|  |  |
| --- | --- |
| December 20, 2013 | Matt Landreman |

# Technical Documentation for SFINCS - single species version

## Introduction

In this document, we detail the equations implemented in SFINCS: the Stellarator Fokker-Planck Iterative Neoclassical Conservative Solver. The normalizations and input and output quantities are also defined.

## Kinetic equation

We begin with the following drift-kinetic equation:



where ,



is the total energy,  is the ion charge in units of the proton charge ,  is the temperature,  is the ion mass,  is the  drift,



is the magnetic drift,  is the gyrofrequency, and  is the speed of light. Subscripts on partial derivatives indicate quantities held fixed in differentiation. We assume the electrostatic potential  is a flux function to the order of interest. The total distribution function is  where

.

In ,  is the collision operator linearized about . We neglect contributions from the inductive electric field to , writing  where  is the toroidal flux. Let  be the thermal speed, and let .

The independent variables used in SFINCS are  where  and . Changing velocity variables to  on the left side of ,



where

,

,

and

.

Applying  to we find

,

so simplifies to

.

Similarly, applying  to , we find

.

Thus, may be written

.

Noting



then the two electric field terms in may be combined to give

.

In the present implementation of SFINCS, the  terms in and are neglected, as is the  term in . (This last term must be dropped in order to maintain conservation of .) We are then left with

,

,

.

These are the same terms as in the last section of the appendix of Ref. [1].

We can verify that - still conserve :



As shown in the appendix of Ref. [1], - do not conserve  because the radial magnetic drift has been dropped. However, in an axisymmetric or quasisymmetric field, - do conserve a combination of energy and canonical momentum.

To compare various effective particle trajectories, the code allows the  terms in and to be turned off, in which case

,

.

For comparison with DKES, SFINCS allows the option of using

,

in place of .

One further option allowed in the code is to also include a term



on the left-hand side of . The rationale for including this term is that it allows the left-hand side of to be put into a conservative form when - are used:

.

For the rest of these notes, we will include the term multiplied by , so  will be either 0 or 1.

Now consider the magnetic field in Boozer coordinates:

,

where  is the rotational transform with  the safety factor, and

,

where , ,  is the poloidal current outside the flux surface, and  is the toroidal current inside the flux surface. Notice . The product of with gives the Jacobian

.

Notice also that



for any quantity , and

.

The kinetic equation with - is thus equivalent to



where

,

,

,

.

## Normalizations

Let’s suppose we are given , , , , , , , , , , and  where  is the normalized toroidal flux. The flux at the last closed flux surface is , so the dimensional flux  is related to  by . The input quantities are specified in terms of some dimensions  (e.g. eV),  (e.g. 1020/m3),  (e.g. kV),  (e.g. T), and  (e.g. m). In other words, the quantities we are actually given are

,

,

,

,

,

,

,

,

,

and

.

Notice , and so



for any flux function .

It will be useful to define the following combinations of normalization constants:

,

,

.

and a normalized collisionality



where

.

Notice that - use the actual particle mass , not a reference mass. Notice also that uses the actual  and , not the reference values  and . It will be useful to notice

.

We define a normalized distribution function  as follows:

.

(Notice that we have normalized by the actual density, not by the reference density.)

The kinetic equation is made dimensionless by multiplying through by

,

yielding



where .

## Legendre discretization

SFINCS uses a collocation discretization in the , , and  coordinates, but a modal discretization in the  coordinate. In other words, the distribution function is known at certain grid points in , , and , but it is expanded as modes in . We employ the following modal expansion in terms of Legendre polynomials :

.

We discretize the kinetic equation by applying

.

To evaluate the various integrals that result, the following identities may be used:

,



,



and

.

As a result, may be written



where

,

,

,



,

,

and



## Collision operator

At present, three options are available for the collision operator: pitch-angle scattering without momentum conservation, pitch-angle scattering with a model momentum conserving term, and the full linearized Fokker-Planck operator.

### Pitch-angle scattering

This operator is defined by



where

,

,

,

and



is the error function.

Applying the Legendre discretization,

.

### Model momentum conserving operator

This model operator is defined by



where  is a model field term:



Using the facts that  is self-adjoint and that , it can be verified that  for any , i.e. the operator conserves momentum. The integral in the denominator of can be evaluated numerically:

.

Applying the Legendre discretization,

.

### Full linearized Fokker-Planck operator

The full linearized Fokker-Planck operator (normalized by ) is



where



is the energy scattering operator,

,

,

and

.

Here,  and  are normalized perturbed Rosenbluth potentials, related to the dimensional perturbed Rosenbluth potentials  and  by



and

.

The Rosenbluth potentials are defined in terms of the distribution function by the following pair of Poisson equations:



and

.

A clear derivation of the operator - may be found in Ref. [2], and it is identical to the linearized operator of Ref. [3].

To apply the Legendre discretization,  and  are expanded in the same way as :

,

,

and the operation is applied to -. As - contain no  dependence except through the unknowns, we may simply replace , , and  in these equations. Finally, - become



and

.

The terms - and equations - are implemented in SFINCS using the method detailed in Ref. [4].

## Output quantities

### Flux surface average:

For any quantity , the flux surface average can be computed from



where

.

Notice

.

### Density perturbation

SFINCS returns the density in  normalized by the density in :

.

Upon flux surface averaging, we obtain



### Pressure perturbation

SFINCS also returns the pressure in  normalized by the pressure in :



Upon flux surface averaging, we obtain



### Flow

We choose to normalize the parallel flow at each point as follows:

.

Both numerical and analytic calculations often employ the weights average flow . In SFINCS, this quantity is normalized in the following way:



### Particle flux

We may write the radial particle flux as



where

.

Using



then

.

### Momentum flux

We may write a radial momentum flux as



where

.

Using



then

.

### Heat flux

We may write the radial energy flux as



where

.

Using , then

.`

## Test of quasisymmetry isomorphism

One useful test of any stellarator neoclassical code is to verify that it behaves correctly in the case of perfect quasisymmetry, meaning . In this limit the ion particle flux should be zero (in the limit that ion-electron collisions are neglected in the ion kinetic equation.) Numerically, the flux will not be exactly zero, but it should be orders of magnitude smaller than the heat flux (in code units).

A second test may be formulated as follows. Suppose the helicity integers  and  are varied, at fixed effective collisionality

,

(any average will do in the denominator) and holding fixed , , , , , and other input quantities. In this “helicity scan”, the flow and heat flux should vary in the following way:



and



where  and  are independent of  and . A derivation showing that the flow and heat flux scale as - is given in Ref. [5]. To hold fixed while varying  and , we set the normalized collision frequency to



where  is held fixed.

It was verified that SFINCS passed these tests. The Matlab version has a switch testQuasisymmetryIsomorphism, which if set, outputs the quantities on the left-hand side of - so you can verify they do not change when helicity\_l and helicity\_n are varied. (You must set epsilon\_t=0 for this test).

## Transport matrix

For some applications, it may be useful to separate out the contributions to each flux and flow from the individual drive terms. To this end, we now develop the concept of a transport matrix. Our definitions will differ from those in e.g. Ref. [6] in order to make the matrix dimensionless and symmetric, to avoid introducing the unnecessary dimensional quantities  and , and to clarify which quantities do and do not affect the matrix elements.

### Thermodynamic forces

We begin by using the linearity of the kinetic equation in  to formally write its solution as



where the  and  are all dimensionless, the  are unknown parts of the distribution function proportional to the individual drives , and the  represent the three different inhomogeneous terms on the right-hand side of , distinguished by their velocity dependence:

,

,

.

As dimensionless factors may always be absorbed into the  or , there is not a unique way to define the  and  quantities to satisfy our requirements. However, examination of with



and shows that one reasonable choice is the following:







where  is the  harmonic of the Boozer spectrum. You can verify that all the  are indeed dimensionless. Applying , -, and in , we find the equations satisfied by the  are

,

,

and

.

with a new dimensionless collisionality



and  as before. (Equations - differ in the power of  on the right-hand side.) The  derivatives in - are performed at fixed  and field line, and the electric field terms have been omitted for simplicity. Notice  is independent of all parameters (density, temperature, etc.) It is then evident from - that the  depend on the input parameters only through the combinations , , , and . There is no additional dependence on the density, temperature, , , or  individually.

### Fluxes

The three output quantities of greatest interest are the particle flux

,

the heat flux

,

and the flux-surface-averaged parallel flow

.

The right-hand sides of - resemble the right-hand sides of -. This correspondence suggests that we define three fluxes as follows:





and

.

These definitions are chosen so right-hand sides of - have the same ratio as -, except for the sign of . It turns out this sign change is necessary in order for the matrix to be symmetric. The definitions of the  are not unique in that only the choices - will turn out to yield a symmetric transport matrix (given our choices of ), as we will show below.

If we now define a transport matrix  by the relation

,

the  matrix elements will be dimensionless, unlike those in Ref. [6]. Notice the  elements are integrals of the , with the integrands depending on the input parameters only through  and . Therefore, exactly like the , the  depend on the input parameters only through the combinations , , , and . There is no additional dependence on the density, temperature, , , or  individually.

In summary, the transport matrix equation is

.

### Matrix elements in SFINCS units

The matrix elements of  are computed in SFINCS by solving the kinetic equation for three separate right-hand sides: each one with only one of the  nonzero. The first solve uses , , , and  on the right-hand side, though  is allowed to be nonzero on the left-hand side terms. The second solve uses , , and  to make  but  nonzero. Again,  is allowed to be nonzero on the left-hand side terms, and . For the third solve, ,  and  on the right-hand side,  is nonzero on the left-hand side, and this time . Straightforward but tedious manipulation of -, , , and then gives expressions for the matrix elements:



















Each of these expressions is to be evaluated using the particleFlux, heatFlux, or FSAFlow from the appropriate right-hand side, the right-most quantity in each case is the value 1 used in the associated right-hand side.

### Sign of diagonal elements

Several properties of the  matrix can be proved. We begin with , substituting into the right-hand side of , giving



To obtain the last line, we have noted that  for any . The quantity  represents (negative) entropy generation, and it can be proved that  for the linearized Fokker-Planck operator. Therefore,

.

The analysis and result for  is similar:

.

To determine the sign of , we substitute into the right-hand side of , giving



so

.

It should be noted that while  for the linearized Fokker-Planck operator,  could possibly be positive for model collision operators.

### Onsager symmetry

We can also prove that the matrix  is symmetric, which is the ultimate reason for defining the fluxes  as we have done. To complete the proof, we must separate each  into the parts that are symmetric and antisymmetric with respect to :  where





with analogous definitions for  and . The kinetic equations - may then be separated into symmetric and antisymmetric parts:













To prove , we then substitute , , or into the right-hand side of - as appropriate. The results are then manipulated using the integration-by-parts rule

,

and the self-adjointness property of :

,

(both true for any physical  and ) as well as , , and .

### Tokamak limits

For benchmarking purposes, it is useful to note the values of the transport matrix elements in the case of axisymmetry  in the limit  (since high collisionality requires lower resolution than low collisionality.) In axisymmetry, certain matrix elements can be fact be determined exactly for any value of ; these elements are denoted with (\*) below. These results are derived in separate notes.

**Pure pitch-angle scattering:**



**Momentum-conserving model:**



**Full linearized Fokker-Planck operator:**



## References

[1] Landreman and Catto, “Conservation of energy and magnetic moment in neoclassical calculations for optimized stellarators”, submitted to Plasma Phys Controlled Fusion (2013).

[2] Li and Ernst, Phys. Rev. Lett. 106, 195002 (2011).

[3] Rosenbluth, McDonald, and Judd, Phys. Rev. 107, 1 (1957).

[4] Landreman and Ernst, J. Comp. Phys., <http://dx.doi.org/10.1016/j.jcp.2013.02.041> (2013).

[5] Landreman and Catto, Plasma Phys Controlled Fusion 53, 015004 (2011).

[6] Beidler et al, Nuclear Fusion 51, 076001 (2011).