Notes on Nonlinear Fluxes in General Geometry

W. Dorland, M. Kotschenreuther

1 Background

1.1 General geometry

Our development closely follows that of Beer, *et al.*[1] Since the divergence of the magnetic field is zero, one may use a Clebsch formulation:[2]

$$\mathbf{B} = \nabla\alpha \times \nabla\psi. \tag{1}$$

To represent an equilibrium magnetic field composed of closed surfaces, it is sufficient to define[2] $\alpha = \phi - q(\psi)\theta - \nu(\psi,\theta,\phi)$ and $\psi = \Psi$. Here, θ and ϕ are the physical poloidal and toroidal angles, respectively, $\Psi = (2\pi)^{-2}\int_V d\tau\,\mathbf{B}\cdot\nabla\theta$ is the poloidal flux, $q(\Psi) = d\Psi_T/d\Psi$, $\Psi_T = (2\pi)^{-2}\int_V d\tau\,\mathbf{B}\cdot\nabla\phi$ is the toroidal flux, and $d\tau$ is the volume element. The quantity ν should be periodic in θ and ϕ.

It is convenient to define a new angle $\zeta = \phi - \nu$. With these definitions, Eq. 1 becomes

$$\mathbf{B_0} = \nabla\Psi \times \nabla(q\theta - \zeta),$$

where the subscript on $\mathbf{B}$ is included to emphasize that we are concerned with the equilibrium, unperturbed magnetic field. The field lines are straight in the (ζ,θ) plane, and are labeled by α. Useful coordinates are therefore (ρ,α,θ), where $\rho(\Psi)$ determines the flux surface, α chooses a field line in that surface, and θ measures the distance along that field line.

In an axisymmetric system, one may also represent the magnetic field as

$$\mathbf{B_0} = I(\Psi)\nabla\phi + \nabla\Psi \times \nabla\phi, \tag{2}$$

where $I(\Psi) = RB_T$. We will find it useful to take advantage of this representation, although not necessary.

In the ballooning or field-line following limit, we assume that the perturbed quantities vary as

$$A = \hat{A}(\theta)\exp{(iS)}$$

where $\hat{\mathbf{b}} \cdot \nabla S = 0$. This takes into account the fact that the perturbations tend to be slowly varying along the field line, and allows for rapid variation across the field line.[3]

The latter condition implies

$$(\nabla\alpha \times \nabla\Psi) \cdot \nabla S = 0$$

which, in turn, implies $S = S(\alpha, \Psi)$. To make contact with the ballooning approximation and with field-line following coordinates, one may choose $S = n_0 (\alpha + q\theta_0)$, where n_0 is some (large) integer, and θ_0 is the familiar ballooning parameter, which in field-line-following coordinates, determines k_x through the relation $k_x = -k_\theta \hat{s}\theta_0$. Here, $\hat{s} = \rho/q(dq/d\rho)$, and ρ is an arbitrary flux surface label. The definition of k_θ is provided below, Eq. (6).

1.2 Nonlinear terms, fluxes

This is the key part of this note, and should appear after much of the following sections, since that is where the normalizations are defined. However, I'm sticking this here for now.

Say we are interested in the nonlinear particle flux. This would be something like

$$\mathbf{\Gamma} = \delta n \, \delta \mathbf{v}.$$

The ultimate goal is to derive flux-surface averaged fluxes of quantities like this one. In the usual way (see Hinton and Hazeltine for details), the component we want is

$$\langle \nabla \cdot \mathbf{\Gamma} \rangle = \frac{d\rho}{dV} \frac{d}{d\rho} \left(\frac{dV}{d\rho} \langle \mathbf{\Gamma} \cdot \nabla\rho \rangle \right).$$

The usual case is the one in which the nonlinear simulation uses a different radial flux label ρ than is to be used in the transport equation. We have found that it is easiest to communicate clearly by using the definition of the area of a flux surface

$$A = \frac{dV}{d\rho} \langle \nabla\rho \rangle$$

to rewrite this expression as

$$\langle \nabla \cdot \mathbf{\Gamma} \rangle = \frac{d\rho}{dV} \frac{d}{d\rho} \left[\left(\frac{dV}{d\rho} \langle \nabla\rho \rangle \right) \frac{\langle \mathbf{\Gamma} \cdot \nabla\rho \rangle}{\langle \nabla\rho \rangle} \right] = \frac{d\rho}{dV} \frac{d}{d\rho} \left[A \frac{\langle \mathbf{\Gamma} \cdot \nabla\rho \rangle}{\langle \nabla\rho \rangle} \right]. \tag{3}$$

Diagnostics in `gs2` produce the quantity

$$\Gamma_{\text{sim}} \equiv \frac{\langle \mathbf{\Gamma} \cdot \nabla\rho \rangle}{\langle \nabla\rho \rangle}.$$

2

Now, I'm going to go from this expression to the normalized expression evaluated in `gs2`, for the electrostatic particle flux. The remaining fluxes are completely analogous.

Introduce normalized variables as follows:

$$\tilde{n} \equiv \frac{\delta n}{n_0} \frac{L}{\rho_0}, \qquad \tilde{\Phi} \equiv \frac{|e|\delta\Phi}{T_0} \frac{L}{\rho_0}, \qquad \nabla_N \equiv L\nabla.$$

Here, L is some equilibrium scale length (typically the major radius or minor radius in `gs2` runs), ρ_0 is the gyroradius of the species with mass m_0, temperature T_0, and charge $Z_0|e|$, in a magnetic field of strength B_a. (I use subscript a instead of 0 to differentiate between the normalizing magnetic field value (a scalar) and the normalized magnetic field strength as a function of position along the field line, $B_0 = B_0(\theta)$. The normalizing density is n_0, which is not to be confused with the toroidal mode number introduced later.

With these definitions, I can write

$$\Gamma_{\text{sim}} \equiv \frac{\langle \delta n\, \delta\mathbf{v} \cdot \nabla\rho \rangle}{\langle \nabla\rho \rangle} = \frac{\langle \frac{n_0\rho_0}{L}\tilde{n}\left(\hat{\mathbf{b}} \times \nabla_N\tilde{\Phi} \cdot \nabla_N\rho\right)\frac{\rho_0}{L^2}\frac{cT_0}{|e|B_0}L \rangle}{\langle \nabla_N\rho \rangle}$$

$$\Gamma_{\text{sim}} \equiv n_0 \frac{cT_0}{|e|B_a} \frac{\rho_0^2}{L^3} \frac{\langle \tilde{n}\left(\hat{\mathbf{b}} \times \nabla_N\tilde{\Phi} \cdot \nabla_N\rho\right)(B_a/B_0) \rangle}{\langle \nabla_N\rho \rangle}.$$

Now, use the Fourier representation (with sloppy notation for now) to replace

$$\tilde{\Phi} \to \tilde{\Phi}\exp\left\{in_0(\alpha + q\theta_0)\right\}$$

and thus obtain

$$\Gamma_{\text{sim}} \equiv n_0 \left(\frac{cT_0}{|e|B_a}\right) \frac{\rho_0^2}{L^3} \frac{d\rho}{d\Psi_N} \frac{\langle in_0\,\tilde{n}\tilde{\Phi}\left(\hat{\mathbf{b}} \times \nabla_N\alpha \cdot \nabla_N\Psi_N\right)(B_a/B_0) \rangle}{\langle \nabla_N\rho \rangle}.$$

Using Eq. (1) and the identity

$$\frac{cT_0}{|e|B_a} = \rho_0 v_{t0},$$

this simplifies considerably:

$$\Gamma_{\text{sim}} \equiv n_0 v_{t0} \frac{\rho_0^2}{L^2} \left(i\frac{n_0}{L}\frac{d\rho}{d\Psi_N}\rho_0\right) \frac{\langle \tilde{n}\tilde{\Phi} \rangle}{\langle \nabla_N\rho \rangle}.$$

Since we define

$$k_\theta \equiv \frac{n_0}{L}\frac{d\rho}{d\Psi_N}$$

3

this can be simplifed even further to the familiar form:

$$\Gamma_{\text{sim}} \equiv n_0 v_{t0} \frac{\rho_0^2}{L^2} \left(ik_\theta \rho_0\right) \frac{\langle \tilde{n}\tilde{\Phi} \rangle}{\langle \nabla_N \rho \rangle}.$$

Unfortunately, this is not actually what `gs2` has been writing out, so that comparisons with experimental data with shaped cross sections have some (hopefully minor) errors. The precise magnitude of the problem depends on the degree of the shaping together with the degree of the $\theta-$dependence of the flux before flux-surface averaging.

1.3 Operators and arguments

In general, we wish to simulate the nonlinear electromagnetic gyrokinetic equation in the ballooning, or field-line-following, limit. We choose a field-line-following representation,[1] which has the advantage that the nonlinear terms are easy to evaluate and are independent of the details of the magnetic geometry. Further details may found in Ref. ([1]).

Effects of the magnetic geometry in this limit enter through only a small number of terms, regardless of whether one proceeds with a moment-based approach,[1] a δf approach,[4, 5] or a gyrokinetic approach.[6, 7] Consider, for example, Eqs. (23–24) of Antonsen and Lane:[3]

$$\hat{g} = \hat{h} - \frac{1}{B_0} \frac{\partial F_0}{\partial \mu} \left[J_0 \left(\frac{v_\perp |\nabla S|}{\Omega} \right) \left(q\hat{\phi} - \frac{v_\parallel}{c} q\hat{\psi} \right) + q\hat{\sigma} \frac{v_\perp |\nabla S|}{c} J_1 \left(\frac{v_\perp |\nabla S|}{\Omega} \right) \right], \quad (4)$$

and

$$-i \left(\omega - \omega_d + iv_\parallel \hat{\mathbf{b}} \cdot \nabla \right) \hat{h} = \int_{-\pi}^{\pi} \frac{d\xi}{2\pi} \exp\left(-iL\right) \mathrm{st}\left(\hat{f}_0 \right)$$

$$+ i\omega \left(\frac{\partial F_0}{\partial \epsilon} - \frac{\mathbf{B_0} \times \nabla S \cdot \nabla F_0}{B_0 m \Omega \omega} \right)$$

$$\left[J_0 \left(\frac{v_\perp |\nabla S|}{\Omega} \right) \left(q\hat{\phi} - \frac{v_\parallel}{c} q\hat{\psi} \right) + q\hat{\sigma} \frac{|\nabla S| v_\perp}{c} J_1 \left(\frac{v_\perp |\nabla S|}{\Omega} \right) \right]. \quad (5)$$

Here, $\omega_d \equiv \nabla S \cdot \mathbf{B_0} \times \left(mv_\parallel^2 \hat{\mathbf{b}} \cdot \nabla \hat{\mathbf{b}} + \mu \nabla B_0 + q \nabla \Phi_0 \right) / (mB_0 \Omega)$. The notation is explained in Ref. [3]. Note that the unperturbed magnetic field $B_0 = B_0(\theta)$.

These equations, together with Maxwell's equations, describe the linear properties of a wide range of microinstabilities. In the limit of large toroidal mode number n_0, only the following components of these equations depend on θ: $\hat{\mathbf{b}} \cdot \nabla$, $|\nabla S|^2$, $\mathbf{B_0} \times \left(\hat{\mathbf{b}} \cdot \nabla \hat{\mathbf{b}} \right) \cdot \nabla S$, $(\mathbf{B_0} \times \nabla B_0) \cdot \nabla S$, and $B_0(\theta)$. To perform volume integrations and flux surface averages in the nonlinear simulations, it is also necessary to have the Jacobian J and $|\nabla \rho|$ as functions of θ. We now consider the terms individually.

To make our normalizations clear, we treat the ω_* term in detail. The ω_* term may be written as

$$-i\frac{\mathbf{B_0} \times \nabla S \cdot \nabla F_0}{B_0 m \Omega} q\hat{\chi} = -in_0 \frac{c}{B_0}\hat{\chi}\left[\hat{\mathbf{b}} \times \nabla\left(\alpha + q\theta_0\right) \cdot \nabla F_0\right]$$

where

$$\hat{\chi} = \left(\hat{\phi} - \frac{v_\parallel}{c}\hat{\psi}\right) J_0 + \frac{\hat{\sigma}|\nabla S|v_\perp}{c}J_1.$$

This, in turn, is

$$-in_0\frac{c}{B_0}\hat{\chi}\left[\hat{\mathbf{b}} \times \nabla\left(\alpha + q\theta_0\right) \cdot \nabla F_0\right] = -in_0\frac{c}{B_0}\hat{\chi}\left(\hat{\mathbf{b}} \cdot \nabla\alpha \times \nabla\Psi\right)\frac{\partial F_0}{\partial \Psi} = -in_0 c\hat{\chi}\frac{\partial F_0}{\partial \Psi},$$

where we have assumed that $F_0 = F_0(\Psi)$.

We now introduce normalizing quantities. Lengths are normalized to a, which we choose to be half the diameter of the last closed flux surface (LCFS), measured at the elevation of the magnetic axis. The magnetic field is normalized to the toroidal field on the flux surface at R_a, $(B_a = I(\Psi)/R_a)$ where R_a is the average of the minimum and maximum of R on the flux surface and $I(\psi)$ is as used in Eq. (2). Time is normalized to a/v_t, where $v_t = \sqrt{T/m_i}$. Thus, for example, $\nabla = (1/a)\nabla_N$ and $\Psi = a^2 B_a \Psi_N$. Perturbed quantities are scaled up by a/ρ_{ia}, where $\rho_{ia} = v_t/\Omega_a$ and $\Omega_a = |e|B_a/(m_i c)$. The perturbed field is normalized by $T_i/|e|$, so that, for example, $\hat{\chi}_N = (|e|\hat{\chi}/T_i)(a/\rho_{ia})$. [Here, we consider only the one-species problem. The generalization to multiple species is straightforward.] Finally, we introduce an arbitrary flux surface label ρ, normalized so that $\rho = 0$ at the magnetic axis and $\rho = 1$ at the LCFS. Note that the Larmor radius ρ_i should not be confused with the flux surface label ρ. Upon adopting these normalizations, one finds

$$-in_0 c\hat{\chi}\frac{\partial F_0}{\partial \Psi} = -i\frac{n_0}{a^2}\frac{cT}{eB_a}\frac{\rho_{ia}}{a}\hat{\chi}_N\frac{\partial F_0}{\partial \rho}\frac{d\rho}{d\Psi_N} = -ik_\theta \rho_{ia}\frac{\rho_{ia}v_t}{a^2}\frac{\partial F_0}{\partial \rho}\hat{\chi}_N$$

which serves to define

$$k_\theta \equiv (n_0/a)d\rho/d\Psi_N. \tag{6}$$

In the high aspect ratio, zero β, circular flux surface limit, $k_\theta = n_0 q/r$. For the case in which there is a background density gradient, one finds

$$-ik_\theta \rho_{ia}\frac{\rho_{ia}v_t}{a^2}\frac{\partial F_0}{\partial \rho}\hat{\chi}_N = i(k_\theta \rho_{ia})\hat{\chi}_N\frac{F_0}{(L_n)_N}\frac{\rho_{ia}v_t}{a^2} = i(k_\theta \rho_{ia})\hat{\chi}_N F_0 \frac{a}{L_n}\left(\frac{\rho_{ia}v_t}{a^2}\right)$$

in which the dimensionless quantity $(L_n)_N^{-1} = -(1/n)dn/d\rho$, and may also be written as L_n/a. With the specified normalizations for time, space, and perturbed quantities,

the factor $\rho_{ia}v_t/a^2$ scales out of the gyrokinetic equation. Compare, for example, the ω_* term with the first term in Eq. (5),

$$i\omega\hat{h} = i\omega_N\hat{h}_N\left(\frac{\rho_{ia}v_t}{a^2}\right).$$

The factor in parentheses is common to all terms in the equation, and does not appear in any other form. It may therefore be considered to be arbitrary.

In the ω_* term, note that k_θ is multiplied by ρ_{ia}, confirming that it is natural to consider perpendicular gradients normalized by the gyroradius ρ_{ia} rather than to the minor radius a, as expected in the ballooning or field-line-following limit.

To summarize, upon adopting the above normalizations, the ω_* term in Eq. (5) in field-line-following coordinates becomes

$$-i\frac{\mathbf{B_0}\times\nabla S\cdot\nabla F_0}{B_0 m\Omega}q\hat{\chi} = i\omega_{*N}\hat{\chi}_N F_0\left(\frac{\rho_{ia}v_t}{a^2}\right) = -ik_\theta\rho_{ia}\frac{1}{F_0}\frac{dF_0}{d\rho}\hat{\chi}_N F_0\left(\frac{\rho_{ia}v_t}{a^2}\right) \qquad (7)$$

Note that $\omega_{*N} = -k_\theta\rho_{ia}(1/F_0)(dF_0/d\rho)$ is dimensionless, independent of θ, and related to the dimensional ω_* by $\omega_* = \omega_{*N}v_t/a$.

We now turn to the $\hat{\mathbf{b}}\cdot\nabla$ operator. We begin by using the $\mathbf{B}$ field in the form of Eq. (1) to find α:

$$\mathbf{B}\cdot\nabla\phi = \nabla\theta\times\nabla\Psi\cdot\nabla\phi\frac{\partial\alpha}{\partial\theta}$$

which implies

$$\alpha = \int_0^\theta d\theta\frac{\mathbf{B_0}\cdot\nabla\phi}{\nabla\theta\times\nabla\Psi\cdot\nabla\phi}. \qquad (8)$$

For an axisymmetric $\mathbf{B}$ field, this integral may be evaluated with the use of Eq. (2). In this case, the $\hat{\mathbf{b}}\cdot\nabla$ operator may be explicitly evaluated. It is

$$\hat{\mathbf{b}}\cdot\nabla\hat{h}(\theta) = \frac{\mathbf{B_0}\cdot\nabla\theta}{B_0}\frac{\partial\hat{h}}{\partial\theta} = -\frac{I_N}{aB_N}\left(\frac{\partial\alpha}{\partial\theta}\right)^{-1}|\nabla_N\phi|^2\frac{\partial\hat{h}}{\partial\theta},$$

which serves to define

$$\left(\hat{\mathbf{b}}\cdot\nabla\right)_N = -\frac{I_N}{B_N}\left(\frac{\partial\alpha}{\partial\theta}\right)^{-1}|\nabla_N\phi|^2. \qquad (9)$$

In the high aspect ratio, zero β, circular flux surface limit, $\left(\hat{\mathbf{b}}\cdot\nabla\right)_N = a/qR_0$, where R_0 is the major radius at the center of the flux surface.

Next, we consider the ∇B part of the ω_d operator. This term is given by

$$\frac{v_\perp^2}{2}\frac{\hat{h}}{\Omega B_0^2}\mathbf{B_0}\times\nabla B_0\cdot\nabla S = \left(\frac{\rho_{ia}v_t}{a^2}\right)\left(\frac{k_\theta\rho_{ia}}{2}\right)\frac{v_{\perp N}^2}{2}\hat{h}_N\left[\frac{2}{B_N^2}\frac{d\Psi_N}{d\rho}\hat{\mathbf{b}}\times\nabla_N B_N\cdot\nabla_N\left(\alpha+q\theta_0\right)\right].$$

The module released here produces the factors in square brackets, *i.e.*,

$$\omega_{\nabla B} = \frac{2}{B_N^2}\frac{d\Psi_N}{d\rho}\hat{\mathbf{b}} \times \nabla_N B_N \cdot \nabla_N \alpha \quad \text{and} \quad \omega_{\nabla B}^{(0)} = \frac{2}{B_N^2}\frac{d\Psi_N}{d\rho}\hat{\mathbf{b}} \times \nabla_N B_N \cdot \nabla_N q. \quad (10)$$

In the high aspect ratio, zero β, circular flux surface limit, $\omega_{\nabla B} = 2a/R_0\,(\cos\theta + \hat{s}\theta\sin\theta)$, and $\omega_{\nabla B}^{(0)} = -2\,(a/R_0)\,\hat{s}\sin\theta$.

The curvature drift is nearly the same as the ∇B drift, except that $v_\perp^2 \to 2v_\parallel^2$, and the fact that there is an additional component of the curvature drift given by

$$v_\parallel^2 \frac{4\pi\hat{h}}{\Omega B_0^2}\hat{\mathbf{b}} \times \nabla p \cdot \nabla S = \left(\frac{\rho_{ia}v_t}{a^2}\right)\left(\frac{k_\theta \rho_{ia}}{2}\right)\hat{h}_N v_{\parallel N}^2 \left[\frac{1}{B_N^3}\frac{d\Psi_N}{d\rho}\hat{\mathbf{b}} \times \nabla_N \beta_a \cdot \nabla_N(\alpha + q\theta_0)\right]. \quad (11)$$

The module released here produces the factors in square brackets, *i.e.*,

$$\omega_\kappa = \omega_{\nabla B} + \frac{1}{B_N^3}\frac{d\Psi_N}{d\rho}\hat{\mathbf{b}} \times \nabla_N \beta_a \cdot \nabla_N \alpha, \quad \omega_\kappa^{(0)} = \omega_{\nabla B}^{(0)} \quad (12)$$

Here, $\beta_a = 8\pi p/B_a^2$. Note that a perpendicular gradient of β_a gets no contribution from the gradient of the magnetic field, since B_a is a constant.

We do not explicitly consider the remaining component of ω_d, proportional to $\nabla\Phi_0$. To the extent that the electrostatic potential is constant on a flux surface, this term may be specified using the information provided by the module.

To summarize, in field-line-following coordinates, the term in Eq. (5) that is proportional to ω_d is given by

$$i\omega_d \hat{h} = i\left(\frac{k_\theta \rho_{ia}}{2}\right)\hat{h}_N\left(\frac{\rho_{ia}v_t}{a^2}\right)\left[\frac{v_{\perp N}^2}{2}\left(\omega_{\nabla B} + \theta_0\,\omega_{\nabla B}^{(0)}\right) + v_{\parallel N}^2\left(\omega_\kappa + \theta_0\,\omega_\kappa^{(0)}\right)\right]$$

The form of Eqs. (4–5) and of the gyrokinetic Maxwell's equations[3] (not shown) guarantees that $|\nabla S|$ always appears as the square, $|\nabla S|^2$. In general geometry, this term may be written

$$|\nabla S|^2 = \frac{n_0^2}{a^2}|\nabla_N(\alpha + q\theta_0)|^2 = k_\theta^2\left(\frac{d\Psi_N}{d\rho}\right)^2|(\nabla_N\alpha + \theta_0\nabla_N q)\cdot(\nabla_N\alpha + \theta_0\nabla_N q)|.$$

The module released here produces the factors (g_1, g_2, g_3), where

$$|\nabla S|^2 = k_\theta^2\left|g_1 + 2\theta_0 g_2 + \theta_0^2 g_3\right| = k_\theta^2\left(\frac{d\Psi_N}{d\rho}\right)^2\left|\nabla_N\alpha \cdot \nabla_N\alpha + 2\theta_0\nabla_N\alpha \cdot \nabla_N q + \theta_0^2\nabla_N q \cdot \nabla_N q\right|. \quad (13)$$

In the high aspect ratio, zero β, circular flux surface limit, $g_1 = 1 + \hat{s}^2\theta^2$, $g_2 = -\theta\hat{s}^2$, and $g_3 = \hat{s}^2$. Note that $|\nabla S|^2$ typically appears with a factor of $1/\Omega^2$, which is not included in Eq. (13).

The remaining quantities are straightforward. The variation of the unperturbed magnetic field along the field line is reported by the module as B_N, with

$$B_N(\theta) = B_0(\theta)/B_a. \tag{14}$$

The quantity $|\nabla_N\rho|$ is also reported by the module, and is unity in the high aspect ratio, zero β, circular flux surface limit.

For numerical applications, it is sometimes necessary to choose the field line coordinate so that $(\hat{\mathbf{b}}\cdot\nabla)_N$ is constant. This choice allows the straightforward evaluation of terms proportional to $|k_\parallel|$ in the transform space. Thus, we use (ρ, α, θ') coordinates, where θ' is the equal arc periodic coordinate defined by

$$\theta'(\theta) = 2\pi L_N(\theta)/L_N(\pi) - \pi \tag{15}$$

between $-\pi$ and π, and $L_N(\theta) = \int_{-\pi}^{\theta} d\theta \left(\hat{\mathbf{b}}\cdot\nabla\right)_N^{-1}$. In this coordinate system, the coefficient of the parallel gradient operator of Eq. (9) becomes

$$\left(\hat{\mathbf{b}}\cdot\nabla\right)_N' = 2\pi/L_N(\pi). \tag{16}$$

The Jacobian is $J_N = (d\Psi_N/d\rho)\left(L_N/2\pi B_N\right)$. With these definitions, the flux surface average of a quantity Γ is defined to be

$$\langle\Gamma\rangle = \frac{\int \Gamma J_N \, d\theta' \, d\alpha}{\int J_N \, d\theta' \, d\alpha}.$$

The normalized area of the flux surface is $A_N = 2\pi\langle |\nabla_N\rho| \rangle \int J d\theta'$.

The field-line variation of the quantities $\omega_{\nabla B}$ and $\omega_{\nabla B}^{(0)}$ [Eq. (10)], ω_κ and $\omega_\kappa^{(0)}$, [Eq. (12)], (g_1, g_2, g_3) [Eq. (13)], $B_N(\theta')$ [Eq. (14)], and $\left(\hat{\mathbf{b}}\cdot\nabla\right)_N$ [Eq. (16)], together with the quantities $|\nabla_N\rho|$, $d\rho/d\Psi_N$ and $d\beta/d\rho$ are the outputs of this geometry module, available from *bdorland@ipr.umd.edu* or *mtk@peaches.ph.utexas.edu*. These coefficients contain all of the geometric information necessary for numerical calculations of high-n microstability and turbulence in axisymmetric toroidal configurations with nested magnetic surfaces.

1.4   Module details

Input numerical equilibria may be specified in numerous ways, as documented in the module. Interfaces to direct and inverse Grad-Shafranov equilibrium solvers are

available. These include using output from several equilibrium codes in use in the fusion community, such as TOQ,[8, 9] EFIT,[10] VMOMS,[11] JSOLVER,[12] and CHEASE,[13] as well as the local equilibrium model of Miller, *et al.*[14]

Here, we describe our implementation of the Miller local equilibrium model[14] for completeness. This model extends the usual zero-beta, high-aspect ratio equilibrium to arbitrary aspect ratio, cross section and beta, and allows one to consider geometric effects on microinstabilities in a controlled way.

The shape of the reference flux surface and its perpendicular derivative are specified in the (R, Z) plane by

$$R_N(\theta) = R_{0N}(\rho) + \rho \cos \left[\theta + \delta(\rho) \sin \theta\right], \tag{17}$$

$$Z_N(\theta) = \kappa(\rho)\rho \sin \theta. \tag{18}$$

Here, $R_N = R/a$, *etc.*, $R_{0N}(\rho) = R_{0N}(\rho_f) + R'_{0N} \, d\rho$, $\delta(\rho) = \delta(\rho_f) + \delta' \, d\rho$, $\kappa(\rho) = \kappa(\rho_f) + \kappa' \, d\rho$, and ρ_f denotes the flux surface of interest. In the remainder of this section, the "N" subscripts will be dropped, since no ambiguities will arise.

As emphasized in Ref. [14], the actual shape of neighboring flux surfaces ($\rho \neq \rho_f$) is not determined by Eqs. (17) and (18). Instead, this is determined by solving the Grad-Shafranov equation in the neighborhood of ρ_f. As noted by Mercier and Luc,[15] one may find this solution provided $R(\theta)$, $Z(\theta)$, $B_p(\theta)$, $p'(\rho_f)$, and $I'(\rho_f)$. One additional piece of information is required to determine either the safety factor q or $d\Psi/d\rho$. Finally, the normalization of the magnetic field determines $I(\rho_f)$.

In our implementation, we take q to be an input parameter, and upon noting that $\oint \alpha \, d\theta = -2\pi q$, use it to define $d\Psi/d\rho$ from Eq. (8):

$$\frac{d\Psi}{d\rho} = \frac{I}{2\pi q} \oint \frac{d\theta}{R^2} \left(\nabla \theta \times \nabla \rho \cdot \nabla \phi\right)^{-1}. \tag{19}$$

[For numerical equilibria, $d\Psi/d\rho$ may be calculated directly, and this expression defines the safety factor.] The poloidal magnetic field $B_p(\rho_f)$ is specified by

$$B_p = \frac{d\Psi}{d\rho} \frac{|\nabla \rho|}{R},$$

where $|\nabla \rho|$ may be found from Eqs. (17) and (18).

The remaining steps may be used with the Miller local equilibrium model or with full numerical equilibria. We allow arbitrary values of $dp/d\rho$ and $\hat{s}$ by using the Mercier-Luc expressions to find ∇S.[14, 15, 16] As noted in Ref. ([14]), the result is exactly equivalent to the generalized $s - \alpha$ analysis of Greene and Chance.[17] To proceed, we define

$$A(\theta) = \int \frac{d\theta}{\nabla \theta \times \nabla \Psi \cdot \nabla \phi} \left[\frac{1}{R^2} + \left(\frac{I}{B_p R^2}\right)^2\right], \qquad B(\theta) = I \int \frac{d\theta}{\nabla \theta \times \nabla \Psi \cdot \nabla \phi} \left[\frac{1}{(B_p R)^2}\right],$$

$$C(\theta) = I \int \frac{d\theta}{\nabla\theta \times \nabla\Psi \cdot \nabla\phi} \left[\frac{\sin u + R/R_c}{B_p R^4} \right],$$

where $u(\theta)$ is the angle between the horizontal and the tangent to the magnetic surface in the poloidal plane, and R_c is the local radius of curvature of the surface in the poloidal plane. If we define $\bar{A} = \oint \cdots$, *etc.*, it can be shown that

$$\hat{s} = \frac{\rho}{q} \frac{dq}{d\rho} = \frac{\rho}{2\pi q} \frac{d\Psi}{d\rho} \left(\bar{A} I' + \bar{B} p' + 2\bar{C} \right) \qquad (20)$$

where the primes denote derivatives with respect to Ψ. Thus, one may specify any two of p', I', and $\hat{s}$. This freedom is a direct consequence of the two free functions in the Grad-Shafranov equation.

It can also be shown[16, 14] that the perpendicular component of the gradient of α is given by

$$\nabla\alpha \cdot \hat{e}_\Psi = |\nabla\Psi| \left(A I' + B p' + 2C \right).$$

The parallel component of the gradient of α may be easily found from Eq. (8). With $\nabla\alpha$ in hand, the remainder of the calculation is straightforward. We note that ∇B may also be calculated using the Mercier-Luc formulas; our treatment is the same as can be found in Refs. ([14]) and ([16]). To wit, the perpendicular component is

$$\nabla B \cdot \hat{e}_\Psi = \frac{B_p}{B_0} \left(\frac{B_p}{R_c} + R p' - \frac{I^2 \sin u}{R^3 B_p} \right),$$

and since $B(\rho_f)$ does not depend on p' or I', the component of ∇B along the field line depends on neither quantity.

The expressions for $\hat{s}$ and the gradients of α and B make it clear that once the safety factor, the shape of the flux surface, and B_p are determined (either from a numerical equilibrium or from the local equilibrium), one may vary p' and $\hat{s}$ independently to find a family of solutions, all of which satisfy the Grad-Shafranov equation. This flexibility allows one to carry out the Greene-Chance kind of analysis for microinstabilities. Such an analysis simplifies the interpretation of the numerical calculations, since all other parameters can easily be held fixed.

Within the context of the local equilibrium model,[14] one may also vary individual shape parameters one at a time, to explore the dependences in a controlled fashion.

The eleven dimensionless parameters that determine the local MHD equiliibrium in this implementation of the Miller model are summarized in Table I.

*Minor radius	ρ_f
*Safety factor	q
Magnetic shear	$\hat{s} = (\rho/q)dq/d\rho$
Elongation	κ
$d\kappa/d\rho$	κ'
Triangularity	δ
$d\delta/d\rho$	δ'
Center of LCFS	R_{geoN}
Center of flux surface	R_{0N}
$dR_0/d\rho$	R'_{0N}
*$d\beta/d\rho$	β'

In addition to these eleven parameters, there are two normalizing dimensional parameters, a and B_a. In all, there are two more parameters than are found in Miller, *et al.*[14] We include the additional parameters to allow a somewhat more natural correspondence between *reported* equilibria and the input variables. We emphasize that there is nothing "extra" in our implementation of the model as result; it is only modestly easier to use for some applications. For example, our choice of the normalization of the magnetic field (B_a) is the vacuum magnetic field at R_{geo}, the center of the LCFS. This quantity is the most commonly reported magnetic field value. By allowing R_0 to be specified separately, we also make it conceptually easier to separate the effects of Shafranov shift from the derivative of the Shafranov shift. The inclusion of the normalized minor radius as a separate variable is a natural choice as soon as one allows for separate specification of R_0 and R_{geo}.

The starred quantities (ρ_f, $\hat{s}$, and $d\beta/d\rho$) may be specified when reading in numerical equilibria. Values of the latter two quantities that are different from the actual equilibrium values are incorporated by using Eq. (20) to define I'.

Finally, when using numerically generated equilibria, the module allows one to choose from the most common definitions of ρ, such as the normalized poloidal or toroidal fluxes, the horizontal minor radius, *etc.* The user may also provide his or her own definition of ρ by supplying a simple function.

References

References

[1] M. A. Beer, S. C. Cowley, and G. W. Hammett, Phys. Plasmas **2**, 2687 (1995).

[2] M. D. Kruskal and R. M. Kulsrud, Phys. Fluids **1**, 265 (1958).

[3] T. Antonsen and B. Lane, Phys. Fluids **23**, 1205 (1980).

[4] A. M. Dimits and W. W. Lee, J. Comput. Phys. **107**, 309 (1993).

[5] R. Denton and M. Kotschenreuther, J. Comp. Phys. **119**, 283 (1995).

[6] G. Rewoldt, W. M. Tang, G. Rewoldt, and M. S. Chance, Phys. Fluids **25**, 480 (1982).

[7] M. Kotschenreuther, G. Rewoldt, and W. M. Tang, Comp. Phys. Comm. **88**, 128 (1995).

[8] R. L. Miller and J. W. VanDam, Nucl. Fusion **28**, 2101 (1987).

[9] P. M. de Zeeuw, J. Comput. Appl. Math. **33**, 1 (1990).

[10] L. L. Lao, J. R. Ferron, R. J. Groebner, W. Howl, H. S. John, E. J. Strait, and T. S. Taylor, Nucl. Fusion **30**, 1035 (1990).

[11] L. L. Lao, S. P. Hirshman, and R. M. Wieland, Phys. Fluids **24**, 1431 (1981).

[12] J. Delucia, S. C. Jardin, and A. M. M. Todd, J. Comput. Phys. **37**, 183 (1980).

[13] H. Luetjens, A. Bondeson, and O. Sauter, Comput. Phys. Comm. **97**, 219 (1996).

[14] R. L. Miller, M. S. Chi, J. M. Greene, Y. R. Lin-Liu, and R. E. Waltz, Phys. Plasmas **5**, 973 (1998).

[15] C. Mercier and N. Luc, Technical Report No. EUR 5127e, Commission of the European Communities, Brussels (unpublished).

[16] C. M. Bishop, P. Kirby, J. W. Connor, R. J. Hastie, and J. B.Taylor, Nuclear Fusion **24**, 1579 (1984).

[17] J. M. Greene and M. S. Chance, Nucl. Fusion **21**, 453 (1981).