1 The current diffusion equation

On the diffusion time scale, the (perpendicular) transport in an axisymmetric tokamak can be described by flux-surface averaged transport (diffusion-convection) equations.

$$\frac{\partial \langle y \rangle}{\partial t} - \frac{\partial}{\partial x}\left(D \frac{\partial \langle y \rangle}{\partial x} + v_y \langle y \rangle \right) = S_y \tag{1}$$

Here, $\langle y \rangle$ corresponds to flux-averaged quantities,

$$\langle y \rangle = \frac{\partial}{\partial V} \int y \mathrm{d}V = \frac{\oint \frac{y}{B_{\mathrm{pol}}} \mathrm{d}l_\theta}{\oint \frac{1}{B_{\mathrm{pol}}} \mathrm{d}l_\theta} \tag{2}$$

ψ is the poloidal magnetic flux and x is a normalized flux coordinate, defined as

$$x = \frac{\rho}{\rho_1}, \quad \rho = \sqrt{\frac{\Phi}{\pi B_0}} \tag{3}$$

Φ is the toroidal magnetic flux, ρ_1 is ρ at the last closed flux surface. In particular, for the magnetic flux diffusion, generally called the current diffusion equation (CDE), we have [1]

$$\begin{gathered} \frac{\partial \psi}{\partial t} - \frac{\left\langle |\nabla \rho|^2 / R^2 \right\rangle}{\mu_0 \sigma_\parallel \rho_1^2 \langle 1/R^2 \rangle} \frac{\partial^2 \psi}{\partial x^2} - \\ \left\{ \frac{\left\langle |\nabla \rho|^2 / R^2 \right\rangle}{\mu_0 \sigma_\parallel \rho_1^2 \langle 1/R^2 \rangle} \frac{\partial}{\partial x} \left[\ln \left(\frac{V' \left\langle |\nabla \rho|^2 / R^2 \right\rangle}{F} \right) \right] + \frac{x}{\rho_1} \frac{\mathrm{d}\rho_1}{\mathrm{d}t} \right\} \frac{\partial \psi}{\partial x} = \frac{B_0}{\sigma_\parallel F \langle 1/R^2 \rangle} j_{\mathrm{ni}} \end{gathered} \tag{4}$$

where

$$V' = \partial V / \partial \rho \tag{5}$$

After using

$$\begin{aligned} g_1 &= \left\langle 1/R^2 \right\rangle \\ g_2 &= \left\langle |\nabla \rho|^2 / R^2 \right\rangle \end{aligned} \tag{6}$$

the equation can be written as

$$\frac{\partial \psi}{\partial t} - \frac{g_2}{\mu_0 \sigma_\parallel \rho_1^2 g_1} \left[\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial}{\partial x} \ln \left(\frac{V' g_2}{F} \right) \frac{\partial \psi}{\partial x} \right] - \frac{x}{\rho_1} \frac{\mathrm{d}\rho_1}{\mathrm{d}t} \frac{\partial \psi}{\partial x} = \frac{B_0}{\sigma_\parallel F g_1} j_{\mathrm{ni}} \tag{7}$$

1.1 Boundary conditions

On the magnetic axis we have (from the geometry)

$$\left. \frac{\partial \psi}{\partial x} \right|_{x=0} = 0 \tag{8}$$

On the plasma boundary ($x = 1$), the most common boundary condition is a prescribed total plasma current

$$I_{\mathrm{p}} = -\frac{1}{2\pi\mu_0} V' g_2 \left. \frac{\partial \psi}{\partial \rho} \right|_{x=1} \tag{9}$$

In case of free-boundary equilibrium simulations, the plasma current is no longer presribed. Hence different boundary conditions must be used. As the magnetic flux must be consistent in the transport and equilibrium equations, the natural boundary condition (at $x = 1$) would be

$$\psi^{\mathrm{diff}} = \psi^{\mathrm{equi}} \tag{10}$$

This is similar to prescribing the loop voltage in fixed boundary simulation, which is known to be prone to numerical errors. For this reason, we have derived two different boundary conditions for FBE simulations. The first one follows from (10) and using $L_{\mathrm{i}} I_{\mathrm{p}} = \psi_0 - \psi_1$. This allows us to calculate an I_{p} predictor, which enforces the ψ consistency:

$$I_{\mathrm{p}}^{*} = I_{\mathrm{p}} \left(1 + \frac{\psi_1^{\mathrm{diff}} - \psi_1^{\mathrm{eq}}}{\psi_0^{\mathrm{eq}} - \psi_1^{\mathrm{eq}}} \right) \tag{11}$$

which is then used in (10). The second possibility is similar to the approach in DINA [3]:

$$\frac{\psi_1}{\tilde{L}_{\mathrm{ext}}} - \gamma C \left. \frac{\partial \psi}{\partial x} \right|_{x=1} = \frac{1}{\tilde{L}_{\mathrm{ext}}} \left(\tilde{\psi}_1 + \psi_0^{\mathrm{ext}} - \tilde{\psi}_0^{\mathrm{ext}} \right) + \tilde{I}_{\mathrm{p}}. \tag{12}$$

where $\gamma = L_{\mathrm{ext}} / \tilde{L}_{\mathrm{ext}}$.

2 Equilibrium

MHD equilibrium is described by the Grad-Shafranov equation

$$-\Delta^{*} \psi = \mu_0 R j_{\phi} = \mu_0 R^2 \frac{\mathrm{d}p}{\mathrm{d}\psi} + F \frac{\mathrm{d}F}{\mathrm{d}\psi} \tag{13}$$

On the diffusion time scale, this equation is valid for every time instant. On the right-hand side appears $p'(\psi)$—the pressure gradient—and $FF'(\psi)$. p' can be calculated from $p(x)$ and $\partial\psi/\partial x$. The calculation of FF' is more difficult. One possibility, which is currently used in CRONOS and ETS-C, is averaging the G-S equation. One obtains

$$FF' = \frac{\mu_0}{g_1} \left(\langle j_{\phi} / R \rangle - p' \right) \tag{14}$$

The average current term can be calculated as

$$\langle j_{\phi} / R \rangle = - \frac{\frac{\partial}{\partial x} \left(V' g_2 \frac{\partial \psi}{\partial x} \right)}{\rho_1^2 \mu_0 V'} \tag{15}$$

Since the current density is generally continuous, it follows that

$$\psi \in C^2, \; g_2 \in C^1, \; V' \in C^1 \tag{16}$$

3 (Numerical) challenges

1. Boundary conditions
2. Noise from the G-S equation
3. Geometric coefficients smoothness
4. Calculation of $\langle j_\phi / R \rangle$ using $\frac{\partial^2 \psi}{\partial x^2}$
5. Possible interplay in FF' and G-S calculation

Neumann (10) and Robin (12) boundary conditions are not straightforward in a finite difference solver. On top of that, the solution does not carry the information about the derivatives (an additional bookkeeping is required).

FBE solvers tend to use rather coarse calculation meshes because of the complexity and non-linearity of the problem. The results is typically a numerical noise in ψ_1 and geometric coefficients.

This also implies that the geometric coefficients does not have to be smooth enough (C^1). This is of course a problem in the calculation of $\langle j_\phi / R \rangle$ as well as in the CDE.

We have to use some kind of smooth interpolation or approximation of $\psi(x)$ in order to calculate $\frac{\partial^2 \psi}{\partial x^2}$. Splines under tension are typically used in CRONOS. This means that (1) it is only an approximation, (2) oscillations can (and actually do) appear near $x = 1$ (even if the exact value of $\left.\frac{\partial \psi}{\partial x}\right|_{x=1}$ is provided).

The FF' calculation takes place in the transport-equilibrium iteration scheme. Since the averaged G-S equation contains geometric coefficients, there can be an interplay, which might lead to an instability. This is most recently discussed in [2].

4 A finite elements method approch

4.1 A brief overview

Assume a general partial differential equation (PDE)

$$Lf - g = 0 \tag{17}$$

with boundary conditions

$$Cf - h = 0 \tag{18}$$

The Galerkin finite elements method (FEM) solves this problem in a weak form by integrating by parts the following equation:

$$\int_\Omega \left(L \sum \phi_i F_i - g \right) \phi_k \mathrm{d}\Omega = 0, \quad k = 1 \ldots N \tag{19}$$

Here, ϕ_i are the finite elements, which are basis functions with finite support, and the function f is discretized as

$$f = \sum F_i \phi_i \tag{20}$$

The integration by parts has an important property: it can remove derivatives in L, in in the coefficients that appear in the original equations. These derivatives are often directly unknown and are calculated from interpolations or approximations.

4.2 Hermite elements

1D Hermite elements are polynomials $\mathrm{H}_i(\xi)$, for which

$$\begin{aligned} \mathrm{H}_{ij}^{(k)}(0) &= \delta_{jk} \\ \mathrm{H}_{ij}^{(k)}(\pm 1) &= 0 \end{aligned} \tag{21}$$

where ξ, $-1 \leqslant \xi \leqslant 1$ is a normalized coordinate, the superscript $^{(k)}$ denotes the k^{th} derivative and δ is the Kronecker symbol. As such, the coefficients F_{ij} in the finite element reprosentation of a function f,

$$f = \sum F_{ij} \mathrm{H}_{ij} \tag{22}$$

are directly the values of the j^{th} derivatives of f at a mesh point i. (Two indeces are used for being more explicit; a renumbering to a single index is straightforward.)

Cubic Hermite elements can be expressed as

$$\mathrm{H}_0(\xi) = (|\xi| - 1)^2 (2|\xi| + 1) \tag{23}$$

$$\mathrm{H}_1(\xi) = \xi h_i (|\xi| - 1)^2 \tag{24}$$

(Note that the scaling factor h_i must be properly defined for H_1.)

4.3 Implications for CDE + G-S

1. Boundary conditions on derivatives are more natural (similar to Dirichlet).
2. The solution, i.e. ψ, is C^1 (using cubic Hermite elements). $\psi(x)$ and $\psi'(x)$ is directly known for any x.
3. Some possibly noisy derivative terms from CDE can be eliminated.
4. Perhaps, a finite element G-S solver (CEDRES++) migh use p and F^2 instead of p' and FF'.

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