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Fast elliptic solvers in cylindrical coordinates and the Coulomb collision operator

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ABSTRACT

In this paper, we describe a new class of fast solvers for separable elliptic partial differential equations in cylindrical coordinates (r,θ,z) with free-space radiation conditions. By combining integral equation methods in the radial variable r with Fourier methods in θ and z, we show that high-order accuracy can be achieved in both the governing potential and its derivatives. A weak singularity arises in the Fourier transform with respect to z that is handled with special purpose quadratures. We show how these solvers can be applied to the evaluation of the Coulomb collision operator in kinetic models of ionized gases.

1. Introduction

A variety of problems in computational physics require the solution of the Poisson and biharmonic equations in cylindrical coordinate systems, particularly when the source distribution (the right-hand side) is axisymmetric or involves only a few azimuthal modes. The present paper was motivated by the need to compute the Coulomb collision operator $C(f_a,f_b)$ in kinetic simulations of the Boltzmann–Fokker–Planck equation [4,5,31–33]:

$$\partial_t f_a + \boldsymbol{v}\cdot\nabla f_a + \frac{e_a}{m_a}(\boldsymbol{E}+\boldsymbol{v}\times\boldsymbol{B})\cdot\partial_{\boldsymbol{v}} f_a = \sum_b (f_a,f_b). \tag{1}$$

Here, $f_a(\boldsymbol{x},\boldsymbol{v},t)$ denotes the state of an ionized gas for plasma species a and the index b runs over all species present. In the Fokker–Planck–Landau formalism [26],

$$C(f_a,f_b) = \gamma_{ab}\partial_{\boldsymbol{v}}\cdot\int \mathbb{S}(\boldsymbol{v}-\boldsymbol{v}')\left(\frac{\partial_{\boldsymbol{v}} f_a(\boldsymbol{v})}{m_a} f_b(\boldsymbol{v}') - f_a(\boldsymbol{v})\frac{\partial_{\boldsymbol{v}'} f_b(\boldsymbol{v}')}{m_b}\right) d\boldsymbol{v}' \tag{2}$$

where

$$\mathbb{S}(\boldsymbol{v}-\boldsymbol{v}')_{ij} = \delta_{ij}\frac{1}{|\boldsymbol{v}-\boldsymbol{v}'|} - \frac{(v_i-v_i')\left(v_j-v_j'\right)}{|\boldsymbol{v}-\boldsymbol{v}'|^3}. \tag{3}$$

An alternative representation makes use of the Rosenbluth potentials [32]:

$$C(f_a,f_b) = \frac{\gamma_{ab}}{m_a}\partial_{\boldsymbol{v}}\cdot\left[\partial_{\boldsymbol{v}}\cdot(f_a\partial_{\boldsymbol{v}}\partial_{\boldsymbol{v}}G_b) - 2\left(1+\frac{m_a}{m_b}\right)f_a\partial_{\boldsymbol{v}}H_b\right] \tag{4}$$

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where

$$H_b(\boldsymbol{v}) = \int \frac{1}{|\boldsymbol{v} - \boldsymbol{v}'|} f_b(\boldsymbol{v}') d\boldsymbol{v}' \quad \text{or} \quad \Delta H_b = -4\pi f_b \tag{5}$$

and

$$G_b(\boldsymbol{v}) = \int |\boldsymbol{v} - \boldsymbol{v}'| f_b(\boldsymbol{v}') d\boldsymbol{v}' \quad \text{or} \quad \Delta^2 G_b = -8\pi f_b \tag{6}$$

Note that four derivatives of G_b are required in (4), while G_b itself satisfies the inhomogeneous biharmonic Eq. (6). Thus, direct discretization of the partial differential equation, followed by evaluation of the collision operator via (4) would require eight steps of numerical differentiation, with significant loss of accuracy.

It is natural, therefore, to consider alternative methods with the dual goals of achieving high order accuracy and minimizing the condition number of the solution process. Because of the design of magnetic confinement devices for plasmas, it is also important to be able to construct numerical methods in cylindrical coordinate systems, since the distribution functions $f_b(\boldsymbol{v})$ are often axisymmetric or involve only a few azimuthal modes.

There is, of course, a substantial literature on computing Coulomb collisions and on solving elliptic partial differential equations in cylindrical coordinates. We refer the reader to [5,7,11,19,22,24,28,29,31–33] for some methods in current use in plasma physics. For a discussion of relativistic effects, see [6]. Most closely related to our approach are the methods of [15,30 and 20,23,24,32]. The first two are fast and achieve high order ("spectral") accuracy, but use Fourier methods in Cartesian coordinates and do not address the axisymmetric (or low azimuthal mode) case. The latter rely on separation of variables in spherical coordinates, for which the axisymmetric case leads naturally to a representation involving Legendre polynomials and the general case to a representation involving associated Legendre functions.

In the numerical analysis literature, most solvers based on cylindrical coordinates tend to concern themselves with periodic (in z) or finite domain boundary conditions rather than free-space boundary conditions (see, for example [9,25]). Here, we develop a method for computing the Rosenbluth potentials using separation of variables and a mix of integral equation and Fourier analysis techniques. We show that free-space (radiation) conditions can be imposed in a straightforward manner and that high order accuracy can be achieved in all derivatives with minimal loss of precision. The solver requires $O(N\log N)$ work, where N is the number of grid points used to sample the distribution function.

Finally, we should make a remark about notation. The collision operator and the Rosenbluth potentials in (5), (6) are defined in velocity variables, for which we will use the standard cylindrical coordinates (r,θ,z) for $\boldsymbol{v}$. In the context of plasma physics, $r = |v_\perp|$, where $|v_\perp|$ is the magnitude of the component of the velocity perpendicular to the magnetic field, θ is the gyrophase angle, and $z = v_\parallel$ is the component of the velocity field parallel to the magnetic field. The problem is purely axisymmetric when the velocity field is independent of the gyrophase angle.

One disadvantage of our solver is that we can be adaptive in the r direction, but not in the z or θ directions, since we use spectral discretizations in the latter variables. For fully adaptive three-dimensional calculations, one could employ fast multipole-accelerated integral equation solvers, as described in [14,27]. These methods directly compute the convolution of the data $f_b(\boldsymbol{v})$ with the free-space Green's function. In the axisymmetric case, one could use an axisymmetric version of the fast multipole method [34]. The constant, however, is larger for these schemes than for methods based on separation of variables, and we limit our attention to methods that rely on a tensor product mesh in r, θ and z, which is adequate for most current simulations of the Boltzmann–Fokker–Planck Eq. (1).

2. The Poisson equation in cylindrical coordinates

In order to compute the Rosenbluth potential H_b, we must solve the Poisson equation in free space

$$\Delta u(\boldsymbol{v}) = f(\boldsymbol{v}).$$

In cylindrical coordinates $\boldsymbol{v} = (r,\theta,z)$, we have

$$u_{rr}(r,\theta,z) + \frac{1}{r} u_r(r,\theta,z) + \frac{1}{r^2} u_{\theta\theta}(r,\theta,z) + u_{zz}(r,\theta,z) = f(r,\theta,z), \tag{7}$$

and we assume that f is identically zero outside the region

$$\Omega = \{(r,\theta,z) : 0 \leqslant r \leqslant R, \quad -A \leqslant z \leqslant A, \quad 0 \leqslant \theta \leqslant 2\pi\}.$$

Since u and f are periodic in θ, we represent them as Fourier series:

$$u(r,\theta,z) = \sum_{n=-\infty}^{\infty} u^{(n)}(r,z) e^{in\theta} \tag{8}$$

$$f(r,\theta,z) = \sum_{n=-\infty}^{\infty} f^{(n)}(r,z) e^{in\theta} \tag{9}$$