Journal of Computational Physics 294 (2015) 58–77

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Accurate spectral numerical schemes for kinetic equations with energy diffusion

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ARTICLE INFO

Article history:
Received 13 February 2014
Received in revised form 15 March 2015
Accepted 23 March 2015
Available online 28 March 2015

Keywords:
Orthogonal polynomials
Continuum kinetic calculations
Fokker–Plank collisions
Sturm–Liouville theory
Continuous spectrum

ABSTRACT

We examine the merits of using a family of polynomials that are orthogonal with respect to a non-classical weight function to discretize the speed variable in continuum kinetic calculations. We consider a model one-dimensional partial differential equation describing energy diffusion in velocity space due to Fokker–Planck collisions. This relatively simple case allows us to compare the results of the projected dynamics with an expensive but highly accurate spectral transform approach. It also allows us to integrate in time exactly, and to focus entirely on the effectiveness of the discretization of the speed variable. We show that for a fixed number of modes or grid points, the non-classical polynomials can be many orders of magnitude more accurate than classical Hermite polynomials or finite-difference solvers for kinetic equations in plasma physics. We provide a detailed analysis of the difference in behavior and accuracy of the two families of polynomials. For the non-classical polynomials, if the initial condition is not smooth at the origin when interpreted as a three-dimensional radial function, the exact solution leaves the polynomial subspace for a time, but returns (up to roundoff accuracy) to the same point evolved to by the projected dynamics in that time. By contrast, using classical polynomials, the exact solution differs significantly from the projected dynamics solution when it returns to the subspace. We also explore the connection between eigenfunctions of the projected evolution operator and (non-normalizable) eigenfunctions of the full evolution operator, as well as the effect of truncating the computational domain.

1. Introduction

First-principles based descriptions of transport processes in plasmas require the solution of high-dimensional kinetic equations for the phase-space distribution function [1,2]. Often, diffusion in velocity-space plays an important physical role, as discussed in [3,4], and the references therein. For example, in kinetic turbulence, there is a cascade of energy in velocity-space in addition to real space, so velocity diffusion cuts off the cascade at small velocity scales. In this sense, velocity diffusion plays a role similar to that of viscosity in conventional hydrodynamic fluid turbulence. Just as viscosity is important in hydrodynamic turbulence no matter how large the Reynolds number, velocity diffusion is important in kinetic

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http://dx.doi.org/10.1016/j.jcp.2015.03.039
0021-9991/

turbulence no matter how small the collisionality. Velocity diffusion is essential to dissipate injected energy and thereby permit a statistically steady state.

Solving these kinetic equations numerically is computationally intensive [5,6], so an important aspect of the theoretical effort is to find new optimized discretization schemes. While high order accurate discretization schemes for the spatial variables have been successfully used for many years, finding an ideal discretization method remains particularly challenging for the discretization of velocity space in situations involving Fokker–Planck collisions [7]. Since the Fokker–Planck collision operator has terms involving first and second order derivatives with respect to the velocity variables, the discretization method must allow accurate differentiation. The scheme must also allow accurate integration since physical quantities such as the number density, the mean fluid velocity and the pressure depend on velocity moments of the distribution function.

Recently, promising new approaches based on spectral and pseudo-spectral representations have been investigated [8,9]. It was shown in [8] that a Hermite representation for the parallel velocity has advantages over the more common finite difference schemes used in numerical simulations. In [9], different representations for the speed coordinate are explored. It is found that because the variable has values in $[0,\infty)$ instead of the entire real axis, a little-known family of polynomials (see [10–12] and the references therein) gives much better performance than finite difference schemes and schemes based on classical orthogonal polynomials. High accuracy is obtained on very coarse grids for both differentiation and integration of Maxwellian-like functions, which are the functions of interest in many applications of plasma physics [9].

The purpose of this paper is to explore the suitability of the non-classical polynomials for initial-value calculations of turbulent plasma transport in the presence of collisions [4,13]. To do so, we consider a model one-dimensional problem describing energy diffusion due to Fokker–Planck collisions [14]:

$$\frac{\partial U}{\partial t} = \frac{1}{x^2}\frac{\partial}{\partial x}\left[\Psi(x)x^2 e^{-x^2}\frac{\partial}{\partial x}\left(e^{x^2}U\right)\right], \qquad (x>0,\ t>0), \tag{1.1}$$

where

$$\Psi(x) = \frac{1}{2x^3}\left[\operatorname{erf}(x) - \frac{2}{\sqrt{\pi}}xe^{-x^2}\right], \qquad \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-s^2}\,ds. \tag{1.2}$$

Here, Ψ differs from the usual Chandrasekhar function by an additional factor of $1/x$. Our choice to focus on this particular model problem is motivated by the following characteristic features. First, the right-hand side of (1.1) corresponds exactly to the speed variable part of the energy diffusion piece in the linearized Landau–Fokker–Planck operator for same-species collisions [4,13]. Since many state-of-the-art plasma turbulence codes (e.g. [5,6]) use variants of the linearized Landau–Fokker–Planck operator to describe collisions, the results presented here are directly relevant to the computational effort to simulate transport processes in plasmas. Second, the relative simplicity of (1.1) makes it possible to represent the solution semi-analytically using a spectral transform method [14], which we can then use to study the properties and accuracy of various discretization schemes. Third, (1.1) has several physically satisfying properties. Any well-behaved initial distribution function relaxes to a Maxwellian distribution function $U \propto e^{-x^2}$ as $t\to\infty$ (the "H-theorem"). Also, for all t, $\partial/\partial t\left(\int Ux^2dx\right) = 0$, i.e. the number of particles is conserved. The best time-dependent numerical schemes are designed to satisfy these basic properties exactly [13].

While we consider a single velocity dimension in (1.1), any accurate numerical scheme for this equation is immediately applicable to simulations with more velocity dimensions and more complete collision operators, such as the operator in [4] or the linearized Fokker–Planck operator, for the following reasons. For either of these collision operators in spherical velocity coordinates, the only term involving any $\partial/\partial x$ derivatives of the distribution function is the right-hand side of (1.1). For example, in the pitch-angle diffusion term, the speed x appears only as a parameter, not as a derivative. Thus, (1.1) captures nearly all the complexity associated with the x coordinate in higher-dimensional kinetic problems with linearized collisions, and the issue of how best to discretize the speed coordinate is quite independent of how the other velocity coordinates are discretized. As an example of how different discretizations may be applied to the different velocity coordinates, one may refer to the time-independent problems considered in [9], in which 2D velocity space is discretized using a pseudospectral x discretization related to the approach considered here, combined with a Legendre modal discretization in pitch angle. In a similar manner, time-dependent problems in a 2D velocity space could be solved by combining the x discretization we consider here with a Legendre modal discretization in pitch angle (or some other pitch angle discretization). The third velocity coordinate, gyro-angle, is often averaged out of kinetic equations in plasma physics due to rapid particle gyration in a magnetic field, but this coordinate too could be included using a tensor product approach if desired.

In this article, we compute high-accuracy solutions using a true (Galerkin) spectral method to represent the projected dynamics of (1.1). We discretize velocity space only, integrating the resulting ordinary differential equations exactly in time. In future work, we plan to adapt the methods developed here to implement exponential time differencing schemes [15] and implicit–explicit Runge–Kutta methods [16] for the time-evolution of the coupled problem. However, for the model problem (1.1), any timestepping scheme will decouple into independent eigenmodes that behave as predicted by standard linear stability theory; thus, spatial discretization is our focus here.

In a separate paper [17], pseudo-spectral methods will be developed that preserve the self-adjoint structure of the discrete evolution operator, mimicking the Galerkin operator as closely as possible. Performance on coarse grids, which is