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Bound-preserving discontinuous Galerkin methods for conservative phase space advection in curvilinear coordinates ☆

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ABSTRACT

We extend the positivity-preserving method of Zhang and Shu [49] to simulate the advection of neutral particles in phase space using curvilinear coordinates. The ability to utilize these coordinates is important for non-equilibrium transport problems in general relativity and also in science and engineering applications with specific geometries. The method achieves high-order accuracy using Discontinuous Galerkin (DG) discretization of phase space and strong stability-preserving, Runge–Kutta (SSP-RK) time integration. Special care is taken to ensure that the method preserves strict bounds for the phase space distribution function f; i.e., $f \in [0, 1]$. The combination of suitable CFL conditions and the use of the high-order limiter proposed in [49] is sufficient to ensure positivity of the distribution function. However, to ensure that the distribution function satisfies the upper bound, the discretization must, in addition, preserve the divergence-free property of the phase space flow. Proofs that highlight the necessary conditions are presented for general curvilinear coordinates, and the details of these conditions are worked out for some commonly used coordinate systems (i.e., spherical polar spatial coordinates in spherical symmetry and cylindrical spatial coordinates in axial symmetry, both with spherical momentum coordinates). Results from numerical experiments — including one example in spherical symmetry adopting the Schwarzschild metric — demonstrate that the method achieves high-order accuracy and that the distribution function satisfies the maximum principle.

1. Introduction

In this paper, we design discontinuous Galerkin methods for the solution of the collision-less, *conservative* Boltzmann equation in general curvilinear coordinates

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$$\frac{\partial f}{\partial t}+\frac{1}{\sqrt{\gamma}}\sum_{i=1}^{d_x}\frac{\partial}{\partial x^i}\left(\sqrt{\gamma}\,F^i f\right)+\frac{1}{\sqrt{\lambda}}\sum_{i=1}^{d_p}\frac{\partial}{\partial p^i}\left(\sqrt{\lambda}\,G^i f\right)=0 \tag{1}$$

that preserve, in the sense of local cell averages, the physical bounds on the distribution function $f=f(\boldsymbol{x},\boldsymbol{p},t)$. This function gives the density of particles with respect to the phase space measure $d\boldsymbol{x}d\boldsymbol{p}$. In Eq. (1), $t\in\mathbb{R}^+$ represents time, and x^i and p^i are components of the position vector $\boldsymbol{x}\in\mathbb{R}^{d_x}$ and momentum vector $\boldsymbol{p}\in\mathbb{R}^{d_p}$, respectively. In general, $d_x=d_p=3$, but when imposing symmetries for simplified geometries, some dimensions may not need to be considered. F^i and G^i are coefficients of the position space flux vector $\boldsymbol{F}f$ and the momentum space flux vector $\boldsymbol{G}f$, respectively, while $\sqrt{\gamma}\geq 0$ and $\sqrt{\lambda}\geq 0$ are the determinants of the position space and momentum space metric tensors, respectively. (See Appendix A for more details. In particular, Eq. (1) is obtained from the conservative, general relativistic Boltzmann equation in the limit of a *time-independent* spacetime.) Eq. (1) must be supplemented with appropriate boundary and initial conditions which, at this point, are left unspecified.

The upper and lower bounds on f follow from the *non-conservative* advection equation

$$\frac{\partial f}{\partial t}+\sum_{i=1}^{d_x}F^i\frac{\partial f}{\partial x^i}+\sum_{i=1}^{d_p}G^i\frac{\partial f}{\partial p^i}=0, \tag{2}$$

which is formally equivalent to (1) due to the divergence-free property of the phase space, or "Liouville," flow

$$\frac{1}{\sqrt{\gamma}}\sum_{i=1}^{d_x}\frac{\partial}{\partial x^i}\left(\sqrt{\gamma}\,F^i\right)+\frac{1}{\sqrt{\lambda}}\sum_{i=1}^{d_p}\frac{\partial}{\partial p^i}\left(\sqrt{\lambda}\,G^i\right)=0. \tag{3}$$

Indeed, it is straightforward to show that (2) preserves the bounds of the initial and boundary data. (Here we assume that the distribution function $f(\boldsymbol{x},\boldsymbol{p},t)$ satisfies $f\in[0,1]\ \forall t$.) We employ the conservative form for two major reasons: (1) it is mathematically convenient when discontinuities are present and (2) it leads naturally to numerical methods with conservative properties. The drawback is that preserving point-wise bounds on f becomes non-trivial.

Discontinuous Galerkin (DG) methods (see e.g., [13,12,18] and references therein) for phase space discretization are attractive for several reasons. First, they achieve high-order accuracy on a compact, local stencil so that data is only communicated with nearest neighbors, regardless of the formal order of accuracy. This leads to a high computation to communication ratio, and favorable parallel scalability on heterogeneous architectures [21]. Second, they exhibit favorable properties when collisions are added to the right-hand side of (1). In particular, they recover the correct asymptotic behavior in the diffusion limit [23,1,17], which is characterized by frequent collisions with a material background and long time scales. To leverage these properties, it is important to preserve positivity in the phase space advection step since negative distribution functions are physically meaningless. In the case of fermions, f is also bounded above (i.e., $f\leq 1$), which introduces Pauli blocking factors in the collision operator. Violation of these bounds can result in numerical difficulties due to nonlinearities that can come from material coupling [29]. Simply introducing a cutoff in the algorithm is unacceptable, since this results in loss of conservation — a critical check on physical consistency.

In this paper, we extend the approach introduced in [49] in order to preserve upper and lower bounds of scalar conservation laws. The approach has three basic ingredients. First, one expresses the update of the (approximate) cell average in a forward Euler step as a linear combination of conservative updates. This requires a quadrature representation of the current local polynomial approximation that calculates the cell average exactly. Second, a limiter is introduced which modifies the current polynomial approximation, making point-wise values satisfy the prescribed bound on the quadrature set while maintaining the cell average. These two steps ensure that the Euler update of the cell average satisfies the required bounds. The third and final step is to apply a Strong Stability-Preserving Runge–Kutta (SSP-RK) method (e.g. [15]) which can be expressed as a convex combination of Euler steps and therefore preserves the same bounds as the Euler step.

The method from [49] has been extended and applied in many ways. Positivity-preserving DG and weighted essentially non-oscillatory (WENO) methods have been designed for convection–diffusion equations [52,47], the Euler equations with source terms [51], the shallow water equations [46], multi-material flows [9], the ideal MHD equations [11], moment models for radiation transport [38], and PDEs involving global integral terms including a hierarchical size-structured population model [48]. The specific problem of maintaining a positive distribution function in phase space has been considered in [10,40,43] for the case of Cartesian coordinates. In [10], the authors consider an Eulerian scheme for the Boltzmann–Poisson system with a linear collision operator. In [40,43], semi-Lagrangian schemes are used to approximate the Vlasov–Poisson system, which contains no collisions. In the current work we also ignore the effects of the collision operator, and consider the conservative phase space advection equation in (1). We enforce both the upper and lower bounds on f for general curvilinear coordinates. This introduces some non-trivial differences. In particular,

1. The volume element in each computational phase space cell depends on the coordinates. This means that mass matrices can vary from cell to cell. It also complicates the quadrature needed for exact evaluation of the cell average. Finally, the balance between cell averages and fluxes that gives the proper bounds requires special treatment. These last two properties may lead to a reduced CFL condition.