### jo00aa

Measures error in Beltrami field,  $||\nabla \times \mathbf{B} - \mu \mathbf{B}||$ .

[called by: xspech.] [calls: coords.]

#### contents

1	jo00	aa :	1
	1.1	overview	1
	1.2	construction of current, $\mathbf{j} \equiv \nabla \times \nabla \times \mathbf{A}$	1
	1.3	quantification of the error	1
	1.4	details of the numerics	2
	1.5	comments	2

### 1.1 overview

This routine is called by xspech as a post diagnostic and only if Lcheck = 1.

# 1.2 construction of current, $\mathbf{j} \equiv \nabla \times \nabla \times \mathbf{A}$

1. The components of the vector potential,  $\mathbf{A} = A_{\theta} \nabla + A_{\zeta} \nabla \zeta$ , are

$$A_{\theta}(s,\theta,\zeta) = \sum_{i,l} A_{\theta,e,i,l} \, \overline{T}_{l,i}(s) \cos \alpha_i + \sum_{i,l} A_{\theta,o,i,l} \, \overline{T}_{l,i}(s) \sin \alpha_i, \tag{1}$$

$$A_{\zeta}(s,\theta,\zeta) = \sum_{i,l} A_{\zeta,e,i,l} \, \overline{T}_{l,i}(s) \cos \alpha_i + \sum_{i,l} A_{\zeta,o,i,l} \, \overline{T}_{l,i}(s) \sin \alpha_i, \tag{2}$$

where  $\overline{T}_{l,i}(s) \equiv \overline{s}^{m_i/2} T_l(s)$ ,  $T_l(s)$  is the Chebyshev polynomial, and  $\alpha_j \equiv m_j \theta - n_j \zeta$ . The regularity factor,  $\overline{s}^{m_i/2}$ , where  $\overline{s} \equiv (1+s)/2$ , is only included if there is a coordinate singularity in the domain (i.e. only in the innermost volume, and only in cylindrical and toroidal geometry.)

2. The magnetic field,  $\sqrt{g} \mathbf{B} = \sqrt{g} B^s \mathbf{e}_s + \sqrt{g} B^\theta \mathbf{e}_\theta + \sqrt{g} B^\zeta \mathbf{e}_\zeta$ , is

$$\sqrt{g} \mathbf{B} = \mathbf{e}_{s} \sum_{i,l} \left[ (-m_{i} A_{\zeta,e,i,l} - n_{i} A_{\theta,e,i,l}) \overline{T}_{l,i} \sin \alpha_{i} + (+m_{i} A_{\zeta,o,i,l} + n_{i} A_{\theta,o,i,l}) \overline{T}_{l,i} \cos \alpha_{i} \right] 
+ \mathbf{e}_{\theta} \sum_{i,l} \left[ (-m_{i} A_{\zeta,e,i,l}) \overline{T}'_{l,i} \cos \alpha_{i} + (-m_{i} A_{\zeta,o,i,l} + n_{i} A_{\theta,o,i,l}) \overline{T}'_{l,i} \sin \alpha_{i} \right] 
+ \mathbf{e}_{\zeta} \sum_{i,l} \left[ (-A_{\theta,e,i,l}) \overline{T}'_{l,i} \cos \alpha_{i} + (-A_{\theta,o,i,l}) \overline{T}'_{l,i} \sin \alpha_{i} \right]$$
(3)

3. The current is

$$\sqrt{g}\,\mathbf{j} = (\partial_{\theta}B_{\zeta} - \partial_{\zeta}B_{\theta})\,\mathbf{e}_{s} + (\partial_{\zeta}B_{s} - \partial_{s}B_{\zeta})\,\mathbf{e}_{\theta} + (\partial_{s}B_{\theta} - \partial_{\theta}B_{s})\,\mathbf{e}_{\zeta},\tag{4}$$

where (for computational convenience) the covariant components of  ${\bf B}$  are computed as

$$B_s = (\sqrt{g}B^s) g_{ss} / \sqrt{g} + (\sqrt{g}B^\theta) g_{s\theta} / \sqrt{g} + (\sqrt{g}B^\zeta) g_{s\zeta} / \sqrt{g}, \tag{5}$$

$$B_{\theta} = (\sqrt{g}B^{s}) g_{s\theta} / \sqrt{g} + (\sqrt{g}B^{\theta}) g_{\theta\theta} / \sqrt{g} + (\sqrt{g}B^{\zeta}) g_{\theta\zeta} / \sqrt{g}, \tag{6}$$

$$B_{\zeta} = (\sqrt{g}B^{s}) g_{s\zeta} / \sqrt{g} + (\sqrt{g}B^{\theta}) g_{\theta\zeta} / \sqrt{g} + (\sqrt{g}B^{\zeta}) g_{\zeta\zeta} / \sqrt{g}.$$
 (7)

## 1.3 quantification of the error

1. The measures of the error are

$$||(\mathbf{j} - \mu \mathbf{B}) \cdot \nabla s|| \equiv \int ds \oint d\theta d\zeta ||\nabla g \mathbf{j} \cdot \nabla s - \mu \sqrt{g} \mathbf{B} \cdot \nabla s|, \qquad (8)$$

$$||(\mathbf{j} - \mu \mathbf{B}) \cdot \nabla \theta|| = \int ds \oint d\theta d\zeta ||\nabla g \mathbf{j} \cdot \nabla \theta - \mu \sqrt{g} \mathbf{B} \cdot \nabla \theta|, \qquad (9)$$

$$||(\mathbf{j} - \mu \mathbf{B}) \cdot \nabla \zeta|| \equiv \int ds \oint d\theta d\zeta ||\nabla g \mathbf{j} \cdot \nabla \zeta - \mu \sqrt{g} \mathbf{B} \cdot \nabla \zeta|.$$
(10)

### 1.4 details of the numerics

- 1. The integration over s is performed using Gaussian integration, e.g.,  $\int f(s)ds \approx \sum_k \omega_k f(s_k)$ ; with the abscissae,  $s_k$ , and the weights,  $\omega_k$ , for k=1, Iquad<sub>v</sub>, determined by CDGQF. The resolution,  $\mathbb{N} \equiv \text{Iquad}_v$ , is determined by Nquad (see global and preset). A fatal error is enforced by jo00aa if CDGQF returns an ifail  $\neq 0$ .
- 2. Inside the Gaussian quadrature loop, i.e. for each  $s_k$ ,
  - (a) The metric elements,  $g_{\mu,\nu} \equiv \text{gij}(1:6,0,1:\text{Ntz})$ , and the Jacobian,  $\sqrt{g} \equiv \text{sg}(0,1:\text{Ntz})$ , are calculated on a regular angular grid,  $(\theta_i,\zeta_j)$ , in coords. The derivatives  $\partial_i g_{\mu,\nu} \equiv \text{gij}(1:6,i,1:\text{Ntz})$  and  $\partial_i \sqrt{g} \equiv \text{sg}(i,1:\text{Ntz})$ , with respect to  $i \in \{s,\theta,\zeta\}$  are also returned.
  - (b) The Fourier components of the vector potential given in Eqn.(1) and Eqn.(2), and their first and second radial derivatives, are summed.
  - (c) The quantities  $\sqrt{g}B^s$ ,  $\sqrt{g}B^\theta$  and  $\sqrt{g}B^\zeta$ , and their first and second derivatives with respect to  $(s, \theta, \zeta)$ , are computed on the regular angular grid (using FFTs).
  - (d) The following quantities are then computed on the regular angular grid

$$\sqrt{g}j^{s} = \sum_{u} \left[ \partial_{\theta} (\sqrt{g}B^{u}) g_{u,\zeta} + (\sqrt{g}B^{u}) \partial_{\theta} g_{u,\zeta} - (\sqrt{g}B^{u}) g_{u,\zeta} \partial_{\theta} \sqrt{g} / \sqrt{g} \right] / \sqrt{g}$$

$$- \sum_{u} \left[ \partial_{\zeta} (\sqrt{g}B^{u}) g_{u,\theta} + (\sqrt{g}B^{u}) \partial_{\zeta} g_{u,\theta} - (\sqrt{g}B^{u}) g_{u,\theta} \partial_{\zeta} \sqrt{g} / \sqrt{g} \right] / \sqrt{g}, \tag{11}$$

$$\sqrt{g}i^{\theta} = \sum_{u} \left[ \partial_{\zeta} (\sqrt{g}B^{u}) g_{u,\theta} + (\sqrt{g}B^{u}) \partial_{\zeta} g_{u,\theta} - (\sqrt{g}B^{u}) g_{u,\theta} \partial_{\zeta} \sqrt{g} / \sqrt{g} \right] / \sqrt{g}$$

$$\sqrt{g}j^{\theta} = \sum_{u} \left[ \partial_{\zeta}(\sqrt{g}B^{u}) g_{u,s} + (\sqrt{g}B^{u}) \partial_{\zeta}g_{u,s} - (\sqrt{g}B^{u})g_{u,s} \partial_{\zeta}\sqrt{g}/\sqrt{g} \right] / \sqrt{g} 
- \sum_{u} \left[ \partial_{s}(\sqrt{g}B^{u}) g_{u,\zeta} + (\sqrt{g}B^{u}) \partial_{s}g_{u,\zeta} - (\sqrt{g}B^{u})g_{u,\zeta} \partial_{s}\sqrt{g}/\sqrt{g} \right] / \sqrt{g},$$
(12)

$$\sqrt{g}j^{\zeta} = \sum_{u} \left[ \partial_{s}(\sqrt{g}B^{u}) g_{u,\theta} + (\sqrt{g}B^{u}) \partial_{s}g_{u,\theta} - (\sqrt{g}B^{u})g_{u,\theta} \partial_{s}\sqrt{g}/\sqrt{g} \right] / \sqrt{g}$$

$$- \sum_{u} \left[ \partial_{\theta}(\sqrt{g}B^{u}) g_{u,s} + (\sqrt{g}B^{u}) \partial_{\theta}g_{u,s} - (\sqrt{g}B^{u})g_{u,s} \partial_{\theta}\sqrt{g}/\sqrt{g} \right] / \sqrt{g}. \tag{13}$$

3. The final calculation of the error, which is written to screen, is a sum over the angular grid:

$$E^{s} \equiv \frac{1}{N} \sum_{k} \omega_{k} \sum_{i,j} |\sqrt{g}j^{s} - \mu \sqrt{g}B^{s}|, \tag{14}$$

$$E^{\theta} \equiv \frac{1}{N} \sum_{k} \omega_{k} \sum_{i,j} |\sqrt{g}j^{\theta} - \mu \sqrt{g}B^{\theta}|, \tag{15}$$

$$E^{\zeta} \equiv \frac{1}{N} \sum_{k} \omega_{k} \sum_{i,j} |\sqrt{g}j^{\zeta} - \mu \sqrt{g}B^{\zeta}|, \tag{16}$$

where  $N \equiv \sum_{i,j} 1$ .

### 1.5 comments

- 1. Is there a better definition and quantification of the error? For example, should we employ an error measure that is dimensionless?
- 2. If the coordinate singularity is in the domain, then  $|\nabla \theta| \to \infty$  at the coordinate origin. What then happens to  $||(\mathbf{j} \mu \mathbf{B}) \cdot \nabla \theta||$  as defined in Eqn.(9)?
- 3. What is the predicted scaling of the error in the Chebyshev-Fourier representation scale with numerical resolution? Note that the predicted error scaling for  $E^s$ ,  $E^\theta$  and  $E^\zeta$  may not be standard, as various radial derivatives are taken to compute the components of  $\mathbf{j}$ . (See for example the discussion in Sec.IV.C in [Hudson, Dewar et al., Phys. Plasmas 19, 112502 (2012)], where the expected scaling of the error for a finite-element implementation is confirmed numerically.)
- 4. Instead of using Gaussian integration to compute the integral over s, an adaptive quadrature algorithm may be preferable.

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SPEC subroutines;