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FPPAC--A Two-Dimensional Multispecies
Nonlinear Fokker-Planck Package

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[illegible]

No. of cards in combined program and test deck: 7000 per machine

Card punching code: 026

CPC Library subprograms used: None

Reference to other published version of this program: None

Keywords: Two-Dimensional, Multispecies, Implicit, Nonlinear, Fokker-Planck

SUMMARY

Nature of the Physical Problem

The complete nonlinear multispecies Fokker-Planck collision operator for a plasma in two-dimensional velocity space is solved. The operator is expressed in terms of spherical coordinates (v =speed, θ =angle between velocity and magnetic field directions, ϕ =azimuthal angle) under the assumption of azimuthal symmetry. Provision is made for additional physics contributions.

Method of Solution

The Fokker-Planck equation is solved using finite differences. Spatial derivatives are approximated by central differences. Time-advancement is accomplished through either implicit operator splitting, an alternating direction implicit (ADI) algorithm, or fully implicit differencing. (In the latter case the user must supply his own nine-banded linear systems solver.) The Fokker-Planck coefficients and their derivatives are computed by expanding the distribution functions and the Rosenbluth potentials⁽¹⁾ in Legendre series, and equating the respective series coefficients.

Restrictions on the Complexity of the Problem

The user must adjust the number of meshpoints in the two coordinate directions as well as the number of Legendre polynomials used to calculate the Fokker-Planck coefficients. Sufficient accuracy for most problems is attained on both the CRAY and 7600. However, double precision should be used on a 32-bit-word machine.

Typical Running Time

(CRAY) 9.6 μ s/meshpoint/species are required to compute the Fokker-Planck coefficients. 1.9 μ s/meshpoint are required to time-advance the distribution function for one species using implicit operator splitting. These times vary to some extent with the mesh configuration due to variations in vectorization efficiency. The package runs 10-12 times slower on the CDC-7600.

Unusual Features of the Program

None

References

1. J. Killeen, A.A. Mirin, and M.E. Rensink, "The Solution of the Kinetic Equations for a Multispecies Plasma," in Methods in Computational Physics 16, Academic Press (1976), 389.
2. J. Killeen and A.A. Mirin, "Numerical Solution of the Fokker-Planck Equations for a Multispecies Plasma," in College in Theoretical and Computational Plasma Physics, Trieste (1977), IAEA, Vienna, 27.
3. M.G. McCoy, A.A. Mirin, and J. Killeen, "A Vectorized Fokker-Planck Package for the Cray-1," Scientific Computer Exchange Meeting, Livermore (1979), UCRL-83206.
4. A.I. Shestakov, "Users Manual for ILUCG," Lawrence Livermore Laboratory Internal Document UCID-18560 (1980).

Note: Separate source decks for CRAY-1 and CDC-7600 versions are provided.

LONG WRITE-UP

1. INTRODUCTION

In the simulation of magnetically confined plasmas in which the ions or electrons are non-Maxwellian and where a knowledge of the distribution functions is important, kinetic equations must be solved. In both mirror and tokamak confinement devices non-Maxwellian plasmas may be present. This may be due to the presence of extensive loss regions in velocity space or to the injection of energetic neutral beams. The kinetic equation to be solved is the Boltzmann equation with Fokker-Planck Coulomb collision terms.

This nonlinear partial differential equation, which describes the evolution of the distribution functions of all charged species in the plasma, has seven independent variables (three spatial coordinates, three velocity coordinates and time). Consequently, a number of simplifications must be introduced into the equation to allow any present day computer to solve the problem. One can reduce the number of independent variables to three by neglecting spatial dependence and by assuming azimuthal symmetry of the distribution functions about the direction of the magnetic field. With these simplifications, Rosenbluth, MacDonald and Judd ⁽⁵⁾ succeeded in expressing the equation in a form suitable for solution on a computer.

Subsequently, a number of computer programs have been developed ^{(1),(6)} which solve this equation. These Fokker-Planck codes are frequently incorporated in larger codes which simulate additional physical processes such as quasi-linear diffusion due to radio frequency heating ⁽⁷⁾ and spatial diffusion of the plasma ⁽⁸⁾.

A problem encountered in these programs has been the long run times required to solve the Fokker-Planck equation, and this problem is aggravated in studies for which it is necessary to solve for the operator at a large number of spatial points or when very high resolution is required. A further problem occurs when making improvements to the numerical algorithm, for changes have to be made in the source decks of all of the codes employing the same form of the Fokker-Planck operator. These two difficulties are alleviated by a newly

developed program consisting of a skeleton driver plus package, FPPAC, the latter of which time-advances the Fokker-Planck equations in 2D velocity space for an arbitrary number of charged "general" species in the presence of an arbitrary number of fixed background Maxwellian species.

The driver/package may be run as a stand-alone code, thereby serving as the kernel of a new code, or the package itself may be stripped from the driver and incorporated into an existing code ^{(7),(8),(9)}. Moreover, additional physics (e.g., rf heating ⁽⁷⁾, magnetic compression ⁽¹⁾, neutral injection ⁽¹⁾) may be represented by merely setting existing array elements; detailed instructions are provided in the source listing. There are two versions of the package--one optimized for the CRAY-1 and the other optimized for the CDC-7600. The CRAY version runs an order of magnitude faster than the 7600 version.

2. THE FOKKER-PLANCK OPERATOR

The Boltzmann equation for the distribution function of each plasma species is given by

$$\frac{\partial f_a}{\partial t} + \underline{v} \cdot \frac{\partial f_a}{\partial \underline{x}} + \frac{\underline{F}}{m_a} \cdot \frac{\partial f_a}{\partial \underline{v}} = \left(\frac{\partial f_a}{\partial t} \right)_c, \quad (1)$$

where f_a is the distribution function of species type "a", $\underline{F}$ is a force field and $\left(\frac{\partial f_a}{\partial t} \right)_c$ is the Fokker-Planck operator representing the rate of change of the distribution function due to Coulomb collisions.

With the simplifying assumption that the Fokker-Planck operator depends only on the velocity, $\underline{v}$, and not upon spatial position, $\underline{x}$, the operator as derived by Rosenbluth et al. ⁽⁵⁾ has the form

$$\left(\frac{\partial f_a}{\partial t}\right)_c = \Gamma_a \left\{ -\frac{\partial}{\partial v_i} \left(f_a \frac{\partial h_a}{\partial v_i} \right) + \frac{1}{2} \frac{\partial^2}{\partial v_i \partial v_j} \left(f_a \frac{\partial^2 g_a}{\partial v_i \partial v_j} \right) \right\}, \quad (2)$$

where the usual summing conventions over repeated indices "i" and "j" are to be used and where $\Gamma_a = 4\pi Z_a^4 e^4 / m_a^2$. The "Rosenbluth potentials" are written as

$$g_a = \sum_b \left(\frac{Z_b}{Z_a} \right)^2 \ln \Lambda_{ab} \int f_b(\underline{v}') |\underline{v} - \underline{v}'| d\underline{v}' \quad (3a)$$

$$h_a = \sum_b \frac{m_a + m_b}{m_b} \left(\frac{Z_b}{Z_a} \right)^2 \ln \Lambda_{ab} \cdot \int f_b(\underline{v}') |\underline{v} - \underline{v}'|^{-1} d\underline{v}'. \quad (3b)$$

The Coulomb logarithm, which depends on both interacting species, is

$$\ln \Lambda_{ab} = \ln \left\{ \left(\frac{m_a m_b}{m_a + m_b} \right) \frac{2\alpha c \lambda_D}{e^2} \cdot \sup \left(\frac{2E_k}{m_k} \right)_{a,b}^{\frac{1}{2}} \right\} - \frac{1}{2},$$

where $\alpha = 0.0073$ is the fine structure constant, $\lambda_D = \sqrt{E_e / 6\pi n_e e^2}$ is the Debye length, E_k is the energy of species k, n_e is the electron density, and E_e is the electron mean energy. (The electrons may be treated either as a general species with distribution function f_e or as a background Maxwellian.)

Under the further assumption that the distribution functions f_a are azimuthally symmetric about the direction of the magnetic field, the formulation given above may be recast as a two dimensional problem when written in spherical polar coordinates (v, θ, ϕ) , where v is the speed, θ is the angle between the velocity vector and the magnetic field, and ϕ is the azimuthal angle. In this case the density and energy-density of species "a" are defined according to

$$n_a = 2\pi \iint f_a(v, \theta) v^2 \sin \theta \, dv \, d\theta \quad (4a)$$

$$n_a E_a = m_a \iint f_a(v, \theta) v^4 \sin \theta \, dv \, d\theta. \quad (4b)$$

Equation (2) then becomes

$$\frac{1}{\Gamma_a} \left(\frac{\partial f_a}{\partial t} \right)_c = \frac{1}{v^2} \frac{\partial G_a}{\partial v} + \frac{1}{v^2 \sin \theta} \frac{\partial H_a}{\partial \theta}, \quad (5)$$

where

$$G_a = A_a f_a + B_a \frac{\partial f_a}{\partial v} + C_a \frac{\partial f_a}{\partial \theta} \quad (6)$$

$$H_a = D_a f_a + E_a \frac{\partial f_a}{\partial v} + F_a \frac{\partial f_a}{\partial \theta}. \quad (7)$$

The coefficients A_a , B_a , C_a , D_a , E_a and F_a are given by:

$$A_a = \frac{v^2}{2} \frac{\partial^3 g_a}{\partial v^3} + v \frac{\partial^2 g_a}{\partial v^2} - \frac{\partial g_a}{\partial v} - v^2 \frac{\partial h_a}{\partial v} - \frac{1}{v} \frac{\partial^2 g_a}{\partial \theta^2} + \frac{1}{2} \frac{\partial^3 h_a}{\partial v \partial \theta^2} - \frac{\cot \theta}{v} \frac{\partial g_a}{\partial \theta} + \frac{\cot \theta}{2} \frac{\partial^2 g_a}{\partial v \partial \theta} \quad (8)$$

$$B_a = \frac{v^2}{2} \frac{\partial^2 g_a}{\partial v^2} \quad (9)$$

$$C_a = -\frac{1}{2v} \frac{\partial g_a}{\partial \theta} + \frac{1}{2} \frac{\partial^2 g_a}{\partial v \partial \theta} \quad (10)$$

$$D_a = \frac{\sin \theta}{2v^2} \frac{\partial^3 g_a}{\partial \theta^3} + \frac{\sin \theta}{2} \frac{\partial^3 g_a}{\partial v^2 \partial \theta} + \frac{\sin \theta}{v} \frac{\partial^2 g_a}{\partial v \partial \theta} - \frac{1}{2v^2 \sin \theta} \frac{\partial g_a}{\partial \theta} + \frac{\cos \theta}{2v^2} \frac{\partial^2 g_a}{\partial \theta^2} - \sin \theta \frac{\partial h_a}{\partial \theta} \quad (11)$$

$$E_a = \sin \theta \left[-\frac{1}{2v} \frac{\partial g_a}{\partial \theta} + \frac{1}{2} \frac{\partial^2 g_a}{\partial v \partial \theta} \right] \quad (12)$$

$$F_a = \frac{\sin \theta}{2v^2} \frac{\partial^2 g_a}{\partial \theta^2} + \frac{\sin \theta}{2v} \frac{\partial g_a}{\partial v}. \quad (13)$$

As suggested by Rosenbluth et al.⁽⁵⁾, the "Rosenbluth potentials" and the distribution functions themselves may be represented by expansions in Legendre polynomials. For this purpose we let

$$f_b(v, \theta, t) = \sum_{l=0}^{\infty} v_l^b(v, t) P_l(\cos \theta) \quad (14)$$

where

$$v_l^b(v, t) = \frac{2l+1}{2} \int_{-1}^{+1} f_b(v, \cos \theta, t) P_l(\cos \theta) d(\cos \theta). \quad (15)$$

The expansions for the potentials are

$$g_a(v, \theta, t) = \sum_{l=0}^{\infty} \sum_b \left(\frac{z_b}{z_a} \right)^2 \epsilon_n \lambda_{ab} v_l^b(v, t) P_l(\cos \theta) \quad (16)$$

and

$$h_a(v, \theta, t) = \sum_{l=0}^{\infty} \sum_b \left(\frac{m_a + m_b}{m_b} \right) \left(\frac{z_b}{z_a} \right)^2 \epsilon_n \lambda_{ab} A_l^b(v, t) P_l(\cos \theta) \quad (17)$$

with coefficients

$$A_l^b = \frac{4\pi}{2l+1} \left[\int_0^v \frac{(v')^{l+2}}{v^{l+1}} v_l^b(v', t) dv' + \int_v^\infty \frac{v^l}{(v')^{l-1}} v_l^b(v', t) dv' \right] \quad (18)$$

$$B_l^b = - \frac{4\pi}{4l^2-1} \left[\int_0^v \frac{(v')^{l+2}}{v^{l-1}} \cdot \left(1 - \frac{l-1/2}{l+3/2} \frac{(v')^2}{v^2} \right) v_l^b(v', t) dv' + \int_v^\infty \frac{v^l}{(v')^{l-3}} \left(1 - \frac{l-1/2}{l+3/2} \frac{v^2}{(v')^2} \right) \cdot v_l^b(v', t) dv' \right]. \quad (19)$$

It is notationally convenient to define four functionals

$$M_l(w)(v) = \int_v^\infty w(y) y^{(1-l)} dy \quad (20)$$

$$N_l(w)(v) = \int_0^v w(y) y^{(2+l)} dy \quad (21)$$

$$R_l(w)(v) = \int_v^\infty w(y) y^{(3-l)} dy \quad (22)$$

$$E_l(w)(v) = \int_0^v w(y) y^{(4+l)} dy. \quad (23)$$

Using these functionals, Eqs. (18) and (19) become

$$A_l^b = \frac{4\pi}{(2l+1)} \left[v^{-l-1} N_l(v_l^b) + v^l M_l(v_l^b) \right]. \quad (24)$$

$$B_l^b = \frac{4\pi}{2l+1} \left\{ \frac{1}{(2l+3)} \left[v^{-l-1} E_l(v_l^b) + v^{l+2} M_l(v_l^b) \right] - \frac{1}{(2l-1)} \left[v^{l-1} N_l(v_l^b) + v^l R_l(v_l^b) \right] \right\}. \quad (25)$$

Evaluation of the coefficients defined in Eqs. (8)-(13) requires derivatives of the "Rosenbluth potentials". These may be obtained through term by term differentiation of Eqs. (16)-(17). To obtain derivatives with respect to v requires differentiation of the right side of Eqs. (24)-(25). This is done analytically.

The resulting expressions are

$$\frac{\partial A_l^b}{\partial v} = \frac{4\pi}{(2l+1)} \left[l v^{l-1} M_l(v_l^b) - (l+1) v^{-l-2} N_l(v_l^b) \right] \quad (26)$$

$$\begin{aligned} \frac{\partial B_l^b}{\partial v} = & \frac{4\pi}{(2l+1)} \left\{ \frac{1}{(2l+3)} \left[(l+2) v^{l+1} M_l(v_l^b) - (l+1) v^{-l-2} E_l(v_l^b) \right] \right. \\ & \left. - \frac{1}{(2l-1)} \left[l v^{l-1} R_l(v_l^b) - (l-1) v^{-l} N_l(v_l^b) \right] \right\} \quad (27) \end{aligned}$$

$$\begin{aligned} \frac{\partial^2 B_l^b}{\partial v^2} = & \frac{4\pi}{(2l+1)} \left\{ \frac{(l+1)(l+2)}{(2l+3)} \left[v^{-l-3} E_l(v_l^b) + v^l M_l(v_l^b) \right] \right. \\ & \left. - \frac{l(l-1)}{(2l-1)} \left[v^{-l-1} N_l(v_l^b) + v^{l-2} R_l(v_l^b) \right] \right\} \end{aligned} \quad (28)$$

$$\begin{aligned} \frac{\partial^3 B_l^b}{\partial v^3} = & \frac{4\pi}{(2l+1)} \left\{ \frac{1}{(2l+3)} \left[l(l+1)(l+2) v^{l-1} M_l(v_l^b) \right. \right. \\ & \left. - (l+1)(l+2)(l+3) v^{-l-4} E_l(v_l^b) \right] \\ & - \frac{1}{(2l-1)} \left[l(l-1)(l-2) v^{-l-3} R_l(v_l^b) \right. \\ & \left. \left. - (l+1)(l)(l-1) v^{-l-2} N_l(v_l^b) \right] \right\} \end{aligned} \quad (29)$$

Derivatives with respect to θ are also done analytically.

3. BOUNDARY CONDITIONS

Eq. (5) may be solved either in full velocity space or in some subspace. The full velocity-space boundary conditions are

$$f_a(v = 0, \theta) \text{ is independent of } \theta \quad (30)$$

$$\frac{\partial f_a}{\partial v}(v = 0, \theta = \pi/2) = 0 \quad (31)$$

$$f(v = \infty, \theta) = 0 \quad (32)$$

$$\frac{\partial f_a}{\partial \theta}(v, \theta = 0) = \frac{\partial f_a}{\partial \theta}(v, \theta = \pi) = 0. \quad (33)$$

For problems with symmetry about the angle $\theta = \pi/2$, it is assumed that

$$\frac{\partial f_a}{\partial \theta}(v, \theta = \pi/2) = 0. \quad (34)$$

In situations where there is a loss cone or separatrix in velocity space, a Dirichlet-like condition may be substituted, i.e., instead of using Eqs. (30)-(33), one may specify values of f_a along curves $(v, \theta_{\min}^a(v))$, $(v, \theta_{\max}^a(v))$, $(v_{\min}^a(\theta), \theta)$, $(v_{\max}^a(\theta), \theta)$. It is often appropriate to combine such Dirichlet conditions with full velocity space conditions, as in the case of electrons trapped in a magnetic well in the presence of a confining potential.⁽⁹⁾

4. MESH DEFINITION

The independent variables v and θ are represented by meshes $\{v_j\}_{j=1}^J$ and $\{\theta_i\}_{i=1}^I$, respectively. These meshes do not have to be uniform. The first velocity meshpoint, v_1 , will always equal 0. The theta domain may be of two types:

(1) assumed symmetry of the distribution functions about $\theta = \pi/2$, in which case $\theta_1 = \pi/2$. This scenario utilizes an extra reflection point $\theta_{I+1} = \pi - \theta_{I-1}$.

(2) no assumed symmetry of the distribution functions. Here, the theta mesh is taken to be symmetric about $\theta = \pi/2$, with a meshpoint right at $\theta = \pi/2$, so that I must be odd. In either case, θ_1 need not be equal to 0.

5. NUMERICAL INTEGRATION IN VELOCITY SPACE

Numerical integration in velocity space is accomplished through a variation of trapezoidal integration. In the v direction,

$$\int f(v) v^2 dv \approx \sum_{j=1}^J a_j f(v_j), \quad (35)$$

where

$$a_1 = v_2^3 / 24 \quad (36)$$

$$a_j = v_j^2 \left(\frac{v_{j+1} - v_{j-1}}{2} \right), \quad 1 < j < J \quad (37)$$

$$a_J = v_J^2 \left(\frac{v_J - v_{J-1}}{2} \right). \quad (38)$$

Eq. (36) assumes $f(v)$ is constant between $v = 0$ and $v = v_2/2$, so that

$$\int_{v_1=0}^{v_2/2} f(v) v^2 dv = f(v_1) \cdot \left(\frac{v_2}{2} \right)^3 / 3. \quad (39)$$

This procedure is more accurate than the straight-forward scheme having $a_1 = v_1^2 \left(\frac{v_2 - v_1}{2} \right) = 0$. In the θ direction,

$$\int f(\theta) \sin \theta d\theta \approx \sum_{i=1}^I b_i f(\theta_i), \quad (40)$$

where

$$b_1 = \left\{ \begin{array}{ll} \sin^2 \theta_1 \left(\frac{\theta_2 - \theta_1}{2} \right) & \text{if } \theta_1 \neq 0 \\ \theta_2^2/8 & \text{if } \theta_1 = 0 \end{array} \right\} \quad (41)$$

$$b_i = \sin \theta_i \left(\frac{\theta_{i+1} - \theta_{i-1}}{2} \right), \quad 1 < i < I \quad (42)$$

$$b_I = \left\{ \begin{array}{ll} \sin \theta_I \left(\frac{\theta_I - \theta_{I-1}}{2} \right) & \text{if } \theta_I \neq \pi \\ (\pi - \theta_{I-1})^2/8 & \text{if } \theta_I = \pi \end{array} \right\}. \quad (43)$$

Thus, the density of species "a" is computed as

$$n_a = 2\pi \sum_{i,j} a_j b_i f_a(v_j, \theta_i), \quad (44a)$$

and the energy-density of species "a" is

$$n_a E_a = m_a \sum_{i,j} a_j b_i v_j^2 f_a(v_j, \theta_i). \quad (44b)$$

6. COMPUTATION OF FOKKER-PLANCK COEFFICIENTS

The collision operator, $\left(\frac{\partial f_a}{\partial t} \right)_c$, may be written as a sum

$$\left(\frac{\partial f_a}{\partial t} \right)_c = \sum_b \left(\frac{\partial f_a}{\partial t} \right)_c^b, \quad (45)$$

where $\left(\frac{\partial f_a}{\partial t}\right)_c^b$ represents collisions of species "a" with species "b". In computing $\left(\frac{\partial f_a}{\partial t}\right)_c^b$ for a general species "b", the procedure is that outlined in Eqs. (5) through (29), with the proviso that the sum over "b" in Eqs. (16) and (17) be replaced by the single index "b". The only numerical approximations come about in the integrals of Eqs. (15) and (20) through (23). Eq. (15) is approximated using Eqs. (41)-(43). Eqs. (20)-(23) are approximated by

$$\int_{v_k}^{v_l} f(v) dv = \sum_{j=k}^{l-1} \left(\frac{v_{j+1} - v_j}{2} \right) \left(f(v_j) + f(v_{j+1}) \right). \quad (46)$$

A detailed explanation of the do-loop structure for the vectorized CRAY version is given in Appendix A.

Up to this point the assumption has been made that "b" is a "general" species represented by a 2D velocity space distribution function. Recalling that PPAC allows fixed background Maxwellian species in addition to general species, the procedure when "b" is a Maxwellian simplifies somewhat. Letting n_b denote its density and T_b its temperature,

$$\left(\frac{\partial f_a}{\partial t}\right)_c^b = \frac{\Gamma_a}{v^2} \left(\frac{\partial}{\partial v} \left(A_a^b f_a + B_a^b \frac{\partial f_a}{\partial v} \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(F_a^b \frac{\partial f_a}{\partial \theta} \right) \right), \quad (47)$$

with

$$A_a^b = \left(\frac{Z_b}{Z_a} \right)^2 \lambda_n \lambda_{ab} \frac{m_a}{m_b} n_b \left(-\frac{v}{v_b} \sqrt{\frac{2}{n}} e^{-v^2/2v_b^2} + \phi \left(\frac{v}{\sqrt{2}} \frac{v_b}{v_h} \right) \right) \quad (48)$$

$$B_a^b = \frac{v_b^2}{v} \frac{m_b}{m_a} A_n^b \quad (49)$$

$$F_a^b = \left(\frac{Z_b}{Z_a} \right)^2 n_{ab} \frac{v_b \sin \theta}{2v} \left(\frac{v_b}{v} \sqrt{\frac{2}{\pi}} e^{-v^2/2v_b^2} + \left(1 - \frac{v_b^2}{v^2} \right) \phi \left(\frac{v}{\sqrt{2}v_b} \right) \right). \quad (50)$$

Here, n_b is the density of species "b", $v_b^2 = T_b/m_b$, and ϕ is the error function

$$\phi(x) = 2/\sqrt{\pi} \int_0^x e^{-y^2} dy. \quad (51)$$

For $x < 0.6$, $\phi(x)$ is approximated by a power series:

$$\phi(x) \approx \sum_{k=0}^6 (-1)^k \frac{x^{2k+2}}{k!(2k+1)}, \quad (52)$$

and for $x \geq 0.6$,

$$\phi(x) \approx 1 - \frac{2}{\sqrt{\pi}} e^{-x^2} \sum_{k=1}^5 A_k x^k, \quad (53)$$

with

$$\eta = 1/(1 + px), \quad (54)$$

and $p = 0.3275911$, $A_1 = 0.225836846$, $A_2 = -0.252128668$, $A_3 = 1.25969513$, $A_4 = -1.287822453$ and $A_5 = 0.94064607^{(10)}$.

7. AUGMENTED EQUATIONS

There are many situations in which it is desirable to model not only Coulomb collisions but additional physics as well (e.g., rf heating, electric field acceleration). This is provided for to the extent that the equations to be time-advanced are of the general form (dropping species identifier "a")

$$Q \frac{\partial f}{\partial t} = \frac{1}{v^2} \frac{\partial}{\partial v} \left(A f + B \frac{\partial f}{\partial v} + C \frac{\partial f}{\partial \theta} \right) + \frac{1}{v^2 \sin \theta} \frac{\partial}{\partial \theta} \left(D f + E \frac{\partial f}{\partial v} + F \frac{\partial f}{\partial \theta} \right) + K f + J, \quad (55)$$

where A,B,C,D,E,F,J,K and Q are arbitrary functions of v and θ . The coefficients A,B,C,D,E,F include contributions from the collision operator $\left(\frac{\partial f}{\partial t}\right)_c$ as computed in Section 6 and possible user-supplied contributions. The coefficients J, K and Q are also user-supplied, so that neutral beam injection (I) and charge exchange (K) may be conveniently modeled. The quantity Q is normally equal to 1, but it may be specified arbitrarily either for debugging purposes or for representing a species-dependent or spatially varying timestep. Implementation details may be found in the source listing.

8. SPATIAL DISCRETIZATION

Spatial derivatives are discretized as follows:

$$\begin{aligned} \left. \frac{\partial}{\partial v} (A f) \right|_{i,j} &= (A_{i,j+1} f_{i,j+1} - A_{i,j-1} f_{i,j-1}) / 2 \Delta v_j \\ \left. \frac{\partial}{\partial v} \left(B \frac{\partial f}{\partial v} \right) \right|_{i,j} &= \left\{ B_{i,j+1/2} \left(\frac{f_{i,j+1} - f_{i,j}}{\Delta v_{j+1/2}} \right) \right. \end{aligned} \quad (56)$$

$$- B_{1,j-1} / 2 \left(\frac{f_{1,j} - f_{1,j-1}}{\Delta v_{j-1/2}} \right) \Delta v_j \quad (57)$$

$$\begin{aligned} \frac{\partial}{\partial v} \left(C \frac{\partial f}{\partial \theta} \right) \Big|_{1,j} = & \left\{ C_{1,j+1} \left(\frac{f_{1+1,j+1} - f_{1-1,j+1}}{2\Delta\theta_1} \right) \right. \\ & \left. - C_{1,j-1} \left(\frac{f_{1+1,j-1} - f_{1-1,j-1}}{2\Delta\theta_1} \right) \right\} / 2\Delta v_j \end{aligned} \quad (58)$$

where

$$\Delta v_{j\pm 1/2} = \pm (v_{j\pm 1} - v_j) \quad (59a)$$

$$\Delta v_j = \frac{1}{2} (\Delta v_{j-1/2} + \Delta v_{j+1/2}) \quad (59b)$$

$$\Delta\theta_1 = \frac{1}{2} (\theta_{1+1} - \theta_{1-1}) \quad (59c)$$

$$B_{1,j\pm \frac{1}{2}} = \frac{1}{2} (B_{1,j} + B_{1,j\pm 1}) \quad (59d)$$

The terms $\frac{\partial}{\partial \theta} (DF)$, $\frac{\partial}{\partial \theta} (E \frac{\partial f}{\partial v})$ and $\frac{\partial}{\partial \theta} (F \frac{\partial f}{\partial \theta})$ are differenced analogously.

The boundary conditions must also be approximated; their discretization depends on the time-integration technique and will be discussed in a later section.

9. TIME DISCRETIZATION

Eq. (55) is time-integrated using either implicit operator splitting, an alternating direction implicit (ADI) method, or fully implicit differencing.

Because implicit operator splitting and ADI are so similar, of the two only ADI⁽¹¹⁾ will be described in detail. This is a two-step procedure, as follows:

$$Q^n \left(\frac{f^{n+1/2} - f^n}{\Delta t/2} \right) = \frac{1}{v^2} \frac{\delta}{\delta v} \left(A^n f^{n+1/2} + B^n \frac{\delta f^{n+1/2}}{\delta v} + C^n \frac{\delta f^n}{\delta \theta} \right) + \frac{1}{v^2 \sin \theta} \frac{\delta}{\delta \theta} \left(D^n f^n + E^n \frac{\delta f^n}{\delta v} + F^n \frac{\delta f^n}{\delta \theta} \right) + K^n f^{n+1/2} + J^n \quad (60)$$

$$Q^n \left(\frac{f^{n+1} - f^{n+1/2}}{\Delta t/2} \right) = \frac{1}{v^2} \frac{\delta}{\delta v} \left(A^n f^{n+1/2} + B^n \frac{\delta f^{n+1/2}}{\delta v} + C^n \frac{\delta f^{n+1/2}}{\delta \theta} \right) + \frac{1}{v^2 \sin \theta} \frac{\delta}{\delta \theta} \left(D^n f^{n+1} + E^n \frac{\delta f^{n+1/2}}{\delta v} + F^n \frac{\delta f^{n+1}}{\delta \theta} \right) + K^n f^{n+1} + J^n, \quad (61)$$

where the meshpoint indices i, j have been dropped, and where $\frac{\delta}{\delta v}$ and $\frac{\delta}{\delta \theta}$ denote the discretizations of Eqs. (56) - (59). For computational expediency, the mixed derivative terms are treated explicitly. This algorithm executes a good deal faster than a fully implicit method since several small tri-diagonal linear systems are inverted instead of a large nine-banded system. It is generally not necessary to iterate Eqs. (60) and (61), since the Fokker-Planck coefficients depend on integrals of the distribution functions and therefore are slowly varying.

For full velocity space operation, Eqs. (60) and (61), which hold at interior meshpoints, are joined by boundary value equations. Letting

$$G = Af + B \frac{\delta f}{\delta v} + C \frac{\delta f}{\delta \theta} \quad (62)$$

$$H = Df + E \frac{\delta f}{\delta v} + F \frac{\delta f}{\delta \theta}, \quad (63)$$

Eq. (60) is calculated as follows:

At $\theta = 0$ ($i = 1$), $\frac{1}{v^2 \sin \theta} \frac{\delta H}{\delta \theta}$ (the second term on the right hand side) is replaced by

$$\frac{1}{v^2 \sin \theta} \frac{\delta H}{\delta \theta} \Big|_{1,j} = 2H_{3/2,j}^n / v_j^2 \theta_{3/2}^2. \quad (64)$$

In cases where f is symmetric about $\pi/2$, the approximation

$$f_{I+1,j}^{n+1/2} = f_{I-1,j}^{n+1/2} \quad (65)$$

is used, and in cases where $\theta_I = \pi$, $\frac{1}{v^2 \sin \theta} \frac{\delta H}{\delta \theta}$ is replaced by

$$\frac{1}{v^2 \sin \theta} \frac{\delta H}{\delta \theta} \Big|_{I,j} = -2H_{I-1/2,j}^n / v_j^2 (\pi - \theta_{I-1/2})^2. \quad (66)$$

At $\theta = 0$ and π , the $C^n \frac{\delta f^n}{\delta \theta}$ term in Eq. (60) is set to 0. (See Eq. (33).)

At $v = 0$, the first term on the right hand side of Eq. (60) is written as

$$\left. \frac{1}{v^2} \frac{\delta G}{\delta v} \right|_{i,1} = \frac{3}{v} \frac{3}{3/2} G_{i,3/2}^{n+1/2}, \quad (67)$$

and

$$\left. \frac{1}{v^2 \sin \theta} \frac{\delta H}{\delta \theta} \right|_{i,1} = 0, \quad (68)$$

where

$$G^{n+1/2} = A^n f^{n+1/2} + B^n \frac{\delta f^{n+1/2}}{\delta v} + C^n \frac{\delta f^n}{\delta \theta}, \quad (69)$$

with the $C^n \frac{\delta f^n}{\delta \theta}$ term ignored at $\theta = 0$ and π (See Eq. (33)).

Eq. (61), the second half time-step, is calculated analogously: At $\theta = 0$ ($i = 1$), $\frac{1}{v^2 \sin \theta} \frac{\delta H}{\delta \theta}$ is replaced by

$$\frac{1}{v^2 \sin \theta} \frac{\delta H}{\delta \theta} = 2 \frac{H_{j/2,j}^{n+1}}{v_j^2 \theta_{j/2}^2}, \quad (70)$$

and at $\theta = \pi$ (when $\theta_I = \pi$),

$$\frac{1}{v^2 \sin \theta} \frac{\delta H}{\delta \theta} = -2 \frac{H_{I-1/2,j}^{n+1}}{v_j^2 (\pi - \theta_{I-1/2})^2}. \quad (71)$$

Here,

$$H^{n+1} = D^n f^{n+1} + E^n \frac{\delta f^{n+1/2}}{\delta v} + F^n \frac{\delta f^{n+1}}{\delta \theta}, \quad (72)$$

and the $C^n \frac{\delta f}{\delta \theta}$ term in Eq. (60) is again ignored. At $v = 0$,

$$f_{i,1}^{n+1} = \sum_{i=1}^I b_i \left(f_{i,1}^{n+1/2} + \frac{\Delta t}{2L_{i,1}} \frac{3}{v_{3/2}} \bar{G}_{i,3/2}^{n+1/2} \right) \left/ \sum_{i=1}^I b_i \right., \quad (73)$$

where b_i is as in Eqs. (41)-(43) and

$$\bar{G}^{n+1/2} = A^n f^{n+1/2} + B^n \frac{\delta f^{n+1/2}}{\delta v} + C^n \frac{\delta f^{n+1/2}}{\delta \theta}, \quad (74)$$

with the $\frac{\delta f}{\delta \theta}$ term ignored at $\bar{v} = 0$ and π . This procedure assures that, in the absence of sources and losses (and if $Q \equiv 1$), the numerical density (Eq. (44a)) does not change from timestep to timestep. The discrete boundary conditions for the fully implicit algorithm are similar, but actually much simpler since there is no time-splitting.

As mentioned in an earlier section, one is not restricted to full velocity space operation; that is, one may replace a subset of the above boundary conditions by Dirichlet conditions along given curves, which are approximated by open polygons in discrete v, θ space.

The principal difference equations, (Eqs. (60) and (61)) and the boundary conditions (Eqs. (62) - (72) or Dirichlet conditions or a combination thereof), may be cast in the following form:

$$- \alpha_{i,j}^n f_{i,j+1}^{n+1/2} + \beta_{i,j}^n f_{i,j}^{n+1/2} - \gamma_{i,j}^n f_{i,j-1}^{n+1/2} = \delta_{i,j}^n \quad (75)$$

$$- \epsilon_{i,j}^n f_{i+1,j}^{n+1} + \mu_{i,j}^n f_{i,j}^{n+1} - \nu_{i,j}^n f_{i-1,j}^{n+1} = \rho_{i,j}^n, \quad (76)$$

where $\alpha, \beta, \gamma, \delta, \epsilon, \nu, \rho$ are known quantities. The indices i, j range over all meshpoints. Vacuum terms should be ignored; e.g., $\gamma_{1,1}^n$ is 0 since $f_{1,0}^{n+1/2}$ makes no sense. In the event of conservation boundary conditions at $v = 0$, Eqs. (73) and (74), which decouple from Eq. (76), are solved after Eqs. (75) and (76).

The procedure for solving Eqs. (75) and (76) is a standard technique for solving tridiagonal systems⁽¹¹⁾. Eq. (75) is reduced to the form:

$$f_{i,j}^{n+1/2} = \sigma_{i,j} f_{i,j+1}^{n+1/2} + \tau_{i,j} \quad (77)$$

where

$$\sigma_{i,1} = \left(\beta_{i,j}^n - \gamma_{i,j}^n \sigma_{i,j-1} \right)^{-1} \alpha_{i,j}^n \quad (78)$$

$$\tau_{i,j} = \left(\beta_{i,j}^n - \gamma_{i,j}^n \sigma_{i,j-1} \right)^{-1} \left(\delta_{i,j}^n + \gamma_{i,j}^n \tau_{i,j-1} \right) \quad (79)$$

The quantities $\sigma_{i,1}$, $\tau_{i,1}$ and $f_{i,j}^{n+1/2}$ are determined through boundary conditions. Eqs. (77) ~ (79) (in the CRAY version) are vectorized over the index "i". Eq. (78) is reduced in an analogous manner, with vectorization over the index "j".

With fully implicit differencing one obtains a system of the form

$$M f^{n+1} = y, \quad (80)$$

where f^{n+1} , the distribution function at the new timestep, is viewed as a vector with I times J components corresponding to meshpoints ordered rowwise or columnwise. The matrix M is a nine-banded matrix, a consequence of the nine point difference algorithm. The discretization at the boundary points is similar to that for the ADI algorithm. The vector y depends on the distribution function at the old timestep, f^n , and the source term J . Both M and y are computed by FPPAC, whereas it is up to the user to supply an

algorithm for solving Eq. (80). The crucial common blocks, however, are compatible with those of the ILUCG package of Shestakov⁽⁴⁾, and implementation of ILUCG is consequently extremely simple.

10. ENERGY TRANSFER

The rate of energy transfer to (or from) each general species is computed. The rate of energy-density gained by species "a" due to collisions with species "b" is equal to the second moment of the operator which represents collisions between "a" and "b":

$$Q_{ab} = \pi m_a \iint \left(\frac{\partial f_a}{\partial t} \right)^b v^4 \sin \theta \, dv \, d\theta \quad (81a)$$

$$= - 2\pi m_a \Gamma_a \int \sin \theta \, d\theta \int G_a^b v \, dv, \quad (81b)$$

where G_a^b is that portion of G_a (see Eq. (6)) which depends on species "b"; i.e., in Eqs. (16) and (17) the sum over "b" is replaced by "b" itself. (Note that the $\frac{\partial f_a}{\partial \theta}$ term in Eq. (5) does not contribute to energy transfer.) In the case where species "b" is isotropic, Eq. (81b) reduces to

$$Q_{ab} = - (4\pi)^2 m_a \Gamma_a \left(\frac{z_b^2}{z_a} \right) \ln \Lambda_{ab}. \quad (82)$$

$$\int v dv \cdot \left(\frac{m_a}{m_b} N_0(f_b) f_a + \frac{1}{3} \left(\frac{E_0(f_b)}{v} + v^2 M_0(f_b) \right) \frac{\partial f_a}{\partial v} \right),$$

and furthermore if f_b is Maxwellian with temperature T_b ,

$$Q_{ab} = - (4\pi)^2 m_a \Gamma_a \left(\frac{z_b}{z_a} \right)^2 \ln \Lambda_{ab} .$$

$$\int N_0(f_b) \left(\frac{m_a}{m_b} v f_a + \frac{T_b}{m_b} \frac{\partial f_a}{\partial v} \right) dv , \quad (83)$$

with $M_0(f_b)$, $N_0(f_b)$ and $E_0(f_b)$ as defined in Eqs. (20), (21), and (23).

11. STRUCTURE OF PACKAGE

FPPAC is presented as part of a complete code with driver. The driver (MAIN) first calls INITIAL^d, which reads in and initializes certain package and driver variables needed by the program. (A superscript "d" here indicates that the subroutine is part of the driver section of the code whereas a superscript "f" indicates that the routine is properly part of the FPPAC core.) Besides reading in data, INITIAL^d calls several subroutines:

- (a) SETPARS^f -- copies values in PARAMETER statements into COMMON storage.
- (b) XINIT^d -- sets up spatial mesh.
- (c) XINITL^f -- computes constants and constant arrays
- (d) FINIT^d -- initializes distribution functions.
- (e) SOURCE^d -- calculates velocity-space sources.
- (f) GNANDE^d -- computes densities and energies.

The initialization phase ends with a call to EEPINT^d, which prints out various information including the distribution functions.

The next function of the driver is to solve the Fokker-Planck operator for NSTOP time steps. This is carried out through calls to three controlling package routines -- SETITUP^f, which sets up variables; COEF^f, which computes the Fokker-Planck operator, and XSWEEP^f (or XSWEPI^f), which time-advances the distribution functions. Details follow.

(a) SETITUP^f -- SETITUP^f first calls PREPKG1^f, a user-supplied (blank) routine which the user may fill in for the purpose of varying boundary conditions and miscellaneous package variables. (The procedures which must be followed in order to fill in PREPKG1^f and other user-supplied (blank) routines are given in inclusive detail in the comments at the beginning of the source code under the heading "User Responsibilities.") GNANDS^f (also a blank routine) then copies the densities and energies from user arrays into package arrays. The Coulomb logarithms are then computed in GAMMA1^f. A blank routine SETMOD^f is provided in the event the user wishes to modify the Coulomb logarithms. This might be desirable for the purpose of simulating additional physics or debugging.

(b) COEF^f -- The procedure here is to compute for each species (first Maxwellians and then general species) its contribution to the collision operators of all of the general species. The energy transfer rates, which are merely second moments of the collision operators, are computed in ENTRNS^f. Other routines used are:

- (1) DISTS^f (a blank routine), which copies the distribution functions from user storage into package storage;
- (2) COSTR^f, which stores or recovers contributions from a given general species to the collision operator (optional);
- (3) ERF^f, which computes the error function.

(c) XSWEET^f -- Each general species is time-advanced using either ADI or implicit operator splitting. First, a package subroutine BNDEXT^f determines the extreme edges of the plasma domain. Additional physics terms are added to the Fokker-Planck operator in the blank routine FPSETUP^f. The distribution function is transferred from user storage to package storage in the blank routine DISTS^f. Routine DGNSTK^f (also blank) computes diagnostic quantities prior to time-advancement. The first half-time-step is then carried out. If ADI is used, the explicit contributions to the discretized operator are computed in GETDH^f. A

package-routine DGNSTK^f is called for a second time in order to compute diagnostics which depend on the half-time-step distribution function. The second half-time-step is now carried out. If ADI is used, the explicit contributions to the discretized operator are computed in GETDG^f. DGNSTK^f is called for a third and final time. Finally, the updated distribution function is transferred from package storage to user storage in the blank routine DIST2^f.

(c') XSWEEP^f -- Each general species is prepared for time-advancement using a fully implicit (backward Euler) algorithm. Routines BNEXT^f, FPSETUP^f, DIST2^f and DGNSTK^f are called as in XSWEEP^f. The augmented matrix for the fully implicit system is computed in COIMPL^f. In order to solve the banded system, the user must fill in blank subroutine IMPSOLV^f. Routines DGNSTK^f and DIST2^f are then called, as above.

After all of the distribution functions have been advanced, an auxiliary driver routine CHPDST^d is called. This routine, which is used only for test problem number 2, adds the contribution of "passing electrons" (see below) to the electron distribution function array. The MAIN loop is concluded with calls to GNADE and EEPRINT^d (described earlier). After NSTOP timesteps, the driver ends with a final call to EEPRINT^d.

Complete lists of driver and package routines appear in Tables 1 and 2.

TABLE 1 -- DRIVER ROUTINES

INITIAL	XINIT	FINIT
GNADE	SOURCE	EEPRINT
CHPDST		

TABLE 2 -- PACKAGE ROUTINES

BNDXT	COEF	COIMPL
COSTR	ENTRNS	ERF
GAMMAI	GETDH	GETDG
SETITUP	SETPARS	XINITL
XSWEEP	XSWEEPI	FPSETUP
DGNSTK	DISTS	DISTS2
GNANDS	IMPSOLV	PREPKG1
SETMOD		

12. LIBRARY SUBROUTINES

FPPAC makes use of several library and inline subprograms which reside on the National MFE Computer Center (NMFECC) network. For the benefit of users on other systems, these routines, which on the NMFECC network are vectorized, are located toward the end of the source deck. Clearly, they should be deleted by NMFECC users. In fact, in the case of the function "CVMGM", CFT compiler users must delete the FORTRAN coding in the source if the program is to run correctly. A table of these routines follows:

TABLE 3 -- LIBRARY ROUTINES

<u>Routine</u>	<u>Machine</u>	<u>National MFE Origin</u>
BCAST	Cray,7600	FORTLIB
SCOPY	Cray	VECLIB
SSCAL	Cray	VECLIB
CVMGM	Cray	CFT Compiler - in line
QVCOPY	7600	STACKLIB
QVSET	7600	STACKLIB
QVMPY1	7600	STACKLIB
QMA2	7600	STACKLIB
QACOPY	7600	STACKLIB
QVMPY0	7600	STACKLIB

QVADD0	7600	STACKLIB
LINK*	Cray,7600	FORTLIB

13. COMMON VARIABLES

All relevant COMMON variables are described in the source listing. Those variables in COMMON blocks NPARAM1, NPARAM2, NPARAM3, NTEMP, and ITEMF are described in detail. Variables in COMMON blocks NXIN1, NXIN2, NXINS, MTEMP, MCOEF, NVALS1 and NVALS2 are generally worker variables which the user need not access (an exception is the pair of variables TERN1 and TERN2 in block NVALS1, which are described in User Responsibility No. 7).

14. ADDITIONAL PHYSICS

In order to present meaningful test problems, additional physics terms are included, as follows:

(a) Particle Source

To the right hand side of Eq. (1) is added a term

$$S_a = \bar{\alpha}_a e^{-\bar{b}_a \left(v - \bar{b}_a \right)^2} \bar{v}^2 - \bar{c}_a \left(\cos \theta - \bar{d}_a \right)^2, \quad (84)$$

where $\bar{\alpha}_a$ (which defines $\bar{b}_a$ by means of $\bar{\alpha}_a = \frac{1}{2} m_a \bar{b}_a^2$), $\bar{b}_a$, $\bar{c}_a$ and $\bar{d}_a$ are input constants, and where $\bar{\alpha}_a$ is chosen so that the source current equals J_a , also an input constant. The quantity $\bar{v}$ is a velocity normalization constant which is also input.

*This routine sets up input/output and does not appear in the source deck.

(b) Particle Loss

To the right hand side of Eq. (1) is added a term

$$L_a = -f_a/\tau_a, \quad (85)$$

where

$$\tau_a = \tau_{0a} + \tau_{1a} \left(v/v \right)^3. \quad (86)$$

This loss time increases roughly as energy to the three-halves power.

(c) RF Heating

To the right hand side of Eq. (1) is added a term

$$R_a = D_a \left\{ \frac{1}{v^2} \frac{\partial}{\partial v} \left(v^2 \sin \theta \frac{\partial f_a}{\partial v} + v \sin \theta \cos \theta \frac{\partial f_a}{\partial \theta} \right) \right. \\ \left. + \frac{1}{v^2 \sin \theta} \frac{\partial}{\partial \theta} \left(v \cos \theta \sin^2 \theta \frac{\partial f_a}{\partial v} + \sin \theta \cos^2 \theta \frac{\partial f_a}{\partial \theta} \right) \right\}. \quad (87)$$

Here D_a is of the form $D_{0a} \exp(-v^2/c^2)$, which reflects the fact that rf has a smaller effect on the higher energy particles (the rf term is applied to electrons in Test Problem 1).

(d) Initial Distribution Functions

Initially, f_a is of the form

$$f_a = a_a e^{-b_a \left(v - \beta_a \right)^2 / v^2 - c_a \left(\cos \theta - d_a \right)^2} \quad (88)$$

where a_a (which defines β_a by means of $a_a = \frac{1}{2} n_a \beta_a^2$), b_a , c_a and d_a are input constants, and where n_a is chosen so that the initial density equals n_a , also an input constant.

(e) Partial Velocity Domain Option (Species "1" Only)

It is assumed here that the general species are in the presence of a confining magnetic field and ambipolar potential. The domain of interest for species "1" is $0 \leq \theta \leq \pi/2$, $0 \leq v \leq v_m(\theta) = v_c (1 - R \sin^2 \theta)^{-1/2}$, where R is the mirror ratio ($0 < R < 1$) and $v_c^2 = 2|e\phi|/m_1$, ϕ being the plasma potential and m_1 the mass of species "1".

(f) Passing Particles Option (Species "1" On'y)

This option may be used only in conjunction with the above Partial Velocity Domain option. It is assumed that there is a truncated Maxwellian distribution function of "passing particles"; i.e., for $v \geq v_m(\theta)$,

$$f_1(v, \theta) = n_u \left(\frac{m_1}{2\pi T_u} \right)^{3/2} e^{-m_1 v^2 / 2T_u}, \quad (89)$$

where n_u and $E_u = 3/2 T_u$ are input constants. When this option is used, the initial distribution function of confined particles must also be a truncated Maxwellian (but not necessarily of the same density and temperature); i.e., $a_1 = c_1 = d_1 = 0$ and b_1 is inversely proportional to the desired temperature.

15. PACKAGE INPUT AND OUTPUT

The package FPPAC (as opposed to the package plus driver) contains no READ or WRITE statements. All input and output is transmitted between the package and driver via COMMON blocks and blank subroutines which the user must fill in. An extensive I/O description is contained in the comments in the source code under "User Responsibilities".

16. DRIVER INPUT AND OUTPUT

Data is read in on logical unit 2 and is written out on logical unit 3. Assignment of these channels for NMFECC users is accomplished in the CALL LINK statement, which is the first executable statement in the driver. The input data disc file is given the name INTIONS and the printed output file is assigned the name FPOUT. There are also several parameters which are set at compile time via PARAMETER statements. Tables of input variables follow. For further clarification users should refer to the section in which the test problems are described.

TABLE OF PARAMETERS

<u>PARAMETER</u>	<u>Description</u>
JX	Number of points in v mesh
IY	Number of points in θ mesh
NBO	Number of general species
MEQ	Number of Maxwellian ion species
MX	Highest order Legendre polynomial in expansion for Rosenbluth potentials
KSYDM	0 for assumed symmetry about $\theta = \pi/2$; 1 otherwise
MEX	1 if electrons are a general species 0 if electrons are a Maxwellian species

TABLE of DATA CARD (Unit 2) VARIABLES

<u>Variable</u>	<u>Description</u>
ITEST	1 for test problem 1 2 for test problem 2
NSTOP	Number of time steps
NPRINT	Frequency of print-outs

NCOEF	Frequency of computation of Fokker-Planck coefficients
XMAX	Maximum normalized velocity
DTR	Timestep (seconds)
VNORM	Velocity normalization constant $\bar{v}$ (cm/sec) ($XMAX * VNORM$ = maximum ion or electron speed represented on velocity mesh)

Per General Species K

FMASS(K)	Mass (grams)
BNUMB(K)	Atomic number (amu)
REDEN(K)	Density (cm^{-3})
ENIT(K)	a_K (keV) (Eq. (88))
XNIT(K)	b_K (Eq. (88))
YNIT(K)	c_K (Eq. (88))
VNIT(K)	d_K (Eq. (88))
TAUO(K)	τ_{0K} (s) (Eq. (86))
TAUI(K)	τ_{1K} (s) (Eq. (86))
ASOR(K)	Source current J_K ($\text{cm}^{-3}\text{s}^{-1}$)
ESOR(K)	$\bar{a}_K$ (Eq. (84))
XSOR(K)	$\bar{b}_K$ (Eq. (84))
YSOR(K)	$\bar{c}_K$ (Eq. (84))
USOR(K)	$\bar{d}_K$ (Eq. (84))

Per Maxwellian Species K

BNUMB(K)	Atomic number (amu)
FMASS(K)	Mass (grams)
REDEN(K)	Density (cm^{-3})
ENERGY(K)	Mean energy (keV)
EMDRF	$m_1 D_{01}$ (keV/sec) (rf term)
BRATIO	Mirror ratio R (Partial Velocity Domain option)
POTENT	Potential $e\phi$ (keV) (Partial Velocity Domain option)

ENRATIO	n_u/n_c^* (Passing Particles option)
ENPASS	E_u (keV) (Passing Particles option)

The output consists of:

- (a) A listing of the PARAMETER and logical unit 2 variables (at time $t = 0$ only).
- (b) The general species normalized distribution functions (every NPRINT time steps). The normalization is as described online (see note following Eq. (3) in listing) with BNORM(K) equal to the initial density of species K. Also, the densities and mean energies of the general species are printed out.

17. DESCRIPTION OF TEST PROBLEMS

Because of the highly versatile nature of this package, two test problems are presented.

TEST PROBLEM 1

Problem 1 describes a toroidal system in which neutral D^0 and T^0 beams are injected tangentially, but in opposite directions ⁽¹²⁾. Low energy ions are assumed to leave the system through radial diffusion. The equation to be solved is

$$\frac{\partial f_k}{\partial t} = \left(\frac{\partial f_k}{\partial t} \right)_c + S_k + L_k, \quad (90)$$

where "k" indexes D^+ and T^+ . Collisions occur between all charged species including fixed Maxwellian electrons at a temperature T_e and density n_e .

* n_c is the full velocity-space density of the confined Maxwellian. $a_1 \exp(-b_1 v^2/v^2)$ (see Eq. (88) and the above section describing the Passing Particles option.).

A table of input variables follows:

INPUT VARIABLES FOR TEST PROBLEM 1

JX	71
IY	31
NBO	2
MEQ	0
MX	4
KSYDM	1
MEX	1
ITEST	1
NSTOP	1000
NPRINT	250
NCOEF	1
XMAX	1.
DTR (Δt)	$8. \times 10^{-3} \text{ s}$
VNORM ($\tilde{v}$)	$6. \times 10^8 \text{ cm/s}$
FMASS(1) (m_D)	$3.3433 \times 10^{-24} \text{ gm}$
BNUMB(1) (Z_D)	1.
REDEN(1) $n_D(t = 0)$	$3.4 \times 10^{13} \text{ cm}^{-3}$
ENIT(1) a_D	40. keV
XNIT(1) b_D	100.
YNIT(1) c_D	10.
VNIT(1) d_D	1.
TAU0(1) τ_{0D}	0.025 s.
TAU1(1) τ_{1D}	200. s.
ASOR(1) J_D	$6.5 \times 10^{13} \text{ cm}^{-3} \text{ s}^{-1}$
ESOR(1) $\bar{a}_D$	99. keV
XSOR(1) $\bar{b}_D$	940.
YSOR(1) $\bar{c}_D$	275.
USOR(1) $\bar{d}_D$	1.
FMASS(2) $n_T(t = 0)$	$5.01495 \times 10^{-24} \text{ gm}$

BNUMB(2)	(Z_T)	1.
REDEN(2)	$n_T(t = 0)$	$3.4 \times 10^{13} \text{ cm}^{-3}$
ENIT(2)	a_T	45. keV
XNIT(2)	b_T	100.
YNIT(2)	c_T	10.
VNIT(2)	d_T	-1.
TAUO(2)	τ_{OT}	0.025 s.
TAU1(2)	τ_{1T}	200. s.
ASOR(2)	J_T	$6.5 \times 10^{13} \text{ cm}^{-3} \text{ s}^{-1}$
ESOR(2)	$\bar{a}_T$	149. keV
XSOR(2)	$\bar{b}_T$	1400.
YSOR(2)	$\bar{c}_T$	275.
USOR(2)	$\bar{d}_T$	-1.
BNUMB(3)	(Z_e)	1.
EMASS(3)	(m_e)	$9.1066 \times 10^{-28} \text{ gm}$
REDEN(3)	(n_e)	$7. \times 10^{13} \text{ cm}^{-3}$
ENERGY(3)	$(3/2T_e)$	8. keV
EMDRF	(mD_0)	0.

Eq. (90) is time-integrated using implicit operator splitting. Within eight seconds ($t = 8 \text{ s}$) an approximate steady state is reached. The deuteron and triton densities are $7.29 \times 10^{13} \text{ cm}^{-3}$ and $5.27 \times 10^{13} \text{ cm}^{-3}$, respectively. The corresponding mean energies are 36.4 keV and 44.1 keV.

A simplified version of this test problem consists of allowing the initial deuteron and triton distribution functions to relax to (approximate) Maxwellians at the electron temperature T_e . This may be accomplished by setting the source currents (ASOR) equal to 0 and the confinement times (TAUO) equal to 10^{90} (effectively infinity). An even simpler case is obtained by eliminating the tritons and electrons completely and allowing the deuterons to relax to a Maxwellian. Here the triton density (REDEN(2)) and electron density (REDEN(3)) should be set to 10^{-90} (effectively 0).

TEST PROBLEM 2

Problem 2 simulates a tandem mirror system (13). The package solves for the distribution function of trapped electrons in the presence of passing electrons and a confining magnetic field and plasma potential (14). The electrons undergo self-collisions, collisions with a fixed Maxwellian ion background of density n_i and temperature T_i , and are further accelerated by an rf heating term. The effect of the passing electrons is to dictate the value of the electron distribution function along an outer boundary in velocity space.

The equation to be solved is

$$\frac{\partial f_e}{\partial t} = \left(\frac{\partial f_e}{\partial t} \right)_c + R_e, \quad (91)$$

where f_e is the trapped electron distribution function and the latter term describes rf diffusion perpendicular to the magnetic field (see Eq. (87)). Both the Partial Velocity Domain and Passing Particles options are utilized.

In describing the input, it is convenient to define a quantity $\gamma(T)$. Given a Maxwellian of temperature T , $\gamma(T)$ represents the fraction of particles within the velocity space domain $v \leq v_m(\theta)$. The dependence on mirror ratio R and potential $e\phi$, though not explicitly stated, is implied (See Partial Velocity Domain option).

Both the trapped electrons and passing electrons are stored in the same array. The initial density of this composite distribution function is

$$n^* = n_t \gamma(T_t) + n_u (1 - \gamma(T_u)), \quad (92)$$

where n_t and T_t are the full-velocity-space density and temperature of trapped electrons and n_u and T_u are the full-velocity-space density and temperature of passing electrons. The quantities n^* (REDEN(1)) and n_u/n_t (ENRATIO) are input (as opposed to n_t and n_u themselves). Also input are the quantities $E_u = 3/2 T_u$ (ENPASS) and b_1 (XNIT(1)), which is related to T_t via

$$T_t \text{ (ergs)} = \frac{1}{2} m_1 \bar{v}^2 / b_1 . \quad (93)$$

Density and energy printouts include the contributions due to the passing electrons.

The input variables for this problem are as follows:

INPUT VARIABLES FOR THE TEST PROBLEM 2

JX	101
IY	20
NBO	1
MEQ	1
MX	8
KSYDM	0
MEX	0
ITEST	2
NSTOP	30000
NPRINT	7500
NCOEF	100
XM4X	80.
DTR (Δt)	$2. \times 10^{-4} \text{ s}$
VNORM ($\bar{v}$)	$6. \times 10^8 \text{ cm/s}$
FMASS(1) (m_e)	$9.1066 \times 10^{-28} \text{ gm}$
BNUB(1) (Z_e)	1.
REDEN(1) (Eq. (92))	$7.33 \times 10^{12} \text{ cm}^{-3}$
ENIT(1) (a)	0.

XNIT(1)	(b)	5.116×10^{-3}
YNIT(1)	(c)	0.
VNIT(1)	(d)	0.
TAUO(1)*		$1. \times 10^{90} \text{ s}$
TAU1(1)*		$1. \times 10^{90} \text{ s}$
ASOR(1)*		$0. \text{ cm}^{-3} \text{ s}^{-1}$
ESOR(1)*		30. keV
XSOR(1)*		10.
YSOR(1)*		0.
USOR(1)*		0.
BNUMB(2)	$\langle Z_i \rangle$	1.
EMASS(2)	$\langle m_i \rangle$	$3.3433 \times 10^{-24} \text{ gm}$
REDEN(2)	$\langle n_i \rangle$	$7.33 \times 10^{12} \text{ cm}^{-3}$
ENERGY(2)	$\langle 3/2 T_i \rangle$	305. keV
ENDRF	$\langle m_e D_0 \rangle$	60. keV/s
BRATIO	(R)	0.4
POTENT	(e ϕ)	60. keV
ENRATIO	$\langle n_u/n_e \rangle$	12.16
ENPASS	$\langle 3/2 T_u \rangle$	13.5 keV

*Irrelevant for this problem. See Test Problem 1

The Fokker-Planck equation including rf is then time-integrated using implicit operator splitting. Within six seconds ($t = 6 \text{ s}$) an approximate steady-state is reached. The total electron density (trapped plus untrapped) is $2.21 \times 10^{12} \text{ cm}^{-3}$ and the mean energy is 32.3 keV, which is considerably higher than the 13.5 keV energy of the passing electrons alone.

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Appendix A

Computation of Fokker-Planck Coefficients on the CRAY-1 Computer

Since the structure of each of the six coefficients is quite similar, the detailed evaluation of only one of them, namely C_a (see Eq. (10)), is considered.

Letting

$$\begin{aligned} \tilde{C}_L^b(v_j, \theta_1) = & -\frac{1}{2v_j} B_L^b(v_j) \frac{\partial}{\partial \theta} P_L(\cos \theta_1) \\ & + \frac{1}{2} \frac{\partial}{\partial v} B_L^b(v_j) \frac{\partial}{\partial \theta} P_L(\cos \theta_1), \end{aligned} \quad (A1)$$

C_a may be expressed (using Eqs. (10) and (16)) in terms of the various $\tilde{C}_L^b$ coefficients as

$$C_a(v_j, \theta_1) = \sum_b L_n \Lambda_{ab} \left(\frac{Z_b}{Z_a} \right)^2 \sum_{L=0}^M \tilde{C}_L^b(v_j, \theta_1). \quad (A2)$$

Note that the Legendre series is truncated at $M+1$ polynomials. Coefficients $\tilde{A}_L^b$ through $\tilde{F}_L^b$ may be similarly defined and expressed.

The expressions for the coefficients $\tilde{A}_L^b$ through $\tilde{F}_L^b$ are complicated (e.g. Eq. A1) and these coefficients must be evaluated at all of the mesh points. In fact, the computation of these coefficients represents a high percentage of the total number of arithmetic operations required; consequently, it is necessary to calculate these coefficients as rapidly as possible. This is accomplished through a series of nested "do-loops" which the CRAY FORTRAN (CFT) compiler vectorizes.

The coefficients $\tilde{A}_\ell^b(v_j, \theta_i)$ through $\tilde{F}_\ell^b(v_j, \theta_i)$ are functions of the four indices, "b", "l", "j" and "i", and efficiency considerations dictate that the species index "b" and the Legendre index "l" form the outer-most "do-loops", since "b" and "l" are never large. Within these two loops one must evaluate Eq. (A1) for all (v_j, θ_i) mesh points. The procedure may be outlined as follows:

(1) Calculate the Legendre coefficients $\{V_\ell^b(v_j, t)\}_{j=1}^J$ (Eq. (15)). This involves the calculation of J 1-D integrals over θ , and may be calculated in two nested loops with the outermost loop over θ ("i"). This will permit compiler vectorization of the entire procedure, since the inner loop over v ("j") is not recursive.

(2) Evaluate the functionals $\{M_\ell(V_\ell^b)(v_j), N_\ell(V_\ell^b)(v_j), R_\ell(V_\ell^b)(v_j), E_\ell(V_\ell^b)(v_j)\}_{j=1}^J$ (See Eqs. (20) - (23)). This is accomplished in two separate loops over "j". For the functional $N_\ell(V_\ell^b)(v_j)$, the first loop calculates the temporary array $TEM(j) = V_\ell^b(v_j) v_j^{(2+\ell)} \Delta v_j$, where Δv_j is a mesh increment, while in a second separate loop adds these temporaries together to form the functional $N_\ell(V_\ell^b)(v_j)$. This second loop does not vectorize since it is recursive.

(3) Determine the coefficients $\{B_\ell^b(v_j), \frac{\partial}{\partial v} B_\ell^b(v_j), \text{etc}\}_{j=1}^J$ (Eqs. (24) - (29)). This is accomplished through a single vectorizable loop over "j".

(4) Determine $\{\tilde{A}_\ell^b(v_j, \theta_i)\}$ through $\{\tilde{F}_\ell^b(v_j, \theta_i)\}_{i,j=1}^{I,J}$. It is evident from Eq. (A1) that the evaluation procedure is vectorizable. The theta ("i") loop is chosen on the outside, since it is normally much smaller than the velocity ("j") loop. The Legendre polynomials and their derivatives are time-independent and are stored quantities. As the coefficients $\tilde{A}_\ell^b - \tilde{F}_\ell^b$ are calculated, they are simultaneously summed over "l" since it is the sum, $\sum_{\ell=0}^M \tilde{C}_\ell^b$, that is required in Eq. (A1).

(5) Evaluate the contribution of the b^{th} species to the Fokker-Planck coefficients $A_a(v_j, \theta_i, t)$ through $F_a(v_j, \theta_i, t)$ for all species "a" (see Eq. (A2)). This is accomplished within the two outer loops over "b" and "l" and within a third loop over "a". The procedure easily vectorizes.