Computing `vmec`'s `ac` current profile and `curtor` from a bootstrap current code

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March 1, 2018

In this note, we detail how to compute the `vmec` input parameters `curtor` and `ac` (or `ac_aux_f`) from the averaged parallel current computed by neoclassical codes, $\langle \boldsymbol{j} \cdot \boldsymbol{B} \rangle$. Here, $\langle \ldots \rangle$ denotes a flux surface average, $\boldsymbol{j}$ is the current density, and $\boldsymbol{B}$ is the magnetic field. The proper result involves a term that is neglected by the `bootsj` code. This term is small in $\beta = 2\mu_0 p/B^2$, but it does not require much work to keep, so we may as well keep it. Physically, neoclassical codes compute a gyrophase-averaged distribution function and so the current they obtain is parallel to $\boldsymbol{B}$, whereas the total toroidal current also has a contribution from the diamagnetic current perpendicular to $\boldsymbol{B}$. The purpose of this note is to compute the proper relationship between these parallel and perpendicular currents and the net toroidal current.

The calculation here is a more detailed version of Appendix C of [1], except that Gaussian units were used in that paper whereas SI units are used throughout this note.

1 Overview

Bootstrap current codes like `bootsj` and `sfincs` solve the drift kinetic equation for the gyrophase-averaged distribution function f. The parallel velocity moment of f, weighted by species charge and summed over species, yields the parallel current $j_{||} = \boldsymbol{j} \cdot \boldsymbol{b}$, where $\boldsymbol{b} = \boldsymbol{B}/|\boldsymbol{B}|$. The spatial variation of $j_{||}$ over a magnetic surface can be determined analytically for any geometry and collisionality using mass conservation, so the results of a drift-kinetic calculation can be summarized by any weighted average of the parallel current over a flux surface. By convention, the average typically reported is $\langle \boldsymbol{j} \cdot \boldsymbol{B} \rangle$.

The `vmec` code takes as an input the profile of net toroidal current inside a flux surface. Therefore, to interface a bootstrap current code with `vmec`, the relationship between this net toroidal current and the parallel current must be calculated. We now calculate this relationship.

2 Derivation

Let $I(s)$ denote the total toroidal current inside a flux surface labelled by any flux function s, where we require that $s = 0$ on the magnetic axis. This total current is the flux (area integral) of the current density $\boldsymbol{j}$ through a surface of constant toroidal angle ζ:

$$I(s) = \int d^2\boldsymbol{a} \cdot \boldsymbol{j} = \int_0^s ds' \int_0^{2\pi} d\theta \sqrt{g} \boldsymbol{j} \cdot \nabla\zeta, \tag{1}$$

where θ is a poloidal angle, the integrand is evaluated at s' rather than s, and

$$\sqrt{g} = \frac{\partial \boldsymbol{r}}{\partial s} \cdot \frac{\partial \boldsymbol{r}}{\partial \theta} \times \frac{\partial \boldsymbol{r}}{\partial \zeta} = \frac{1}{\nabla s \cdot \nabla\theta \times \nabla\zeta} \tag{2}$$

is the Jacobian of the (s,θ,ζ) coordinates. It turns out to be convenient to write (1) in differential rather than integral form, by applying d/ds:

$$\frac{dI}{ds} = \int_0^{2\pi} d\theta \sqrt{g}\boldsymbol{j}\cdot\nabla\zeta. \tag{3}$$

These expressions so far are all valid for any angle coordinates (θ,ζ) (`vmec`, Boozer, `pest`, Hamada, etc.)

Next, consider that to leading order in $\rho/L \ll 1$, where ρ is a typical gyroradius and L is a typical equilibrium scale length, the current perpendicular to $\boldsymbol{B}$ is given by the diamagnetic current:

$$\boldsymbol{j}_\perp = \frac{1}{B^2}\frac{dp}{ds}\boldsymbol{B}\times\nabla s, \tag{4}$$

where $p(s)$ is the total pressure. This result can be obtained, for example, by applying $\boldsymbol{B}\times(\ldots)$ to the MHD equilibrium relation $\boldsymbol{j}\times\boldsymbol{B} = \nabla p$. Therefore the total current vector is

$$\boldsymbol{j} = \frac{j_{||}}{B}\boldsymbol{B} + \frac{1}{B^2}\frac{dp}{ds}\boldsymbol{B}\times\nabla s. \tag{5}$$

Substituting this result into (3),

$$\frac{dI}{ds} = \int_0^{2\pi} d\theta\sqrt{g}\left[\frac{j_{||}}{B}\boldsymbol{B}\cdot\nabla\zeta + \frac{B_\theta}{B^2}\frac{dp}{ds}\nabla\theta\times\nabla s\cdot\nabla\zeta\right], \tag{6}$$

where to get the last term we have expressed $\boldsymbol{B}$ in components

$$\boldsymbol{B} = B_s\nabla s + B_\theta\nabla\theta + B_\zeta\nabla\zeta. \tag{7}$$

The important message from (6) is that the total toroidal current I needed for `vmec` consists not only of the parallel current determined by neoclassical physics (the first right-hand-side term), but also by the diamagnetic current $\propto dp/ds$ in the last term.

While the calculation so far is true for any angle coordinates (θ,ζ), for the rest of this section it is convenient to use Boozer coordinates. The main result will turn out to be independent of the choice of angle coordinates. In any straight-field-line coordinates such as Boozer coordinates, the magnetic field can be written as

$$\boldsymbol{B} = \frac{d\psi}{ds}\left[\nabla s\times\nabla\theta + \iota\nabla\zeta\times\nabla s\right], \tag{8}$$

where $2\pi\psi$ is the toroidal flux enclosed by surface s, and $\iota(s)$ is the rotational transform. Hence, the geometric factor appearing in the first right-hand-side term of (6) is

$$\boldsymbol{B}\cdot\nabla\zeta = \frac{d\psi}{ds}\nabla s\times\nabla\theta\cdot\nabla\zeta = \frac{d\psi}{ds}\frac{1}{\sqrt{g}}, \tag{9}$$

and so (6) reduces to

$$\frac{dI}{ds} = \int_0^{2\pi} d\theta\left[\frac{d\psi}{ds}\frac{j_{||}}{B} - \frac{B_\theta}{B^2}\frac{dp}{ds}\right]. \tag{10}$$

Furthermore, in Boozer coordinates, B_θ and B_ζ in (7) are flux functions, i.e. they depend only on s, and we can show that B_θ is related to $I(s)$ as follows. The curl of (7) is

$$\nabla\times\boldsymbol{B} = \nabla B_s\times\nabla s + \frac{dB_\theta}{ds}\nabla s\times\nabla\theta + \frac{dB_\zeta}{ds}\nabla s\times\nabla\zeta. \tag{11}$$

Substituting this expression into Ampere's Law $\mu_0 \boldsymbol{j} = \nabla \times \boldsymbol{B}$, and using the result to eliminate $\boldsymbol{j}$ in (1),

$$\begin{aligned}\mu_0 I(s) &= \int_0^s ds' \int_0^{2\pi} d\theta \sqrt{g} \left[\frac{\partial B_s}{\partial \theta} \nabla\theta \times \nabla s \cdot \nabla\zeta + \frac{dB_\theta}{ds} \nabla s \times \nabla\theta \cdot \nabla\zeta \right] \\ &= \int_0^s ds' \int_0^{2\pi} d\theta \left[-\frac{\partial B_s}{\partial \theta} + \frac{dB_\theta}{ds} \right] = \int_0^s ds' \int_0^{2\pi} d\theta \frac{dB_\theta}{ds} \\ &= 2\pi [B_\theta(s) - B_\theta(0)].\end{aligned} \tag{12}$$

At the magnetic axis ($s = 0$), B_θ must vanish, since in (7) it multiplies $\nabla\theta$ which diverges on axis, and the product must be regular. Hence,

$$B_\theta(s) = \frac{\mu_0 I(s)}{2\pi}. \tag{13}$$

Using this result in (10), and applying a toroidal average $(2\pi)^{-1} \int_0^{2\pi} d\zeta(\ldots)$,

$$\frac{dI}{ds} = \frac{1}{2\pi} \frac{d\psi}{ds} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{j_{||}}{B} - \frac{\mu_0 I}{4\pi^2} \frac{dp}{ds} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{1}{B^2}. \tag{14}$$

The angular averages in this last expression can be written in terms of the flux surface average, which for any quantity Q is

$$\langle Q \rangle = \frac{\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \sqrt{g} Q}{\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \sqrt{g}} = \frac{\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \sqrt{g} (Q/B^2)}{\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta / B^2}. \tag{15}$$

In the last equation, we have used the fact that the Jacobian in Boozer coordinates is $\sqrt{g} = (d\psi/ds)(B_\zeta + \iota B_\theta)/B^2$, which follows from the product of (7) and (8). From (15) we see that

$$\langle B^2 \rangle = \frac{4\pi^2}{\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta / B^2}. \tag{16}$$

Using (15)-(16), (14) can be written

$$\boxed{\frac{dI}{ds} + \frac{\mu_0 I}{\langle B^2 \rangle} \frac{dp}{ds} = 2\pi \frac{d\psi}{ds} \frac{\langle j_{||} B \rangle}{\langle B^2 \rangle}.} \tag{17}$$

This result is the key equation for relating the current density $\langle j_{||} B \rangle$ from a neoclassical code to the radial profile of total current in an MHD equilibrium code. While we used Boozer angles to derive this result,it is independent of any particular choice of angles.

There are several ways to implement (17) numerically, which we will now describe. In each case, an iteration must be performed between the MHD equilibrium code and the bootstrap current code. We will use a subscript i to denote the iteration step.

2.1 Low β approximation

It can be seen that the dp/ds term in (17) is smaller than the dI/ds term preceding it by a factor of β. Therefore for $\beta \ll 1$ it is a reasonable approximation to neglect the dp/ds term. Then the current profile is updated according to

$$\frac{dI_{i+1}}{ds} = 2\pi \frac{d\psi}{ds} \frac{\langle j_{||} B \rangle_i}{\langle B_i^2 \rangle}. \tag{18}$$

This is the approach adopted in `bootsj`.

2.2 Lagging the dp/ds term

A more accurate approach to solving (17) numerically is to evaluate the updated dI/ds term using the dp/ds term from the previous iteration:

$$\frac{dI_{i+1}}{ds} = -\frac{\mu_0 I_i}{\langle B_i^2 \rangle}\frac{dp}{ds} + 2\pi\frac{d\psi}{ds}\frac{\langle j_{||}B\rangle_i}{\langle B_i^2\rangle}. \tag{19}$$

For $\beta \ll 1$ this iteration should converge rapidly since the dp/ds term is small, and since the factor of I in the dp/ds term is smoother than dI/ds. This is the approach that is used for the `stellopt` `vboot` iteration using `sfincs`.

2.3 Integrating factor

A third approach to solving (17) is to interpret this expression as an ordinary differential equation for $I(s)$, introducing an integrating factor:

$$\frac{d}{ds}(IF) = 2\pi F\frac{d\psi}{ds}\frac{\langle j_{||}B\rangle}{\langle B^2\rangle}, \tag{20}$$

where the integrating factor is

$$F(s) = \exp\left(\mu_0\int_0^s \frac{ds'}{\langle B^2\rangle}\frac{dp}{ds}\right). \tag{21}$$

(Again, the integrand is evaluated at s' rather than s.) One can see from this definition that $F = 1 + \mathcal{O}(\beta)$. Imposing the boundary condition $I(0) = 0$ (there is no enclosed toroidal current on the magnetic axis), the solution to (20) is then

$$I(s) = \frac{2\pi}{F(s)}\int_0^s ds'' F\frac{d\psi}{ds}\frac{\langle j_{||}B\rangle}{\langle B^2\rangle}, \tag{22}$$

where the integrand is evaluated at s''. From this expression, we obtain the iterative scheme

$$I_{i+1}(s) = \frac{2\pi}{F_i(s)}\int_0^s ds'' F_i\frac{d\psi}{ds}\frac{\langle j_{||}B\rangle_i}{\langle B_i^2\rangle}, \tag{23}$$

3 VMEC definitions

The current profile is provided to `vmec` using two quantities. The first is the number `curtor`, which is the total toroidal current inside the outermost `vmec` magnetic surface. My understanding of `vmec`'s sign convention is that `curtor` is positive when the current is in the $\nabla\zeta$ direction, where ζ is the toroidal angle used in `vmec` (also called ϕ or v in the code and its documentation). I also believe `vmec`'s ζ always increases in the counter-clockwise direction when the plasma is viewed from above, so (R, ζ, Z) is a right-handed system. For comparison, (1) indicates that $I(s)$ is positive if the current is in the direction $\sqrt{g}\nabla\zeta$, which is opposite to the $\nabla\zeta$ direction if $\sqrt{g} < 0$. In my understanding, $\sqrt{g}$ is *always* < 0 in `vmec` output. (The notation $\sqrt{g}$ is confusing, since square roots are normally defined to be positive.) Thus,

$$\texttt{curtor} = \texttt{signgs}\, I(1), \tag{24}$$

where signgs$= -1$ is the name for the sign of $\sqrt{g}$ in the vmec wout*.nc output file. In (24) we have used the vmec convention that $s = 1$ is the outermost magnetic surface in the code. The particular definition of s used in vmec is that s is the toroidal flux normalized to range from 0 on the magnetic axis to 1 at the outermost surface.

The other relevant vmec input parameters are ac or ac_aux_f; I'll write just ac here to denote whichever one is used based on the pcurr_type parameter. The profile determined by ac (using a power series, spline, or other function) corresponds to dI/ds up to an overall scale factor. The ac profile is always scaled by vmec so the total current at the outermost surface is curtor. Hence,

$$\frac{dI/ds}{(dI/ds)_{s=1}} = \frac{\mathtt{ac}(s)}{\mathtt{ac}(1)}. \tag{25}$$

We can therefore set ac equal to (18), to (19), or to the radial derivative of (22) (times any constant.)

To evaluate any of these three expressions, we need $d\psi/ds$. Since $s \propto \psi$ in vmec, $d\psi/ds$ is just the constant ψ_{edge}, the toroidal flux at the outermost magnetic surface. However, we must be careful about the sign. Applying the operation $\int_0^1 ds \int_0^{2\pi} d\theta \sqrt{g} \nabla\zeta \cdot (\ldots)$ to (8) gives

$$\int_0^1 ds \int_0^{2\pi} d\theta \sqrt{g} \boldsymbol{B} \cdot \nabla\zeta = \int_0^1 ds \int_0^{2\pi} d\theta \sqrt{g} \frac{d\psi}{ds} \nabla s \times \nabla\theta \cdot \nabla\zeta = 2\pi \frac{d\psi}{ds} = 2\pi\psi_{edge}. \tag{26}$$

From this equation, we see the sign convention for $d\psi/ds$ in (22) is that a positive value corresponds to the magnetic field pointing in the direction $\sqrt{g}\nabla\zeta$. In contrast, I believe vmec's convention is that the output toroidal flux variable phi is positive if the magnetic field points in the direction $\nabla\zeta$. Also, phi is the flux *not* divided by 2π, in contrast to ψ in this note. Hence, the value of $d\psi/ds$ to use in (22) is

$$\frac{d\psi}{ds} = \mathtt{signgs} \frac{\mathtt{phi}(s = 1)}{2\pi}. \tag{27}$$

Note that the output quantity phips differs from phi by a factor 2πsigngs, so we could equivalently use $d\psi/ds = \mathtt{phips}$.

References

[1] M Landreman and P J Catto. *Phys. Plasmas*, **19**, 056103 (2012).