jo00aa

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

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

contents

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 $\overline{T}_{l,i}(s) \equiv \bar{s}^{m_i/2}\, T_l(s)$, $T_l(s)$ is the Chebyshev polynomial, and $\alpha_j \equiv m_j\theta - n_j\zeta$. The regularity factor, $\bar{s}^{m_i/2}$, where $\bar{s} \equiv (1+s)/2$, 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

$$\begin{array}{cccccccccc}
\sqrt{g}\,\mathbf{B} & = & \mathbf{e}_s & \sum_{i,l}[(& -m_i A_{\zeta,e,i,l} & - & n_i A_{\theta,e,i,l} &)\overline{T}_{l,i}\sin\alpha_i + (& +m_i A_{\zeta,o,i,l} & + & n_i A_{\theta,o,i,l} &)\overline{T}_{l,i}\cos\alpha_i] \\
 & + & \mathbf{e}_\theta & \sum_{i,l}[(& & - & A_{\zeta,e,i,l} &)\overline{T}'_{l,i}\cos\alpha_i + (& & - & A_{\zeta,o,i,l} &)\overline{T}'_{l,i}\sin\alpha_i] \\
 & + & \mathbf{e}_\zeta & \sum_{i,l}[(& A_{\theta,e,i,l} & & &)\overline{T}'_{l,i}\cos\alpha_i + (& A_{\theta,o,i,l} & & &)\overline{T}'_{l,i}\sin\alpha_i]
\end{array} \tag{3}$$

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 $\mathbf{B}$ are computed as

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

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

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

1.3 quantification of the error

1. The measures of the error are

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

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

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

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, ω_k, for $k = 1$, $\texttt{Iquad}_v$, determined by `CDGQF`. The resolution, $\texttt{N} \equiv \texttt{Iquad}_v$, is determined by `Nquad` (see global and preset). A fatal error is enforced by jo00aa if `CDGQF` returns an $\texttt{ifail} \neq 0$.

2. Inside the Gaussian quadrature loop, i.e. for each s_k,

   (a) The metric elements, $g_{\mu,\nu} \equiv$ `gij(1:6,0,1:Ntz)`, and the Jacobian, $\sqrt{g} \equiv$ `sg(0,1:Ntz)`, are calculated on a regular angular grid, (θ_i, ζ_j), in coords. The derivatives $\partial_i g_{\mu,\nu} \equiv$ `gij(1:6,i,1:Ntz)` and $\partial_i \sqrt{g} \equiv$ `sg(i,1: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, θ, ζ), are computed on the regular angular grid (using FFTs).

   (d) The following quantities are then computed on the regular angular grid

$$
\begin{aligned}
\sqrt{g}j^s &= \sum_u \left[\partial_\theta(\sqrt{g}B^u)\, g_{u,\zeta} + (\sqrt{g}B^u)\, \partial_\theta g_{u,\zeta} - (\sqrt{g}B^u) g_{u,\zeta}\, \partial_\theta \sqrt{g}/\sqrt{g}\right]/\sqrt{g} \\
&- \sum_u \left[\partial_\zeta(\sqrt{g}B^u)\, g_{u,\theta} + (\sqrt{g}B^u)\, \partial_\zeta g_{u,\theta} - (\sqrt{g}B^u) g_{u,\theta}\, \partial_\zeta \sqrt{g}/\sqrt{g}\right]/\sqrt{g}, \qquad (11)\\
\sqrt{g}j^\theta &= \sum_u \left[\partial_\zeta(\sqrt{g}B^u)\, g_{u,s} + (\sqrt{g}B^u)\, \partial_\zeta g_{u,s} - (\sqrt{g}B^u) g_{u,s}\, \partial_\zeta \sqrt{g}/\sqrt{g}\right]/\sqrt{g} \\
&- \sum_u \left[\partial_s(\sqrt{g}B^u)\, g_{u,\zeta} + (\sqrt{g}B^u)\, \partial_s g_{u,\zeta} - (\sqrt{g}B^u) g_{u,\zeta}\, \partial_s \sqrt{g}/\sqrt{g}\right]/\sqrt{g}, \qquad (12)\\
\sqrt{g}j^\zeta &= \sum_u \left[\partial_s(\sqrt{g}B^u)\, g_{u,\theta} + (\sqrt{g}B^u)\, \partial_s g_{u,\theta} - (\sqrt{g}B^u) g_{u,\theta}\, \partial_s \sqrt{g}/\sqrt{g}\right]/\sqrt{g} \\
&- \sum_u \left[\partial_\theta(\sqrt{g}B^u)\, g_{u,s} + (\sqrt{g}B^u)\, \partial_\theta g_{u,s} - (\sqrt{g}B^u) g_{u,s}\, \partial_\theta \sqrt{g}/\sqrt{g}\right]/\sqrt{g}. \qquad (13)
\end{aligned}
$$

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

$$
\begin{aligned}
E^s &\equiv \frac{1}{N} \sum_k \omega_k \sum_{i,j} |\sqrt{g}j^s - \mu\sqrt{g}B^s|, \qquad (14)\\
E^\theta &\equiv \frac{1}{N} \sum_k \omega_k \sum_{i,j} |\sqrt{g}j^\theta - \mu\sqrt{g}B^\theta|, \qquad (15)\\
E^\zeta &\equiv \frac{1}{N} \sum_k \omega_k \sum_{i,j} |\sqrt{g}j^\zeta - \mu\sqrt{g}B^\zeta|, \qquad (16)
\end{aligned}
$$

   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^θ and E^ζ 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.