Commun. Comput. Phys.
doi: 10.4208/cicp.010113.160813s

Vol. **15**, No. 4, pp. 996-1011
April 2014

Exponential Runge-Kutta Methods for the Multispecies Boltzmann Equation

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Received 1 January 2013; Accepted (in revised version) 16 August 2013

Available online 21 January 2014

Abstract. This paper generalizes the exponential Runge-Kutta asymptotic preserving (AP) method developed in [G. Dimarco and L. Pareschi, *SIAM Numer. Anal.*, 49 (2011), pp. 2057–2077] to compute the multi-species Boltzmann equation. Compared to the single species Boltzmann equation that the method was originally applied on, this set of equation presents a new difficulty that comes from the lack of local conservation laws due to the interaction between different species. Hence extra stiff nonlinear source terms need to be treated properly to maintain the accuracy and the AP property. The method we propose does not contain any nonlinear nonlocal implicit solver, and can capture the hydrodynamic limit with time step and mesh size independent of the Knudsen number. We prove the positivity and strong AP properties of the scheme, which are verified by two numerical examples.

AMS subject classifications: 65C20, 65M06, 76D05, 82C40

Key words: Multispecies Boltzmann equation, exponential Runge-Kutta method, hydrodynamic limit, asymptotic preserving property, positivity preserving.

1 Introduction

We are interested in developing efficient numerical methods for the nonlinear multispecies Boltzmann equation [11]:

$$\partial_t f_i + v\cdot\nabla_x f_i = \frac{1}{\varepsilon}Q_i(f,f), \quad t\geq 0, \quad (x,v)\in\mathbb{R}^d\times\mathbb{R}^d. \tag{1.1}$$

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Here $f_i(t,x,v)$ represents the distribution function of the i-th species at time t, position x and velocity v, and $f=(f_1,f_2,\cdots,f_N)^{\mathrm{T}}$, d is the dimensionality and N is the number of species. The collision term is given by

$$Q_i(f,f)=\sum_{k=1}^{N}Q_{ik}(f,f), \tag{1.2a}$$

$$\begin{aligned}Q_{ik}(f,f)(v)&=\int_{S^{d-1}}\int_{\mathbb{R}^d}(f_i'f_{k^*}'-f_if_{k^*})B_{ik}(|v-v_*|,\omega)dv_*d\omega\\&\triangleq Q_{ik}^{+}-f_iQ_{ik}^{-},\end{aligned} \tag{1.2b}$$

where B_{ik} is the symmetric collision kernel (*i.e.* $B_{ik}=B_{ki}$), v and v_* are pre-collisional velocities, v' and v_*' are post-collisional velocities, $f_i'=f_i(t,x,v')$ and $f_{k^*}'=f_k(t,x,v_*')$, ω is a unit vector, and S^{d-1} is the unit sphere defined in $\mathbb{R}^d$ space, $g=v-v_*$ is relative velocity. There are many variations for the collision kernel B_{ik}. One of the simple cases is the Maxwell molecule when $B_{ik}=B_{ik}\left(\frac{g\cdot\omega}{|g|}\right)$. The post-collisional velocities v' and v_*' satisfy:

$$v'=v-\frac{\mu_{ik}}{m_i}(g-|g|\omega),\qquad v_*'=v_*+\frac{\mu_{ik}}{m_k}(g-|g|\omega), \tag{1.3}$$

with $\mu_{ik}=\frac{m_im_k}{m_i+m_k}$ being the reduced mass, and m_i, m_k being the mass for species i and k respectively. This deduction is based on momentum and energy conservations:

$$m_iv+m_kv_*=m_iv'+m_kv_*',\qquad m_i|v|^2+m_k|v_*|^2=m_i|v'|^2+m_k|v_*'|^2.$$

Eq. (1.1) describes the evolution of rarefied gas that has more than two components whose particles usually have different masses. It is often used in modeling the high altitude gas, which is usually considered as a binary mixture of Oxygen and Nitrogen, and the environment at the reentry to the earth of spacecrafts. In (1.2b), the gaining part is marked as Q_{ik}^{+} and the rest is the losing part marked as $f_iQ_{ik}^{-}$ with f_i extracted out of the integration. In (1.1), the ε is called the Knudsen number, indicating the ratio of mean free path over the typical domain size. When $\varepsilon=\mathcal{O}(1)$, the equation is in kinetic (microscopic) regime. As $\varepsilon\to 0$, one gets to fluid (macroscopic) regime with the Euler equations as the first order approximation in Chapman-Enskog Expansion [**?**].

Numerical challenge comes from the time discretization due to the Knudsen number. On the one hand, it is impractical to design an implicit method since it requires the inversion of the nonlocal and nonlinear collision term. On the other hand, if explicit method is used, the time step is limited by the smallest Knudsen number for stability reasons, which usually leads to unaffordable computational cost.

There has been a great amount of literature on removing the numerical stiffness in (1.1), many of which are based on domain decomposition [5, 8, 9, 16, 18, 25–27]. The idea is to solve (1.1) when the Knudsen number is of $\mathcal{O}(1)$, and to solve its Euler limit when the Knudsen number is small. Despite its success in theory, the method encounters two difficulties in practice: 1. It is hard to identify how small the Knudsen number should