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Discontinuous Galerkin finite element methods with shock-capturing for nonlinear convection dominated models

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ABSTRACT

In this paper, convection-diffusion-reaction models with nonlinear reaction mechanisms, which are typical problems of chemical systems, are studied by using the upwind symmetric interior penalty Galerkin (SIPG) method. The local spurious oscillations are minimized by adding an artificial viscosity diffusion term to the original equations. A discontinuity sensor is used to detect the layers where unphysical oscillations occur. Finally, the proposed method is tested on various single- and multi-component problems.

1. Introduction

Unsteady nonlinear convection diffusion reaction problems are often studied in many engineering problems such as fluid dynamics problems in the presence of body forces, electrochemical interaction flows and chemically reactive flows (Helmig, 1997; Warnatz, Maas, & Dibble, 2009). In this paper, we consider the following nonlinear system of coupled diffusion-convection-reaction equations as a model problem for our investigations:

$$\partial_t u_i - \epsilon_i \Delta u_i + \beta_i \cdot \nabla u_i + \alpha_i u_i + r_i(\mathbf{u}) = f_i \quad \text{in} \quad \Omega_i, \tag{1.1a}$$

$$u_i = g_i^D \quad \text{on} \quad \Gamma_i^D, \tag{1.1b}$$

$$\epsilon \frac{\partial u_i}{\partial n} = g_i^N \quad \text{on} \quad \Gamma_i^N, \tag{1.1c}$$

$$u_i(\cdot, t_0) = u_i^0 \quad \text{in} \quad \Omega_i \tag{1.1d}$$

for $i = 1, \cdots, m$. Here, $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$ with $\mathbf{u} = (u_1, \cdots, u_m)^T$ denotes the vector of unknowns where Ω_i is a bounded, convex domain in $\mathbb{R}^2$ with boundary $\Gamma_i = \overline{\Gamma_i^D \cup \Gamma_i^N}$, $\Gamma_i^D \cap \Gamma_i^N = \emptyset$ and $t \in (0, T]$ for some $T > 0$. The source functions and boundary conditions, i.e., Dirichlet boundary condition (1.1b) and Neumann boundary condition (1.1c), are defined such as $f_i \in L^2(0, T; L^2(\Omega))$, $g_i^D \in L^2(0, T; H^{3/2}(\Gamma_i^D))$ and $g_i^N \in L^2(0, T; H^{1/2}(\Gamma_i^N))$, respectively. Moreover, the diffusion coefficients ϵ_i are small positive numbers such that $0 < \epsilon_i \ll 1$, $\alpha_i \in L^\infty(\Omega)$ are the reaction coefficients and $\beta_i \in L^\infty(0, T; (W^{1,\infty}(\Omega))^2)$ are the velocity fields (see Adams, 1975 for details). The initial conditions are also defined such that $u_i^0 \in H^1(\Omega)$. We have the following assumptions for the nonlinear reaction parameters $r_i(\mathbf{u})$:

$$r_i(\mathbf{u}) \in C^1(\mathbb{R}_0^+), \quad r_i(0) = 0, \quad r_i'(s) \geq 0 \quad \forall s \geq 0, \quad s \in \mathbb{R} \tag{1.2}$$

to satisfy the boundedness of $r_i'(u)$ in terms of above compact intervals of u. In large chemical systems the reaction terms $r_i(\mathbf{u})$ are assumed to be expressions which are products of some function of the concentrations of the chemical component and an exponential function of the temperature, called Arrhenius kinetics expression. As an example, the rate of conversion of u_1 and u_2 in the reaction

$$u_1 + u_2 \rightarrow \text{ products}$$

can be expressed as

$$k_0 u_1^a u_2^b e^{-(E/(\mathcal{R}T))},$$

where u_1 and u_2 are the concentrations of reactants, a and b are the orders of reaction, k_0 is the preexponential factor, E is the activation energy, $\mathcal{R}$ is the universal gas constant and T is the absolute reaction temperature.

Problems of the form (1.1) are strongly coupled such that inaccuracies in one unknown directly affect all other unknowns.

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Prediction of these unknowns is very important for the safe and economical operation of biochemical and chemical engineering processes. Typically, in (1.1) the size of the diffusion parameter ϵ is smaller compared to the size of velocity field β. Then, such a convection diffusion system is called convection-dominated.

For convection-dominated problems, especially in the presence of boundary and/or interior layers, the standard finite element methods may result in spurious oscillations causing in turn a severe loss of accuracy and stability. To avoid these oscillations, some stabilization techniques are applied such as the streamline upwind Galerkin method (SUPG) for single linear convection dominated equations (John & Schmeyer, 2008). Nevertheless, spurious localized oscillations, in particular in cross-wind direction, may still be present. Recently, higher order discontinuous Galerkin (DG) methods have become popular for convection dominated problems (Cockburn, 1998; Cockburn & Shu, 2001) since DG methods possess inherent stability at discontinuities. However, the stability condition sometimes is not satisfied by the DG space discretization itself at discontinuities and therefore, numerical solutions might suffer from unphysical oscillations near the discontinuities.

The most straightforward approach consists in avoiding the presence of sharp gradients with some non-linear projection operators, namely slope limiters, introduced in Cockburn, Hou, and Shu (1990); Cockburn and Shu (1989). Nevertheless, these limiters are not suitable for higher-order reconstructions, i.e., they drastically reduce the order of the approximation to linear or constant. Alternatively, a high-order reconstruction scheme, known as weighted non-oscillatory approach is used in Qiu and Shu (2005) as a slope limiter. However, it requires structured grids with a very wide stencil and therefore the compactness of DG may become less attractive. In addition, the extension to multiple dimensions is still an open issue for both slope limiters. Another classical way to avoid spurious oscillations is the artificial viscosity proposed in von Neumann and Richtmyer (1950), which is used with in many numerical techniques, i.e., finite difference methods (Lapidus, 1967), SUPG discretization (John & Schmeyer, 2008) for linear convection dominated problems and in Bause (2010); Bause and Schwegler (2012) for nonlinear convection dominated problems. Within the DG framework, it is mostly used for Euler equations (Persson & Peraire, 2006) as an alternative to slope limiters.

In this paper, we solve the convection dominated problems with various nonlinear reaction terms by using the upwind symmetric interior penalty Galerkin (SIPG) method. If necessary, we use a shock-capturing method proposed in Persson and Peraire (2006) based on the element size and the polynomial degree in order to prevent unphysical oscillations. It is used in conjunction with a discontinuity detection strategy.

The rest of the paper is organized as follows: In the next section we introduce the model problem as scalar convection dominated reaction-diffusion equation with nonlinear reaction term. Section 3 specifies the upwind SIPG discretization in space with shock-capturing and time discretization. In the final section we present numerical results that illustrate the performance of discontinuous Galerkin approximation with shock-capturing.

2. Scalar equation as model problem

We use the following scalar equation as a model problem

$$\partial_t u - \epsilon \Delta u + \boldsymbol{\beta} \cdot \nabla u + \alpha u + r(u) = f \qquad \text{in} \quad \Omega, \tag{2.1}$$

equipped with appropriate initial and boundary conditions, i.e., Dirichlet and Neumann boundary conditions, to make the notation easier for the readers. Let us first consider the weak formulation of the state equation (2.1). The state space and the space of the test functions are

$$U = \{u \in H^1(\Omega) : \quad u = g_D \quad \text{on} \quad \Gamma_D\} \quad \text{and} \quad V = H_0^1(\Omega),$$

respectively. Then, it is well known that the weak formulation of the state equation (2.1) is such that Elman, Silvester, and Wathen (2005)

$$(\partial_t u, v) + a(u, v) + \int_\Omega r(u)v \;\; dx = l(v), \qquad \forall v \in V,$$

where

$$a(u, v) = \int_\Omega (\epsilon \nabla u \cdot \nabla v + \beta \cdot \nabla u v + \alpha u v) \;\; dx,$$

$$l(v) = \int_\Omega f v \;\; dx + \int_{\Gamma_N} g_N v \;\; ds.$$

When shock-capturing is applied, we add an artificial viscosity $(\nabla \cdot (\mu \nabla u))$ to the weak formulation of the problem (2.1). It is an unphysical diffusion term whose sole purpose is to damp out high frequency components of the solution encountered wherever Gibbs phenomenas are present. Then, the weak formulation with the artificial viscosity is given by

$$(\partial_t u, v) + a(u, v) + \int_\Omega r(u)v \;\; dx + \int_\Omega \nabla \cdot (\mu \nabla u) v \;\; dx = l(v), \quad \forall v \in V,$$

where μ is the amount of viscosity. The viscosity parameter μ is chosen as a function of the mesh size and order of approximating polynomials. It will be described in Section 3.2 in more details.

3. Discretization scheme

3.1. DG discretization in space

The DG discretization here is based on the SIPG discretization for the diffusion and the upwind discretization for the convection. The same discretization is used, e.g., in Houston, Schwab, and Süli (2002); Schötzau and Zhu (2009) for scalar linear convection diffusion equations. In this paper, we follow the notation in Schötzau and Zhu (2009).

Let $\{\mathcal{T}_h\}_h$ be a family of shape regular meshes such that $\overline{\Omega} = \cup_{K \in \mathcal{T}_h} \overline{K}$, $K_i \cap K_j = \emptyset$ for $K_i, K_j \in \mathcal{T}_h$, $i \neq j$. The diameter of an element K and the length of an edge E are denoted by h_K and h_E, respectively.

For an integer ℓ and $K \in \mathcal{T}_h$ let $\mathbb{P}^\ell(K)$ be the set of all polynomials on K of degree at most ℓ. We define the discrete state and test spaces to be

$$V_h = U_h = \left\{ u \in L^2(\Omega) : u|_K \in \mathbb{P}^\ell(K) \quad \forall K \in \mathcal{T}_h \right\}. \tag{3.1}$$

Note that since discontinuous Galerkin methods impose boundary conditions weakly, the space U_h of discrete states and the space of test functions V_h are identical.

We split the set of all edges $\mathcal{E}_h$ into the set $\mathcal{E}_h^0$ of interior edges, the set $\mathcal{E}_h^D$ of Dirichlet boundary edges and the set $\mathcal{E}_h^N$ of Neumann boundary edges so that $\mathcal{E}_h = \mathcal{E}_h^\partial \cup \mathcal{E}_h^0$ with $\mathcal{E}_h^\partial = \mathcal{E}_h^D \cup \mathcal{E}_h^N$. Let $\mathbf{n}$ denote the unit outward normal to $\partial\Omega$. We define the inflow boundary

$$\Gamma^- = \left\{ x \in \partial\Omega \; : \beta \cdot \mathbf{n}(x) < 0 \right\},$$

and the outflow boundary $\Gamma^+ = \partial\Omega \setminus \Gamma^-$. The boundary edges are decomposed into edges $\mathcal{E}_h^- = \left\{ E \in \mathcal{E}_h^\partial : E \subset \Gamma^- \right\}$ that correspond to inflow boundary and edges $\mathcal{E}_h^+ = \mathcal{E}_h^\partial \setminus \mathcal{E}_h^-$ that correspond to outflow boundary.