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New velocity-space discretization for continuum kinetic calculations and Fokker–Planck collisions

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ABSTRACT

Numerical techniques for discretization of velocity space in continuum kinetic calculations are described. An efficient spectral collocation method is developed for the speed coordinate – the radius in velocity space – employing a novel set of non-classical orthogonal polynomials. For problems in which Fokker–Planck collisions are included, a common situation in plasma physics, a procedure is detailed to accurately and efficiently treat the field term in the collision operator (in the absence of gyrokinetic corrections). When species with disparate masses are included simultaneously, a careful extrapolation of the Rosenbluth potentials is performed. The techniques are demonstrated in several applications, including neoclassical calculations of the bootstrap current and plasma flows in a tokamak.

1. Introduction

A ubiquitous situation in numerical kinetic calculations is that the distribution function must be discretized in a manner allowing both accurate integration and accurate differentiation. Integration is needed because typically moments of the distribution function, such as density and velocity, are of interest. Differentiation is needed both for the collisionless terms in the kinetic equation and also for velocity-space diffusion in collisions. Spherical or cylindrical coordinates are natural for velocity space, meaning the normalized spherical or cylindrical radius (speed) coordinate x lies in the semi-infinite domain $[0,\infty)$. The distribution function often has a Maxwellian envelope, meaning it behaves as $\propto \exp(-x^2)$ as $x \to \infty$.

Many discretization schemes for the radial velocity coordinate are possible and many have been explored in the literature [1–7], each with advantages and disadvantages regarding the above requirements. A uniform grid allows modest accuracy at both integration and differentiation using finite difference/volume/element methods. To use a uniform grid, x may either be mapped to a finite interval using a coordinate transformation, or else the fact that the distribution function is exponentially small for $x \gtrsim 6$ may be used to truncate the x grid above some $x_{\max}$. Alternatively, Gaussian abscissa permit extremely accurate integration but generally only low-order differentiation if finite difference/volume/element methods are applied to the unequally spaced grid. A Chebyshev grid permits both spectrally accurate differentiation and integration [8,9]. However, Chebyshev grids involve a high density of nodes near the endpoints of a finite interval, so unless a transformation is applied, Chebyshev grids are therefore poorly suited for the semi-infinite domain of x and for the $\propto \exp(-x^2)$ dependence typical of distribution functions. Methods using Laguerre or associated Laguerre polynomials have also been used, but as we will show,

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these methods do not always perform as well as one might hope due to a nonanalytic Jacobian in the coordinate transformation from energy to speed [2].

In this work, we present a new approach for discretizing velocity space. The approach permits both spectrally accurate integration and differentiation on the semi-infinite domain $[0,\infty)$ for functions with Maxwellian-like $\propto \exp(-x^2)$ dependence for large normalized speed x. The method is collocation rather than modal in nature, i.e. the function is known on a set of grid points (abscissae) rather than being explicitly expanded in a set of modes. As such, the method is well suited for nonlinear computations in addition to linear ones.

Our method derives from a set of previously unexplored orthogonal polynomials. The semi-infinite integration domain in the orthogonality relation for these new polynomials is identical to that of the Laguerre polynomials. However, the use of a different weight e^{-x^2} in place of e^{-y} results in polynomials with superior properties for the calculations of interest.

In kinetic calculations for plasmas, it is often important to accurately include collisions in the kinetic equation, and the Fokker–Planck operator [10] is the best available description of collisions. This operator may be written in terms of "Rosenbluth potentials", which are defined in terms of the distribution function through a pair of Poisson equations. A complication of the Fokker–Planck operator is that the Rosenbluth potentials vary as powers of x rather than as $\exp(-x^2)$ for large x, which means discretization schemes that work well for the distribution function may not work well for the potentials. Accurate numerical schemes for handling the Fokker–Planck operator in plasma computations have been a subject of great interest [11,12,5,13]. Here we will develop an efficient approach to incorporating the Rosenbluth potentials in the kinetic equation, carefully accounting for their behavior at large x to maintain high precision even for coarse grid resolution.

The new techniques we discuss are demonstrated in several applications. First, we compute the resistivity of a plasma. Second, we compute the bootstrap current in a tokamak plasma. Lastly, we calculate the flows of multiple ion species in a tokamak. These computations require the solution of equations in which both the collision operator and other kinetic terms appear. Using the new velocity discretization described here, we find that only 4–6 grid points in x are required for the desired level of convergence. For gyrokinetic simulations of plasma turbulence, which commonly use ~ 16 energy gridpoints, this new energy grid may reduce requirements of time, memory, or number of processors.

2. Spectral collocation scheme for velocity space

For a variety of problems in kinetic theory, either with or without collisions, it is useful to represent the distribution function in either spherical or cylindrical coordinates in velocity space. The dimensional coordinates v (the spherical radius in velocity space) or $v_\perp$ (the cylindrical radius in velocity space) then arise. Either coordinate may be normalized for numerical work by the thermal speed $v_{\text{th}} = \sqrt{2T/m}$ where T is a typical temperature and m is the mass of the particle species. We define $x = v/v_{\text{th}}$ or $x = v_\perp/v_{\text{th}}$ as appropriate.

For large x, distribution functions decay exponentially as $\propto \exp(-x^2)$. It is therefore natural to represent the distribution function as $\exp(-x^2)$ times a sum of polynomials P_n^k that are orthogonal according to the relevant weight and domain:

$$\int_0^\infty P_N^k(x) P_n^k(x) x^k e^{-x^2} dx = M_n^k \delta_{N,n} \tag{1}$$

where k is any number greater than -1, and M_n^k is some normalization. Notice (1) differs from the defining orthogonality relations for both the associated Laguerre and Hermite polynomials, which are, respectively,

$$\int_0^\infty L_N^m(y) L_n^m(y) y^m e^{-y} dy = \frac{\Gamma(n+m+1)}{n!} \delta_{N,n} \tag{2}$$

(i.e. polynomials in x^2 rather than x) and

$$\int_{-\infty}^\infty H_N(x) H_n(x) e^{-x^2} dx = 2^n n! \sqrt{\pi} \delta_{N,n} \tag{3}$$

(different range of integration than (1)). Laguerre polynomials are the special case of associated Laguerre polynomials with $m = 0$. There are several reasons why it is preferable to use polynomials in speed x rather than polynomials in energy $y = x^2$, i.e. why the new polynomials are preferable to Laguerre or associated Laguerre polynomials. These reasons will be developed throughout the remainder of this section. As initial motivation, consider that the new polynomials can represent both even and odd powers of v or $v_\perp$, whereas the associated Laguerre polynomials can represent only even powers.

In our experience, the choice $k = 0$ tends to yield the fastest convergence for the problems we consider in the following sections, so for the rest of this paper we consider the polynomials $P_n = P_n^0$. It is straightforward to generalize all results and algorithms presented below to the case of different k.

The first few polynomials may be computed iteratively using the following Gram-Schmidt procedure (though this method turns out to be poorly conditioned when n is large). The polynomial $P_n(x)$ has $n+1$ coefficients, which may be determined by imposing orthogonality with respect to P_0 through P_{n-1} and enforcing the normalization, for a total of $n+1$ constraints. The first few polynomials P_n, normalized so the leading coefficient is 1, are thus