

Gaussian Radial Basis Functions for Plasma Physics: Numerical Aspects

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A magnetized plasma is described by the Vlasov equation and the non-linear Fokker-Planck collision operator [1]. The Vlasov part describes phase-space advection and the collision operator adds dissipation due to collisional energy and momentum exchange. Numerical discretization of the collision operator, however, is far from trivial. Recently, we have developed a new approach [2] to address this issue. The new approach is based on an expansion in Gaussian Radial Basis Functions (RBFs), a method widely used in neural network calculations [3]. In this paper, we discuss useful details regarding the numerical implementation of the RBF method.

Introduction In Ref. [2], we addressed the kinetic equation and the collision operator by expressing the distribution function as a sum of shifted Maxwellians, i.e., as Gaussian RBFs. In the continuous summation limit, an equivalent expression for the distribution becomes

$$f_a(\mathbf{v}, t) = \int \left(\frac{\gamma}{\pi} \right)^{3/2} \exp \left[-\gamma (\mathbf{v} - \mathbf{u})^2 \right] W_a(\mathbf{u}, \gamma, t) d\mathbf{u} d\gamma,$$

where the weight function $W_a(\mathbf{u}, \gamma, t)$ is normalized to the density of the species a according to $\int W_a(\mathbf{u}, \gamma, t) d\mathbf{u} d\gamma = n_a(t)$. The Rosenbluth potentials, which are needed to describe the non-linear collision operator, can then be calculated analytically according to

$$\begin{aligned} \varphi_b(\mathbf{v}, t) &= -\frac{1}{4\pi} \int \gamma^{1/2} \Phi(\gamma^{1/2} |\mathbf{v} - \mathbf{u}|) W_b(\mathbf{u}, \gamma, t) d\mathbf{u} d\gamma, \\ \psi_b(\mathbf{v}, t) &= -\frac{1}{8\pi} \int \gamma^{-1/2} \Psi(\gamma^{1/2} |\mathbf{v} - \mathbf{u}|) W_b(\mathbf{u}, \gamma, t) d\mathbf{u} d\gamma, \end{aligned}$$

where $\Phi(s) = \text{erf}(s)/s$, $\Psi(s) = [s + 1/(2s)]\text{erf}(s) + \exp(-s^2)/\sqrt{\pi}$, and $\text{erf}(s)$ is the error function.

For numerical considerations, the integration is changed into a discrete sum by defining the weight-function to be a sum of delta-functions: in 3D velocity space one chooses $W_a(\mathbf{u}, \gamma, t) = \sum_i w_a^i(t) \delta(\mathbf{u} - \mathbf{v}_i) \delta(\gamma - \gamma_a^i)$ and in the axisymmetric case one can choose cylindrical velocity space coordinates and $W_a(\mathbf{u}) = \sum_i w_a^i(t) \frac{1}{2\pi v_{\perp i}} \delta(u_{\parallel} - v_{\parallel i}) \delta(u_{\perp} - v_{\perp i}) \delta(\gamma - \gamma_a^i)$. As was shown in Ref. [2] the collisional part of the Fokker-Planck equation then reduces to

$$\sum_i \frac{\partial w_a^i}{\partial t} F_a^i = \sum_{b,k,\ell} w_b^k(t) w_a^{\ell}(t) L_{ab} \left[\frac{m_a}{m_b} F_b^k F_a^{\ell} + \mu_{ab} \frac{\partial \varphi_b^k}{\partial \mathbf{v}} \cdot \frac{\partial F_a^{\ell}}{\partial \mathbf{v}} - \frac{\partial^2 \psi_b^k}{\partial \mathbf{v} \partial \mathbf{v}} \cdot \frac{\partial^2 F_a^{\ell}}{\partial \mathbf{v} \partial \mathbf{v}} \right], \quad (1)$$

where $\mu_{ab} = m_a/m_b - 1$, $L_{ab} = (e_a e_b / m_a \varepsilon_0)^2 \ln \Lambda_{ab}$, $\ln \Lambda_{ab}$ is the Coulomb logarithm, and w_a^i are the expansion weights. The RBF basis functions become $F_a^i = (\gamma_a^i / \pi)^{3/2} \exp[-\gamma_a^i (\mathbf{v} - \mathbf{v}_a^i)^2]$, for the 3D weight-function, and $F_a^i = (\gamma_a^i / \pi)^{3/2} I_0(2\gamma_a^i v_{i,\perp} v_\perp) e^{-\gamma_a^i (v_\parallel - v_{i,\parallel})^2 - \gamma_a^i (v_\perp^2 + v_{i,\perp}^2)}$, corresponding to the 2D axisymmetric weight function. $I_0(x)$ is the zeroth modified Bessel function of the second kind. The only notable difference between the 3D and 2D axisymmetric case is that in 3D, the weight function completely eliminates the \mathbf{u} -integral in the potential functions, while in 2D the potentials φ_b^i and ψ_b^i have to be computed numerically as *ring-like* averages of the functions Φ and Ψ .

In this paper, we provide a detailed discussion of some of the key aspects needed for an efficient implementation of Eq. (1). We will focus on the evaluation of the right-hand-side and also on the specific case of axisymmetry.

Equation for the weights Even after the expansion, the Fokker-Planck equation, Eq. (1), has a velocity space dependence. In order to obtain an equation for the weights only, this dependence has to be eliminated.

Multiplying Eq. (1) with a test function Θ^i and integrating over velocity space gives

$$\sum_j M_a^{ij} \frac{\partial w_a^j}{\partial t} = \sum_{b,k,\ell} w_b^k(t) w_a^\ell(t) C_{ab}^{ik\ell}, \quad (2)$$

where the so-called *mass* matrix $M_a^{ij} = \int d\mathbf{v} \Theta^i F_a^j$ and the tensor like collision term $C_{ab}^{ik\ell}$ is

$$C_{ab}^{ik\ell} = \int d\mathbf{v} \Theta^i L_{ab} \left[\frac{m_a}{m_b} F_b^k F_a^\ell + \mu_{ab} \frac{\partial \varphi_b^k}{\partial \mathbf{v}} \cdot \frac{\partial F_a^\ell}{\partial \mathbf{v}} - \frac{\partial^2 \psi_b^k}{\partial \mathbf{v} \partial \mathbf{v}} : \frac{\partial^2 F_a^\ell}{\partial \mathbf{v} \partial \mathbf{v}} \right] \equiv \int d\mathbf{v} \Theta^i C_{ab}^{kl}.$$

The traditional Galerkin projection is obtained by choosing $\Theta^i = F_a^i$, and the center collocation method by choosing $\Theta^i = \delta(\mathbf{v} - \mathbf{v}_i)$. In the center collocation, the matrix is thus simply $M_a^{ij} = F_a^j(\mathbf{v}_i)$ and the collision tensor becomes $C_{ab}^{ik\ell} = C_{ab}^{kl}(\mathbf{v}_i)$.

The true challenge in solving Eq. (2) is that the right hand side contains a rank-3 tensor, which is not sparse: introducing the Gaussian RBF-basis is advantageous in the sense that the expression for the collision operator in 3D velocity space becomes analytic but, simultaneously, each basis function extends to infinity, making both the matrix and the tensor full. The specific structure of the collision tensor, however, can be used to reduce the memory demands significantly, especially if the center collocation method is used.

Consider the evaluation of the collision operator at a set of points $\{\mathbf{v}_i\}_{i=1}^N$. Since $C_{ab}^{kl}(\mathbf{v})$ can be expressed as a sum of products of two different functions we can compute the value of the collision operator at the points \mathbf{v}_i according to

$$C = L_{ab} \left[\frac{m_a}{m_b} ([\mathbf{F}_b] \mathbf{w}_b)^T ([\mathbf{F}_a] \mathbf{w}_a) + \mu_{ab} ([\partial \varphi_b^\sigma] \mathbf{w}_b)^T ([\partial \mathbf{F}_a^\sigma] \mathbf{w}_a) - ([\partial \partial \psi_b^{\sigma\nu}] \mathbf{w}_b)^T ([\partial \partial \mathbf{F}_a^{\sigma\nu}] \mathbf{w}_a) \right],$$

where summation over repeated indices σ and ν is assumed, \mathbf{w}_a is a vector containing the weights, \mathbf{F}_a is a matrix with components $(\mathbf{F}_a)_{ij} = F_a^j(\mathbf{v}_i)$, the derivative matrices in Cartesian 3D velocity space have the components

$$[\partial\varphi_b^\sigma]_{ij} = \frac{\partial\varphi_b^j(\mathbf{v}_i)}{\partial v^\sigma}, \quad [\partial\partial\psi_b^{\sigma\nu}]_{ij} = \frac{\partial^2\psi_b^j(\mathbf{v}_i)}{\partial v^\sigma\partial v^\nu},$$

and similarly for the distribution function. Later we give the expressions in cylindrical coordinates. The upper index T denotes a matrix transpose. Thus, instead of storing a full rank-3 tensor to evaluate the right hand side in Eq. (2), it is enough to compute and store the matrices $[\mathbf{F}_a]$, $[\partial\varphi_a^\sigma]$, $[\partial\mathbf{F}_a^\sigma]$, $[\partial\partial\psi_a^{\sigma\nu}]$, and $[\partial\partial\mathbf{F}_a^{\sigma\nu}]$ for each of the plasma species of interest.

In the center collocation method, the matrix sizes are $N \times N$ for N basis functions, and the discretized equation for the weights can then be expressed in a matrix form as

$$[\mathbf{F}_a] \frac{\partial \mathbf{w}_a}{\partial t} = \mathbf{C}(\mathbf{w}_a, \mathbf{w}_b).$$

In the Galerkin projection, one has to compute the integrals over the velocity space but, as it has to be done numerically, it can be formulated into a similar form

$$[\mathbf{M}_a] \frac{\partial \mathbf{w}_a}{\partial t} = \mathbf{K}(\mathbf{w}_a, \mathbf{w}_b),$$

where the mass matrix and the integral of the collision operator are defined by

$$[\mathbf{M}_a]_{ij} = \sum_\ell b_\ell F_a^i(\mathbf{v}_\ell) F_a^j(\mathbf{v}_\ell), \quad \mathbf{K}_i(\mathbf{w}_a, \mathbf{w}_b) = \sum_\ell b_\ell F_a^i(\mathbf{v}_\ell) C_\ell(\mathbf{w}_a, \mathbf{w}_b),$$

and b_ℓ are the integration weights. Using the described method one avoids storing a full rank-3 tensor.

Velocity space axisymmetry Using cylindrical velocity space coordinates $(v_{\parallel}, v_{\perp})$ the relative magnitude of two vectors \mathbf{v} and \mathbf{u} is $|\mathbf{v} - \mathbf{u}| = \sqrt{(v_{\parallel} - u_{\parallel})^2 + v_{\perp}^2 + u_{\perp}^2 - 2v_{\perp}u_{\perp}\cos(\theta_v - \theta_u)}$ from which it is easy to observe that $(\partial_{\theta_v} + \partial_{\theta_u})|\mathbf{v} - \mathbf{u}| = 0$, and then further show that the Rosenbluth potentials become independent of the cylindrical angle θ_v when the 3D potentials are integrated over the angle θ_u . In order to compute the axisymmetric collision operator in cylindrical velocity-space coordinates, we thus need the expressions

$$\begin{aligned} \frac{\partial\varphi_b^k}{\partial\mathbf{v}} \cdot \frac{\partial F_a^\ell}{\partial\mathbf{v}} &= \frac{\partial\varphi_b^k}{\partial v_{\parallel}} \frac{\partial F_a^\ell}{\partial v_{\parallel}} + \frac{\partial\varphi_b^k}{\partial v_{\perp}} \frac{\partial F_a^\ell}{\partial v_{\perp}}, \\ \frac{\partial^2\psi_b^k}{\partial\mathbf{v}\partial\mathbf{v}} \cdot \frac{\partial^2 F_a^\ell}{\partial\mathbf{v}\partial\mathbf{v}} &= \frac{\partial^2\psi_b^k}{\partial v_{\perp}^2} \frac{\partial^2 F_a^\ell}{\partial v_{\perp}^2} + 2 \frac{\partial^2\psi_b^k}{\partial v_{\perp}\partial v_{\parallel}} \frac{\partial^2 F_a^\ell}{\partial v_{\perp}\partial v_{\parallel}} + \frac{1}{v_{\perp}^2} \frac{\partial\psi_b^k}{\partial v_{\perp}} \frac{\partial F_a^\ell}{\partial v_{\perp}} + \frac{\partial^2\psi_b^k}{\partial v_{\parallel}^2} \frac{\partial^2 F_a^\ell}{\partial v_{\parallel}^2}. \end{aligned}$$

As these expressions are also summations of products of two functions the equation for the weights is obtained in the same manner as was described above.

Derivatives of the distribution function are simple to calculate analytically and the derivatives of the potential functions ψ_i become

$$\begin{aligned}\frac{\partial^2 \psi_i}{\partial v_{\parallel}^2} &= -\frac{\gamma_i^{1/2}}{8\pi} \left\langle \frac{\Psi'(\gamma_i^{1/2}|\mathbf{v} - \mathbf{v}_i|)}{\gamma_i^{1/2}|\mathbf{v} - \mathbf{v}_i|} + \gamma_i(v_{\parallel} - v_{i,\parallel})^2 \left(\frac{\Psi''(\gamma_i^{1/2}|\mathbf{v} - \mathbf{v}_i|)}{\gamma_i|\mathbf{v} - \mathbf{v}_i|^2} - \frac{\Psi'(\gamma_i^{1/2}|\mathbf{v} - \mathbf{v}_i|)}{\gamma_i^{3/2}|\mathbf{v} - \mathbf{v}_i|^3} \right) \right\rangle_{\theta_i}, \\ \frac{\partial \psi_i}{\partial v_{\perp}} &= -\frac{1}{8\pi} \left\langle \gamma_i^{1/2} [v_{\perp} - v_{i,\perp} \cos(\theta - \theta_i)] \frac{\Psi'(\gamma_i^{1/2}|\mathbf{v} - \mathbf{v}_i|)}{\gamma_i^{1/2}|\mathbf{v} - \mathbf{v}_i|} \right\rangle_{\theta_i}, \\ \frac{\partial^2 \psi_i}{\partial v_{\perp}^2} &= -\frac{\gamma_i^{1/2}}{8\pi} \left\langle \frac{\Psi'(\gamma_i^{1/2}|\mathbf{v} - \mathbf{v}_i|)}{\gamma_i^{1/2}|\mathbf{v} - \mathbf{v}_i|} + \gamma_i(v_{\perp} - v_{i,\perp} \cos(\theta - \theta_i))^2 \left[\frac{\Psi''(\gamma_i^{1/2}|\mathbf{v} - \mathbf{v}_i|)}{\gamma_i|\mathbf{v} - \mathbf{v}_i|^2} - \frac{\Psi'(\gamma_i^{1/2}|\mathbf{v} - \mathbf{v}_i|)}{\gamma_i^{3/2}|\mathbf{v} - \mathbf{v}_i|^3} \right] \right\rangle_{\theta_i}, \\ \frac{\partial^2 \psi_i}{\partial v_{\perp} \partial v_{\parallel}} &= -\frac{\gamma_i^{1/2}}{8\pi} \left\langle \gamma_i(v_{\parallel} - v_{i,\parallel}) [v_{\perp} - v_{i,\perp} \cos(\theta - \theta_i)] \left[\frac{\Psi''(\gamma_i^{1/2}|\mathbf{v} - \mathbf{v}_i|)}{\gamma_i|\mathbf{v} - \mathbf{v}_i|^2} - \frac{\Psi'(\gamma_i^{1/2}|\mathbf{v} - \mathbf{v}_i|)}{\gamma_i^{3/2}|\mathbf{v} - \mathbf{v}_i|^3} \right] \right\rangle_{\theta_i},\end{aligned}$$

where $\langle \cdot \rangle_{\theta}$ refers to integration over the angle θ . Similarly one would calculate the derivatives for the potential φ_i . For the results presented in Ref. [2] these integrals were evaluated numerically using the Simpson's rule which is a particularly good method for periodic integrands. High level of accuracy can be obtained already with 100 integration points, as the integrands are periodic with respect to the angle θ .

Summary We have described in detail the numerical implementation of the Gaussian radial basis function method to discretize the Fokker-Planck collision operator in both full 3D and in axisymmetric 2D velocity space. Especially, we focused explicitly on decomposing the rank-3 tensor that appears in the collision operator into a form that only requires storing rank-2 matrices. This approach saves both memory and computation time. In addition, we gave explicit formulas for evaluating the axisymmetric velocity space derivatives of the Rosenbluth potentials that are needed for the axisymmetric implementation.

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