Interfacing vacuum to M3D and M3D-C1*

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Introduction

- The vacuum equations are intrinsically linear so that the solutions obtained with the 2 dimensional VACUUM code are still applicable for nonlinear problems *provided that the boundary conditions are still approximately linearized, and the "background" equilibrium is still approximately two-dimensional*.
- One way to perhaps accomplish this is with a "buffer zone" between the fully developed nonlinear plasma and the vacuum. In this zone would be a transition from the nonlinear regime to an approximately linearized, two-dimensional boundary outside of which the vacuum solution is valid and can be applied as outlined below to establish the outer boundary conditions. Nonlinear codes such as M3D-C1, M3D or NIMROD would treat both the plasma core and the buffer zone with the VACUUM code treating the region to infinity or to a conducting shell.
- We assume that the buffer zone is bounded by either:

  I. A toroidally symmetric virtual boundary. Or

  II. A toroidally symmetric resistive shell.

The field representation in M3D and M3D-C1

The parameter m determines the applicability for M3D ($m = 1$) and M3D-C1 ($m = 2$).

In the cylindrical coordinate system (R, ϕ, Z), the magnetic field, $\mathbf{B}$ is derived from a vector potential, $\mathbf{A}$ involving two scalar variables f and ψ:

$$\mathbf{A} = \psi\nabla\phi + R^m\nabla\phi \times \nabla f - R_0 \ln R\, \mathbf{e}_Z \tag{1}$$

$$\mathbf{B} = \nabla\psi \times \nabla\phi - R^{m-2}\nabla_\perp f' + F\nabla\phi \tag{2}$$

with $$F \equiv R^2\nabla\cdot R^{m-2}\nabla_\perp f + R_0 \tag{3}$$

and $$\nabla_\perp f \equiv \nabla f - \frac{\partial f}{\partial\phi}\nabla\phi \equiv \nabla f - f'\nabla\phi. \tag{4}$$

M3D: $$\mathbf{B} = \nabla\psi \times \nabla\phi + R_0\nabla\phi - R^{-1}\nabla_\perp f' + R^2\nabla\cdot R^{-1}\nabla_\perp f \tag{5}$$

M3D-C1: $$\mathbf{B} = \nabla\psi \times \nabla\phi + R_0\nabla\phi - \nabla_\perp f' + R^2\nabla_\perp^2 f \tag{6}$$

VACUUM: $$\mathbf{B}^v = \nabla\psi^v \times \nabla\phi + F^v\nabla\phi + \nabla\chi, \qquad \nabla^2\chi = 0 \tag{7}$$

The terms involving ψ^v and F^v are the axisymmetric ($n = 0$) contributions to the field.

- Note the similarity between the representations of VACUUM and M3D-C1.

The Current, $k_1\mathbf{J} = \nabla \times \mathbf{B}$

$$k_1\mathbf{J} = \nabla F^* \times \nabla\phi + \frac{1}{R^2}\nabla_\perp\psi' - \left[\Delta^*\psi - (m-2)R^{m-2}f_z'\right]\nabla\phi$$
$$-(m-2)R^{m-4}f''\nabla Z \qquad (8)$$
$$= \left(\nabla F + R^{m-2}\nabla f''\right) \times \nabla\phi + \frac{1}{R^2}\nabla_\perp\psi' - \left[\Delta^*\psi - (m-2)R^{m-2}f_z'\right]\nabla\phi \qquad (9)$$

where

$$\Delta^* \equiv R^2\nabla\cdot\frac{1}{R^2}\nabla_\perp = \frac{\partial^2}{\partial R^2} - \frac{1}{R}\frac{\partial}{\partial R} + \frac{\partial^2}{\partial Z^2}. \qquad (10)$$

In component form,

$$k_1\mathcal{J}\mathbf{J}\cdot\nabla\mathcal{Z} = \frac{\partial F}{\partial\theta} + R^{m-2}\frac{\partial f''}{\partial\theta} + \frac{\mathcal{J}}{R^2}\nabla\mathcal{Z}\cdot\nabla_\perp\psi' \qquad (11)$$
$$k_1R^2\mathbf{J}\cdot\nabla\phi = -\Delta^*\psi - (m-2)R^{m-2}f_z' \qquad (12)$$
$$k_1R^2\nabla\phi\times\mathbf{J} = \nabla_\perp F^* + R^{m-2}\nabla_\perp f'' + \nabla\phi\times\nabla_\perp\psi'. \qquad (13)$$

The response to the magnetic scalar potential, χ

The VACUUM code solves for the magnetic scalar potential, χ, as a response $\mathcal{C}$, to B_n, the normal component of the magnetic field at the surface which separates the MHD region from the vacuum region. This surface is parameterized by $[R^s(\theta), Z^s(\theta)],\ 0 \leq \theta \leq 2\pi$ in a local coordinate system $(\mathcal{Z}, \theta, \phi)$. $\nabla\mathcal{Z}$ is normal to the surface with $\mathcal{J} = (\nabla\mathcal{Z} \times \nabla\theta{\cdot}\nabla\phi)^{-1}$. The response relation is written as

$$\chi(\theta, \phi) = \sum_l \mathcal{C}_l(\theta)\mathcal{B}_l^v e^{-in\phi}, \quad n \neq 0 \tag{14}$$

where the normal field, written as an angular flux density, $\mathcal{B}^v(\theta) \equiv \mathcal{J}\nabla\chi{\cdot}\nabla\mathcal{Z}$ (since the flux is $\int \mathcal{B}^s\, d\theta\, d\phi$), is expanded in a set of suitably chosen (orthonormal) basis functions appropriate for the source surface,

$$\mathcal{B}^v(\theta) = \sum_l \mathcal{B}_l^v \varphi_l(\theta). \tag{15}$$

The response $\mathcal{C}_l(\theta)$, contains the effects of the external vacuum region, including the option of an external conducting shell. It depends only on the geometry of the boundary and the conductors and need only be calculated once for the number of expansion functions required for the application.

Matching across a virtual boundary – no shell: All components continuous

- We assume here that the plasma is highly resistive at the virtual boundary so that there is no support for the existence of a skin current.
  - Hence, in addition to the usual continuity of B_n we require that all components of the field are continuous.
- The normal component of $\mathbf{B}$ (angular flux):

$$\mathcal{B}^p \equiv \mathcal{J}\mathbf{B}\cdot\nabla\mathcal{Z} \;=\; \frac{\partial\psi}{\partial\theta} - R^{m-2}\mathcal{J}\nabla\mathcal{Z}\cdot\nabla_\perp f'. \tag{16}$$

The covariant surface components of $\mathbf{B}$, e.g., $B_\theta = \mathcal{J}\nabla\phi\times\nabla\mathcal{Z}\cdot\mathbf{B}$ etc., are

$$B_\theta = -\left(\frac{\mathcal{J}}{R^2}\nabla\mathcal{Z}\cdot\nabla\psi + R^{m-2}\frac{\partial f'}{\partial\theta}\right) \tag{17}$$

$$B_\phi = F \;=\; R^2\nabla\cdot R^{m-2}\nabla_\perp f + R_0. \tag{18}$$

$k_1\mathcal{J}\mathbf{J}\cdot\nabla\mathcal{Z}$ can be written as

$$k_1\mathcal{J}\mathbf{J}\cdot\nabla\mathcal{Z} = \frac{\partial}{\partial\theta}R^2\nabla\cdot R^{m-2}\nabla_\perp f + \frac{\partial}{\partial\phi}\left(\frac{\mathcal{J}}{R^2}\nabla\mathcal{Z}\cdot\nabla\psi + R^{m-2}\frac{\partial f'}{\partial\theta}\right) \tag{19}$$

$$= \frac{\partial}{\partial\theta}B_\phi - \frac{\partial}{\partial\phi}B_\theta \tag{20}$$

as expected using Eqs. (17) and (18).

Matching across a virtual boundary – 2

Since B_n is continuous across a surface, we can substitute $\mathcal{B}^p$ for $\mathcal{B}^v$ in Eq. (14), i.e.,

$$\chi(\theta,\phi) = \sum_l \mathcal{C}_l(\theta) \left[\frac{\partial\psi}{\partial\theta} - R^{m-2}\mathcal{J}\nabla\mathcal{Z}\cdot\nabla_\perp f'\right]_l e^{-in\phi}, \tag{21}$$

using Eq. (16). this gives a relation between χ and the plasma quantities, ψ and f. we assumed here that the plasma quantities are expanded in $\varphi_l(\theta)$.

Under the assumption that the fields are continuous χ can be eliminated as follows. For the covariant component along the poloidal direction, we have

$$B^v_\theta = \mathcal{J}\nabla\phi\times\nabla\mathcal{Z}\cdot\mathbf{B}^v = \frac{\partial\chi}{\partial\theta} = \sum_l \frac{\partial\mathcal{C}_l(\theta)}{\partial\theta}\left[\frac{\partial\psi}{\partial\theta} - R^{m-2}\mathcal{J}\nabla\mathcal{Z}\cdot\nabla_\perp f'\right]_l e^{-in\phi}, \tag{22}$$

(23)

Substitute Eq. (16):

$$\boxed{\frac{\mathcal{J}}{R^2}\nabla\mathcal{Z}\cdot\nabla\psi + R^{m-2}\frac{\partial f'}{\partial\theta} = -\sum_l \frac{\partial\mathcal{C}_l(\theta)}{\partial\theta}\left[\frac{\partial\psi}{\partial\theta} - R^{m-2}\mathcal{J}\nabla\mathcal{Z}\cdot\nabla_\perp f'\right]_l e^{-in\phi}.} \tag{24}$$

Thus, together with the continuity of the normal component of the magnetic field used above, Eq. (24) provides a constraint on ψ and f for the vacuum boundary conditions.

Matching across a virtual boundary – continuous B_ϕ

For the covariant ϕ component, we find another relation between ψ and f at the boundary:

$$\boxed{R^2\nabla\cdot R^{m-2}\nabla_\perp f = -in\sum_l \mathcal{C}_l(\theta)\left[\frac{\partial\psi}{\partial\theta} - R^{m-2}\mathcal{J}\nabla\mathcal{Z}\cdot\nabla_\perp f'\right]_l e^{-in\phi}, \quad n\neq 0} \tag{25}$$

These are equivalent in a vacuum: differentiate Eq. (24) with respect to ϕ and Eq. (25) with respect to θ:

$$\frac{\partial}{\partial\phi}\left(\frac{\mathcal{J}}{R^2}\nabla\mathcal{Z}\cdot\nabla\psi + R^{m-2}\frac{\partial f'}{\partial\theta}\right) = in\sum_l \frac{\partial\mathcal{C}_l(\theta)}{\partial\theta}\left[\frac{\partial\psi}{\partial\theta} - R^{m-2}\mathcal{J}\nabla\mathcal{Z}\cdot\nabla_\perp f'\right]_l e^{-in\phi}. \tag{26}$$

$$\frac{\partial}{\partial\theta}\left(R^2\nabla\cdot R^{m-2}\nabla_\perp f\right) = -in\sum_l \frac{\partial\mathcal{C}_l(\theta)}{\partial\theta}\left[\frac{\partial\psi}{\partial\theta} - R^{m-2}\mathcal{J}\nabla\mathcal{Z}\cdot\nabla_\perp f'\right]_l e^{-in\phi}. \tag{27}$$

The left sides are the terms in the perpendicular current given by Eq. (20). Either one can then be used as the constraint that relates ψ and f at the boundary.

The vanishing of $\mathbf{J}\cdot\nabla\mathcal{Z}$ can be imposed as an extra constraint or it will occur naturally if the plasma resistivity at the interface is high enough.

Derivatives in Rectangular Coordinates, (R, Z)

Relations valid at the surface $[R(\theta), Z(\theta)]$:

$$\frac{\partial}{\partial\theta} = R_\theta \frac{\partial}{\partial R} + Z_\theta \frac{\partial}{\partial Z}, \tag{28}$$

$$\mathcal{J}\nabla\mathcal{Z}\cdot\nabla = R\left[R_\theta \frac{\partial}{\partial Z} - Z_\theta \frac{\partial}{\partial R}\right]. \tag{29}$$

In the expansion space of φ_l:

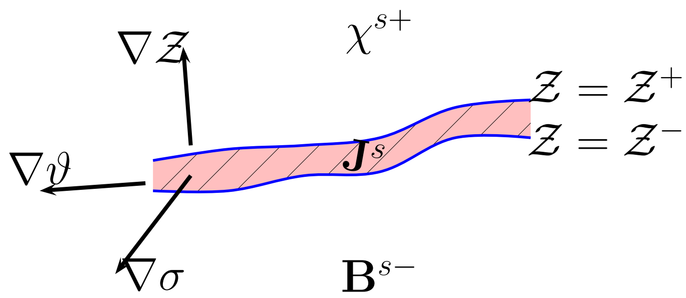
$$\left[\frac{1}{R}(R_\theta\psi_Z - Z_\theta\psi_R) - inR^{m-2}(R_\theta f_R + Z_\theta f_Z)\right]_l = \tag{30}$$

$$-\sum_{l'}\left(\frac{\partial\mathcal{C}}{\partial\theta}\right)_{ll'}\left[R_\theta\psi_R + Z_\theta\psi_Z + inR^{m-1}(R_\theta f_Z - Z_\theta f_R)\right]_{l'}, \tag{31}$$

$$\left[R^2\nabla\cdot R^{m-2}\nabla_\perp f\right]_l = -in\sum_{l'}\mathcal{C}_{ll'}\left[R_\theta\psi_R + Z_\theta\psi_Z + inR^{m-1}(R_\theta f_Z - Z_\theta f_R)\right]_{l'} \tag{32}$$

Here, R_θ, Z_θ can be calculated from the parameterization of the boundary $[R(\theta), Z(\theta)]$. The VACUUM code provides the response matrices, $\mathcal{C}_{ll'}$ and $(\partial\mathcal{C}/\partial\theta)_{ll'}$.

Current in Thin Surfaces



- Consider current carrying discontinuities whose resistivity and small but finite thickness δ can be spatially varying.
- In a local generalized shell coordinate system $(\mathcal{Z}, \vartheta, \sigma)$ the shell, bounded by surfaces of constant $\mathcal{Z}$, is of uniform thickness $\Delta\mathcal{Z} = \mathcal{Z}^{+} - \mathcal{Z}^{-}$.
- A divergence free representation of the shell current density $\mathbf{J}^{s}$ can be written in terms of a current potential $\mathcal{I}^{s}$ as

$$\mathbf{J}^{s} = \frac{\nabla\mathcal{Z} \times \nabla\mathcal{I}^{s}}{\Delta\mathcal{Z}} \tag{33}$$

  where $\mathcal{I}(\vartheta)^{s}$ is assumed to be independent of $\mathcal{Z}$.
- We first obtain the relation between the shell current and magnetic field then calculate the jump in the fields across the shell.

Faraday's Law

The normal component of Faraday's law, $\nabla \times \mathbf{E} = -k_3\, \partial_t \mathbf{B}$, together with Ohm's law $\mathbf{E} = \eta \mathbf{J}$ relates the surface Laplacian of $\mathcal{I}^s$ to $\mathbf{B}$:

$$\nabla \cdot \left[\eta \frac{\nabla \mathcal{Z} \times \nabla \mathcal{I}^s}{\Delta \mathcal{Z}} \times \nabla \mathcal{Z} \right] = -k_3 \frac{\partial}{\partial t} \mathbf{B} \cdot \nabla \mathcal{Z}. \tag{34}$$

In the global wall coordinate system, $(\mathcal{Z}, \theta, \phi)$ and using $\Delta \mathcal{Z} \approx |\nabla \mathcal{Z}| \delta(\theta)$ where $\delta(\theta)$ is the thickness of the (thin) shell, Eq. (34) becomes after Fourier analysis in ϕ,

$$\frac{\partial}{\partial \theta} \left(\frac{\eta}{\delta} \frac{R}{(R_\theta^2 + Z_\theta^2)^{1/2}} \frac{\partial}{\partial \theta} \mathcal{I}^s \right) - n^2 \frac{\eta}{\delta} \frac{(R_\theta^2 + Z_\theta^2)^{1/2}}{R} \mathcal{I}^s = -k_3 \frac{\partial \mathcal{B}}{\partial t}. \tag{35}$$

Introducing amplitudes and dimensionless profile functions for resistivity, $\eta \to \eta f^\eta(\theta)$, and shell thickness, $\delta \to \delta f^\delta(\theta)$, one obtains,

$$\mathcal{L} \mathcal{I}^s = -k_3 \frac{\delta}{\eta} \frac{\partial \mathcal{B}}{\partial t}, \tag{36}$$

where $\mathcal{L}$ is the self-adjoint operator

$$\mathcal{L} = \frac{\partial}{\partial \theta} \left(\frac{f^\eta}{f^\delta} \frac{R}{(R_\theta^2 + Z_\theta^2)^{1/2}} \frac{\partial}{\partial \theta} \right) - n^2 \frac{f^\eta}{f^\delta} \frac{(R_\theta^2 + Z_\theta^2)^{1/2}}{R}. \tag{37}$$

Straight cylinder

For a straight cylinder shell of constant thickness and resistivity, periodic length $2\pi R_0$, and radius a, i.e., $R = R_0 + a\cos\theta$, $z = a\sin\theta$, the solution to Eq. (36) is directly found by expanding both $\mathcal{I}^s$ and $\mathcal{B}$ in a Fourier series with coefficients $\mathcal{I}_l^s$ and b_l so that to the lowest order in a

$$\mathcal{I}^s = \sum_l \mathcal{I}_l^s e^{il\theta} \tag{38}$$

with

$$\mathcal{I}_l^s = k_3 \frac{\delta}{\eta} \frac{a/R_0}{l^2 + n^2 \frac{a^2}{R_0^2}} \frac{\partial b_l}{\partial t} \tag{39}$$

For more complicated geometries a standard procedure for obtaining the solution of Eq. (36) is to construct the Green's function of $\mathcal{L}$ from its eigensolutions, i.e.,

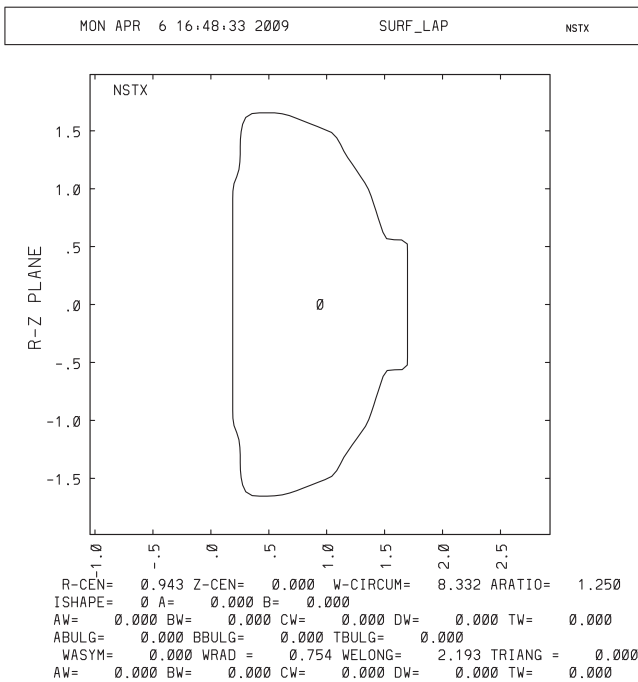
$$\mathcal{L} K_i(\theta) = -h(\theta)\lambda_i K_i(\theta) \tag{40}$$

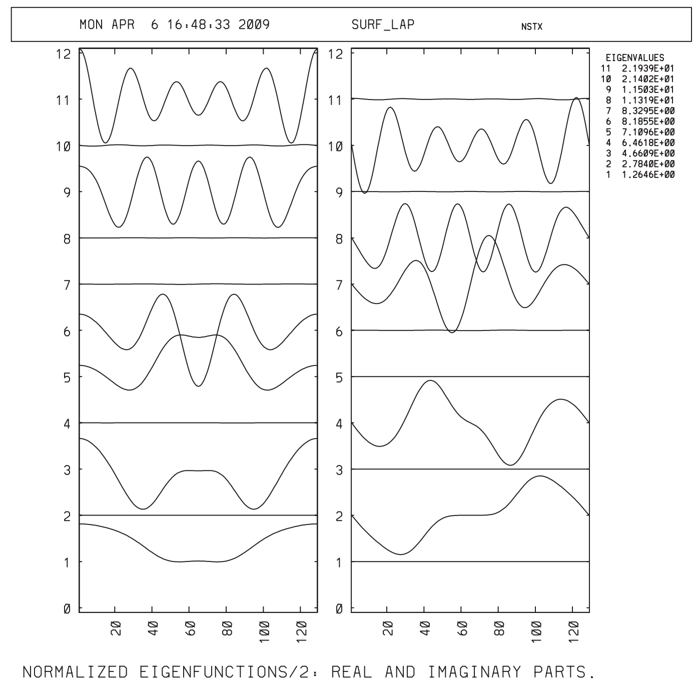
where $h(\theta)$ can be a convenently chosen weight function, and normalize the eigenfunctions so that

$$\frac{1}{N} \int K_i^*(\theta) K_j(\theta) h(\theta)\, d\theta = \delta_{ij}. \tag{41}$$

N can be suitably chosen.

Cross-section of the NSTX shell. Real and imaginary parts of the Eigenfunctions, $K(\theta)$, and the corresponding eigenvalues





Relation between the coefficients, $\mathcal{I}_j^s$ and b_j

Expand the fields in terms of the eigenfunctions,

$$\mathcal{I}^s(\theta) = \sum_i \mathcal{I}_i^s K_i(\theta), \qquad \frac{1}{h(\theta)}\frac{\partial \mathcal{B}}{\partial t} = \sum_j \frac{\partial b_j}{\partial t} K_j(\theta). \tag{42}$$

One readily obtains

$$\mathcal{I}_j^s = k_3 \frac{\delta}{\eta \lambda_j} \frac{\partial b_j}{\partial t} \tag{43}$$

so that the relation between the current potential and $\mathbf{B}_n$ is:

$$\mathcal{I}^s(\theta) = k_3 \frac{\delta}{\eta} \sum_j \frac{1}{\lambda_j} \frac{\partial b_j}{\partial t} K_j(\theta). \tag{44}$$

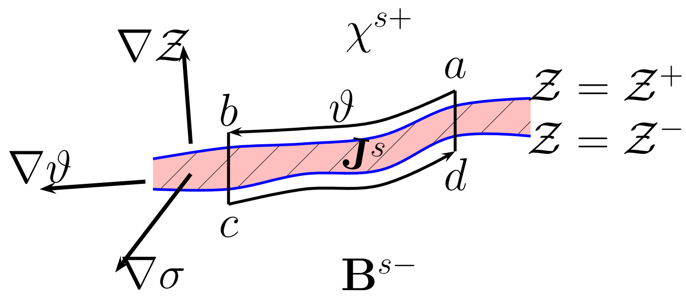
Note: The Green's function, $G(\theta, \theta')$:

$$\mathcal{I}^s(\theta) = \frac{1}{N} \int d\theta' \sum_j \frac{K_j(\theta) K_j^*(\theta')}{\lambda_j} k_3 \frac{\delta}{\eta} \frac{\partial \mathcal{B}}{\partial t}\, d\theta' \tag{45}$$

$$\equiv -\frac{1}{N} \int G(\theta, \theta') k_3 \frac{\delta}{\eta} \frac{\partial \mathcal{B}}{\partial t}\, d\theta' \tag{46}$$

Ampere's Law

Ampere's law, $\nabla \times \mathbf{B} = k_1 \mathbf{J}^s$, together with Stoke's theorem gives the jump in the fields from the inner (-) side to the outer (+) side of the shell.



In a local coordinate system, $(\sigma, \mathcal{Z}, \vartheta)$,where the coordinate ϑ is aligned along an arbitrary direction along the surface one obtains:

$$\oint \mathbf{B}\cdot d\mathbf{l} = k_1 \int \mathbf{J}^s \cdot d\mathbf{S}_\sigma \tag{47}$$

with $d\boldsymbol{\vartheta} = \mathcal{J}\nabla\sigma \times \nabla\mathcal{Z}\, d\vartheta$ and $d\mathbf{S}_\sigma = \mathcal{J}\nabla\sigma\, d\mathcal{Z}\, d\vartheta$, so that

$$\int_a^b \mathbf{B}^+ \cdot d\boldsymbol{\vartheta} + \int_c^d \mathbf{B}^- \cdot d\boldsymbol{\vartheta} = \int_0^\vartheta \left[\mathbf{B}^+ - \mathbf{B}^-\right] \cdot d\boldsymbol{\vartheta} \;=\; k_1 \int_a^b \frac{\partial \mathcal{I}^s}{\partial \vartheta}\, d\vartheta, \tag{48}$$

$$\mathcal{J}\left[\mathbf{B}^+ - \mathbf{B}^-\right] \cdot \nabla\sigma \times \nabla\mathcal{Z} = B^+_\vartheta - B^-_\vartheta \;=\; k_1 \frac{\partial \mathcal{I}^s}{\partial \vartheta}. \tag{49}$$

Ampere's Law – 2

- If the outer region is current free then Eq. (49) becomes

$$B_\vartheta^{s-} = \frac{\partial \chi^{s+}}{\partial \vartheta} - k_1 \frac{\partial \mathcal{I}^s}{\partial \vartheta}. \tag{50}$$

- The VACUUM code calculates $\chi^{s+}(\theta)$ as a response to the normal field:

$$\chi^{s+}(\theta) = \sum_j \mathcal{C}_j^{s+}(\theta) b_j e^{-in\phi} \tag{51}$$

- Eq. (44) relates $\mathcal{I}^s$ to b_j, so that Eq. (50) becomes

$$B_\vartheta^{s-}(\theta) = \sum_j \frac{\partial}{\partial \vartheta} \left[\mathcal{C}_j^{s+}(\theta) b_j - k_1 k_3 \frac{\delta}{\eta} \frac{1}{\lambda_j} \frac{\partial b_j}{\partial t} K_j(\theta) \right] e^{-in\phi}. \tag{52}$$

(53)

Relations between ψ and f with the resistive shell

Letting the coordinate ϑ in turn be θ or ϕ, we obtain respectively

$$B_\theta^{s-}(\theta) = \sum_j \frac{\partial}{\partial\theta}\left[\mathcal{C}_j^{s+}(\theta)b_j - k_1k_3\frac{\delta}{\eta}\frac{1}{\lambda_j}\frac{\partial b_j}{\partial t}K_j(\theta)\right]e^{-in\phi} \tag{54}$$

$$B_\phi^{s-}(\theta) = -in\sum_j \left[\mathcal{C}_j^{s+}(\theta)b_j - k_1k_3\frac{\delta}{\eta}\frac{1}{\lambda_j}\frac{\partial b_j}{\partial t}K_j(\theta)\right]e^{-in\phi}. \tag{55}$$

Recall that b_j, $B_\theta^{s-}(\theta)$ and $B_\phi^{s-}(\theta)$ can be cast in terms of the scalar variables ψ and f of the MHD or MHD-C1 code, i.e.,

$$\frac{\partial b_j}{\partial t} = N\int K_j^*(\theta)\frac{\partial\mathcal{B}}{\partial t}\,d\theta \tag{56}$$

$$\mathcal{B}^p = \frac{\partial\psi}{\partial\theta} - R^{m-2}\mathcal{J}\nabla\mathcal{Z}\cdot\nabla_\perp f' \tag{57}$$

$$B_\theta = -\left(\frac{\mathcal{J}}{R^2}\nabla\mathcal{Z}\cdot\nabla\psi + R^{m-2}\frac{\partial f'}{\partial\theta}\right) \tag{58}$$

$$B_\phi = R^2\nabla\cdot R^{m-2}\nabla_\perp f + R_0 \tag{59}$$

- These equations, Eqs. (54) to (59) are the generalization of their no shell counterparts.
- Taking the limit of large η recovers the no-shell case.