $Ma=5$ and 8 with NSF and NCCR models

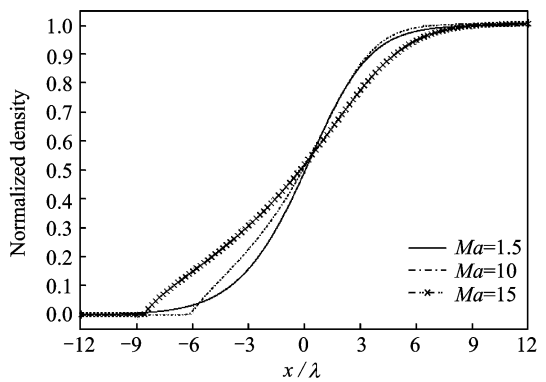

Fig. 6 Normalized density profiles at various Mach numbers with NCCR model

5 CONCLUSION

An explicit modal DG scheme has been developed for simulating the shock wave structures. The mixed DG scheme based on the idea of adding auxiliary unknowns is employed in spatial discretization of the Burgers, NSF and NCCR equations. The proposed scheme is limited to the one dimensional problem for simplicity, but it can be readily extended to the more complicated multi-dimensional situations.

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