# SPEC

3.10

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# 1 Todo List

### Subprogram bnorml (mn, Ntz, efmn, ofmn)

There is a very clumsy attempt to parallelize this which could be greatly improved.

# Subprogram casing (teta, zeta, gBn, icasing)

It would be MUCH faster to only require the tangential field on a regular grid!!!

Please check why  $B_s$  is not computed. Is it because  $B_s \nabla s \times \mathbf{n} = 0$  ?

This needs to be revised.

#### Subprogram curent (Ivol, mn, Nt, Nz, iflag, IdltGp)

Perhaps this can be proved analytically; in any case it should be confirmed numerically.

### Subprogram inputlist::lconstraint

if Lconstraint==2, under reconstruction.

### Subprogram inputlist::wbuild\_vector\_potential

: what is this?

### Type intghs\_module::intghs\_workspace

Zhisong might need to update the documentation of this type.

# Subprogram ma02aa (Ivol, NN)

If Lconstraint = 2, then  $\mu = \mu_1$  is varied in order to satisfy the helicity constraint, and  $\Delta \psi_p = \mu_2$  is not varied, and Nxdof=1. (under re-construction)

# Subprogram pc00aa (NGdof, position, Nvol, mn, ie04dgf)

Unfortunately, E04DGF seems to require approximately 3N function evaluations before proceeding to minimize the energy functional, where there are N degrees of freedom. I don't know how to turn this off!

### Subprogram pc00ab (mode, NGdof, Position, Energy, Gradient, nstate, iuser, ruser)

IT IS VERY LIKELY THAT FFTs WOULD BE FASTER!!!

# Subprogram spec

If Lminimize.eq.1, call pc00aa() to find minimum of energy functional using quasi-Newton, preconditioned conjugate gradient method, E04DGF

### Subprogram stzxyz (Ivol, stz, RpZ)

Please see co01aa() for documentation.

# 2 Module Index

### 2.1 Modules

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# 3 Data Type Index

# 3.1 Data Types List

Here are the data types with brief descriptions:

intghs\_module::intghs\_workspace

This calculates the integral of something related to matrix-vector-multiplication 171

# 4 File Index

# 4.1 File List

Here is a list of all documented files with brief descriptions:

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src/bfield.f90 Returns $\dot{s}\equiv B^s/B^\zeta$ and $\dot{\theta}\equiv B^\theta/B^\zeta$	178
src/bnorml.f90   Computes $B_{Plasma}\cdot e_{\theta}\times e_{\zeta}$ on the computational boundary, $\partial\mathcal{D}$	179

src/brcast.f90 Broadcasts Beltrami fields, profiles,	180
src/casing.f90  Constructs the field created by the plasma currents, at an arbitrary, external location using virtual casing	180
src/coords.f90   Calculates coordinates, ${\bf x}(s,\theta,\zeta)\equiv R{\bf e}_R+Z{\bf e}_Z$ , and metrics, using FFTs	180
src/curent.f90 Computes the plasma current, $I\equiv\int B_{\theta}~d\theta$ , and the "linking" current, $G\equiv\int B_{\zeta}~d\zeta$	181
src/df00ab.f90 Evaluates volume integrals, and their derivatives w.r.t. interface geometry, using "packed" format	181
src/dforce.f90   Calculates $F(x)$ , where $x \equiv \{\text{geometry}\} \equiv \{R_{i,v}, Z_{i,v}\}$ and $F \equiv [[p+B^2/2]]+\{\text{spectral constraints}\}$ , and $\nabla F$	181
src/dfp100.f90 Split the work between MPI nodes and evaluate the global constraint	181
src/dfp200.f90 Given the field consistent with the constraints and the geometry, computes local quantites related to the force evaluation	183
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src/packab.f90	
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src/packxi.f90	
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to the interface geometry	241
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Constructs smooth approximation to wall	241

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Main program 243

# 5 Module Documentation

# 5.1 Diagnostics to check the code

### **Functions/Subroutines**

• subroutine bfield (zeta, st, Bst)

Compute the magnetic field.

• subroutine hesian (NGdof, position, Mvol, mn, LGdof)

Computes eigenvalues and eigenvectors of derivative matrix,  $\nabla_{\xi} \mathbf{F}$ .

• subroutine jo00aa (Ivol, Ntz, Iquad, mn)

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

• subroutine pp00aa

Constructs Poincaré plot and "approximate" rotational-transform (driver).

subroutine pp00ab (Ivol, sti, Nz, nPpts, poincaredata, fittedtransform, utflag)

Constructs Poincaré plot and "approximate" rotational-transform (for single field line).

• subroutine stzxyz (Ivol, stz, RpZ)

Calculates coordinates,  $\mathbf{x}(s, \theta, \zeta) \equiv R \mathbf{e}_R + Z \mathbf{e}_Z$ , and metrics, at given  $(s, \theta, \zeta)$ .

# 5.1.1 Detailed Description

### 5.1.2 Function/Subroutine Documentation

Compute the magnetic field.

Returns the magnetic field field line equations,  $d\mathbf{x}/d\phi = \mathbf{B}/B^{\phi}$  .

# **Equations of field line flow**

• The equations for the fieldlines are normalized to the toroidal field, i.e.

$$\dot{s} \equiv \frac{B^s}{B^{\zeta}}, \qquad \dot{\theta} \equiv \frac{B^{\theta}}{B^{\zeta}}.$$
 (1)

# Representation of magnetic field

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

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

$$A_{\zeta}(s,\theta,\zeta) = \sum_{i,l} A_{\zeta,e,i,l} \, \overline{T}_{l,i}(s) \cos \alpha_i + \sum_{i,l} A_{\zeta,o,i,l} \, \overline{T}_{l,i}(s) \sin \alpha_i, \tag{3}$$

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.)

• 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

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

$$(4)$$

• In Eqn. (1), the coordinate Jacobian,  $\sqrt{g}$ , cancels. No coordinate metric information is required to construct the fieldline equations from the magnetic vector potential.

#### IT IS REQUIRED TO SET IVOL THROUGH GLOBAL MEMORY BEFORE CALLING BFIELD.

The format of this subroutine is constrained by the NAG ode integration routines.

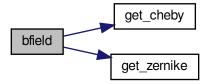
#### **Parameters**

in	$zeta$ toroidal angle $\zeta$	
in	st radial coordinate $s$ and poloidal angle $ heta$	
out $   extit{Bst}  $ tangential magnetic field directions $B_s, B_s$		

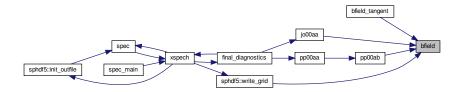
References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::aze, allglobal::aze, allglobal::cpus, allglobal::gbzeta, get\_cheby(), get\_zernike(), constants::half, allglobal::halfmm, allglobal::im, allglobal::in, allglobal::ivol, allglobal::lcoordinatesingularity, inputlist::lrad, allglobal::mn, allglobal::mpi\_comm\_spec, inputlist::mpol, allglobal::myid, allglobal::note, allglobal::note, allglobal::note, allglobal::regumm, numerical::small, constants::two, numerical::vsmall, inputlist::wmacros, and constants::zero.

Referenced by bfield\_tangent(), jo00aa(), pp00ab(), and sphdf5::write\_grid().

Here is the call graph for this function:



Here is the caller graph for this function:



Computes eigenvalues and eigenvectors of derivative matrix,  $\nabla_{\varepsilon} \mathbf{F}$ .

#### **Parameters**

in	NGdof	number of global degrees of freedom
in,out	position	internal geometrical degrees of freedom
in	Mvol	total number of volumes in computation
in	mn	number of Fourier harmonics
in	LGdof	what is this?
	position	internal geometrical degrees of freedom;

# construction of Hessian matrix

- The routine dforce() is used to compute the derivatives, with respect to interface geometry, of the force imbalance harmonics,  $[[p+B^2/2]]_j$ , which may be considered to be the "physical" constraints, and if Igeometry==3 then also the derivatives of the "artificial" spectral constraints,  $I_j \equiv (R_\theta X + Z_\theta Y)_j$ .
- The input variable Lconstraint determines how the enclosed fluxes,  $\Delta \psi_t$  and  $\Delta \psi_p$ , and the helicity multiplier,  $\mu$ , vary as the geometry is varied; see global.f90 and mp00ac() for more details.

### construction of eigenvalues and eigenvectors

- If LHevalues==T then the eigenvalues of the Hessian are computed using the NAG routine F02EBF.
- If LHevectors==T then the eigenvalues and the eigenvectors of the Hessian are computed.
- Note that if Igeometry==3, then the derivative-matrix also contains information regarding how the "artificial" spectral constraints vary with geometry; so, the eigenvalues and eigenvectors are not purely "physical".
- The eigenvalues and eigenvectors (if required) are written to the file .ext.GF.ev as follows:

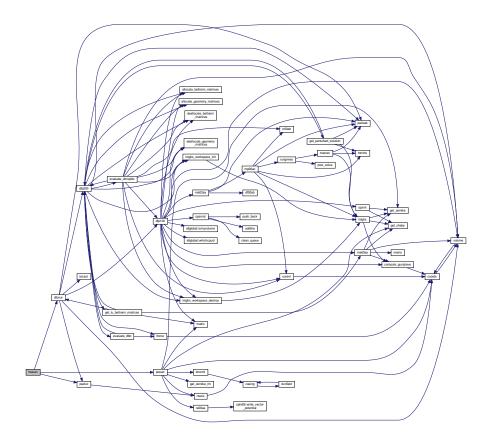
```
open(hunit,file="."//trim(ext)//".GF.ev",status="unknown",form="unformatted")
write(hunit)ngdof,ldvr,ldvi
                                   ! integers; if only the eigenvalues were computed then Ldvr=Ldvi=1;
                                   ! reals ;
write(hunit)evalr(1:ngdof)
                                               real
                                                         part of eigenvalues;
write(hunit)evali(1:ngdof)
                                   ! reals
                                             ; imaginary part of eigenvalues;
                                                         part of eigenvalues; only if Ldvr=NGdof;
write(hunit)evecr(1:ngdof,1:ngdof) ! reals
                                               real
write(hunit)eveci(1:ngdof,1:ngdof) ! reals
                                            ; imaginary part of eigenvalues; only if Ldvi=NGdof;
close(hunit)
```

• The eigenvectors are saved in columns of evecr, eveci, as described by the NAG documentation for F02EBF.

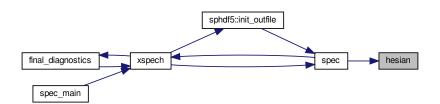
References allglobal::cpus, allglobal::dbbdmp, allglobal::dbbdrz, allglobal::dessian, allglobal::dffdrz, dforce(), allglobal::dmupfdx, inputlist::dpp, inputlist::dqq, allglobal::drbc, allglobal::drbs, allglobal::dzbc, allglobal::dzbc, allglobal::dzbc, allglobal::drbc, allglobal::drbc, allglobal::dzbc, allglobal::inputlist::ipeometry, allglobal::imputlist::lcheck, inputlist::lfindzero, inputlist::lfreebound, allglobal::lhessianallocated, inputlist::lhevalues, inputlist::lhevectors, inputlist::lhevalues, inputlist::lhevalues, inputlist::lhevalues, inputlist::munit, allglobal::myid, allglobal::ncpu, allglobal::notstellsym, inputlist::nvol, constants::one, fileunits::ounit, packxi(), inputlist::pflux, preset(), allglobal::psifactor, numerical::small, numerical::sqrtmachprec, constants::ten, constants::two, numerical::vsmall, inputlist::wmacros, allglobal::yesstellsym, and constants::zero.

Referenced by spec().

Here is the call graph for this function:



Here is the caller graph for this function:



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

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

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

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

$$A_{\theta}(s,\theta,\zeta) = \sum_{i,l} A_{\theta,e,i,l} \overline{T}_{l,i}(s) \cos \alpha_i + \sum_{i,l} A_{\theta,o,i,l} \overline{T}_{l,i}(s) \sin \alpha_i,$$
 (5)

$$A_{\zeta}(s,\theta,\zeta) = \sum_{i,l} A_{\zeta,e,i,l} \, \overline{T}_{l,i}(s) \cos \alpha_i + \sum_{i,l} A_{\zeta,o,i,l} \, \overline{T}_{l,i}(s) \sin \alpha_i, \tag{6}$$

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.)

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

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

· The current is

$$\sqrt{g}\mathbf{j} = (\partial_{\theta}B_{\zeta} - \partial_{\zeta}B_{\theta})\mathbf{e}_{s} + (\partial_{\zeta}B_{s} - \partial_{s}B_{\zeta})\mathbf{e}_{\theta} + (\partial_{s}B_{\theta} - \partial_{\theta}B_{s})\mathbf{e}_{\zeta}, \tag{8}$$

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

$$B_s = (\sqrt{g}B^s) g_{ss} / \sqrt{g} + (\sqrt{g}B^\theta) g_{s\theta} / \sqrt{g} + (\sqrt{g}B^\zeta) g_{s\zeta} / \sqrt{g}, \tag{9}$$

$$B_{\theta} = (\sqrt{g}B^{s})g_{s\theta}/\sqrt{g} + (\sqrt{g}B^{\theta})g_{\theta\theta}/\sqrt{g} + (\sqrt{g}B^{\zeta})g_{\theta\zeta}/\sqrt{g}, \tag{10}$$

$$B_{\zeta} = (\sqrt{g}B^{s}) g_{s\zeta} / \sqrt{g} + (\sqrt{g}B^{\theta}) g_{\theta\zeta} / \sqrt{g} + (\sqrt{g}B^{\zeta}) g_{\zeta\zeta} / \sqrt{g}. \tag{11}$$

# quantification of the error

· The measures of the error are

$$||(\mathbf{j} - \mu \mathbf{B}) \cdot \nabla s|| \equiv \int ds \oint d\theta d\zeta ||\sqrt{g} \mathbf{j} \cdot \nabla s - \mu \sqrt{g} \mathbf{B} \cdot \nabla s|, \qquad (12)$$

$$||(\mathbf{j} - \mu \mathbf{B}) \cdot \nabla \theta|| \equiv \int ds \oint d\theta d\zeta ||\sqrt{g} \mathbf{j} \cdot \nabla \theta - \mu \sqrt{g} \mathbf{B} \cdot \nabla \theta|,$$
(13)

$$||(\mathbf{j} - \mu \mathbf{B}) \cdot \nabla \zeta|| \equiv \int ds \oint d\theta d\zeta ||\sqrt{g} \mathbf{j} \cdot \nabla \zeta - \mu \sqrt{g} \mathbf{B} \cdot \nabla \zeta|.$$
 (14)

#### comments

- Is there a better definition and quantification of the error? For example, should we employ an error measure that is dimensionless?
- 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. (13)?
- 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  ${\bf j}$ . (See for example the discussion in Sec.IV.C in Hudson et al. (2011) [4], where the expected scaling of the error for a finite-element implementation is confirmed numerically.)
- Instead of using Gaussian integration to compute the integral over s, an adaptive quadrature algorithm may be preferable.

#### **Parameters**

in	Ivol	in which volume should the Beltrami error be computed	
in	Ntz	number of grid points in $\theta$ and $\zeta$	
in	Iquad	d degree of Gaussian quadrature	
in	in mn number of Fourier harmonics		

#### details of the numerics

- 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 v, determined by CDGQF. The resolution, N  $\equiv$  Iquad v, is determined by Nquad (see global.f90 and preset()). A fatal error is enforced by jo00aa() if CDGQF returns an ifail  $\neq 0$ .
- Inside the Gaussian quadrature loop, i.e. for each  $s_k$ ,
  - 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  $\partial_i g_{\mu,\nu}\equiv \text{gij}\,(1:6,\text{i},1\leftrightarrow\text{i})$ . Ntz) and  $\partial_i \sqrt{g}\equiv \text{sg}\,(\text{i},1:\text{Ntz})$ , with respect to  $i\in\{s,\theta,\zeta\}$  are also returned.
  - The Fourier components of the vector potential given in Eqn. (5) and Eqn. (6), and their first and second radial derivatives, are summed.
  - 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).
  - The following quantities are then computed on the regular angular grid

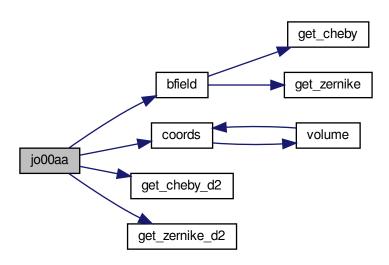
$$\sqrt{g}j^{s} = \sum_{u} \left[ \partial_{\theta}(\sqrt{g}B^{u}) g_{u,\zeta} + (\sqrt{g}B^{u}) \partial_{\theta}g_{u,\zeta} - (\sqrt{g}B^{u})g_{u,\zeta} \partial_{\theta}\sqrt{g}/\sqrt{g} \right] / \sqrt{g} 
- \sum_{u} \left[ \partial_{\zeta}(\sqrt{g}B^{u}) g_{u,\theta} + (\sqrt{g}B^{u}) \partial_{\zeta}g_{u,\theta} - (\sqrt{g}B^{u})g_{u,\theta} \partial_{\zeta}\sqrt{g}/\sqrt{g} \right] / \sqrt{g}, \quad (15) 
\sqrt{g}j^{\theta} = \sum_{u} \left[ \partial_{\zeta}(\sqrt{g}B^{u}) g_{u,s} + (\sqrt{g}B^{u}) \partial_{\zeta}g_{u,s} - (\sqrt{g}B^{u})g_{u,s} \partial_{\zeta}\sqrt{g}/\sqrt{g} \right] / \sqrt{g} 
- \sum_{u} \left[ \partial_{s}(\sqrt{g}B^{u}) g_{u,\zeta} + (\sqrt{g}B^{u}) \partial_{s}g_{u,\zeta} - (\sqrt{g}B^{u})g_{u,\zeta} \partial_{s}\sqrt{g}/\sqrt{g} \right] / \sqrt{g}, \quad (16) 
\sqrt{g}j^{\zeta} = \sum_{u} \left[ \partial_{s}(\sqrt{g}B^{u}) g_{u,\theta} + (\sqrt{g}B^{u}) \partial_{s}g_{u,\theta} - (\sqrt{g}B^{u})g_{u,\theta} \partial_{s}\sqrt{g}/\sqrt{g} \right] / \sqrt{g} 
- \sum_{u} \left[ \partial_{\theta}(\sqrt{g}B^{u}) g_{u,s} + (\sqrt{g}B^{u}) \partial_{\theta}g_{u,s} - (\sqrt{g}B^{u})g_{u,s} \partial_{\theta}\sqrt{g}/\sqrt{g} \right] / \sqrt{g}. \quad (17)$$

• The error is stored into an array called beltramierror which is then written to the HDF5 file in hdfint().

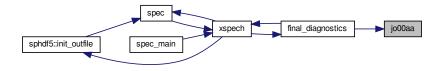
References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::beltramierror, bfield(), allglobal::cfmn, allglobal::cfmn, allglobal::cheby, coords(), allglobal::cpus, allglobal::dpflux, allglobal::dtflux, allglobal::efmn, allglobal::gbzeta, get\_cheby\_d2(), get\_zernike\_d2(), allglobal::guvij, constants::half, inputlist::igeometry, allglobal::im, allglobal::in, allglobal::ivol, allglobal::lcoordinatesingularity, inputlist::lerrortype, inputlist::lrad, allglobal::mpi\_comm\_spec, inputlist::mpol, inputlist::mu, allglobal::myid, inputlist::nfp, allglobal::node, allglobal::notstellsym, allglobal::nt, inputlist::nvol, allglobal::nt, allglobal::ofmn, constants::one, fileunits::ounit, constants::pi2, allglobal::regumm, allglobal::rij, allglobal::rtt, allglobal::sfmn, allglobal::sg, allglobal::tt, constants::two, inputlist::wmacros, allglobal::zernike, constants::zero, and allglobal::zij.

Referenced by final\_diagnostics().

Here is the call graph for this function:



Here is the caller graph for this function:



## **5.1.2.4 pp00aa()** subroutine pp00aa

Constructs Poincaré plot and "approximate" rotational-transform (driver).

# relevant input variables

- The resolution of Poincaré plot is controlled by
  - nPtraj trajectories will be located in each volume;
  - nPpts iterations per trajectory;
  - odetol o.d.e. integration tolerance;
- The magnetic field is given by bfield().
- The approximate rotational transform is determined, in pp00ab(), by fieldline integration.

#### format of output: Poincaré

• The Poincaré data is written to .ext.poincare:xxxx , where xxxx is an integer indicating the volume. The format of this file is as follows:

```
write(svol,'(i4.4)')lvol! lvol labels volume; open(lunit+myid, file="."//trim(ext)//".poincare."//svol, status="unknown", form="unformatted") do until end of file write(lunit+myid) nz, nppts ! integers write(lunit+myid) data(1:4,0:nz-1,1:nppts)! doubles enddo close(lunit+myid) where  -\theta \equiv \text{data}(1,k,j) \text{ is the poloidal angle,} \\ -s \equiv \text{data}(2,k,j) \text{ is the radial coordinate,} \\ -R \equiv \text{data}(3,k,j) \text{ is the cylindrical } R, \\ -Z \equiv \text{data}(4,k,j) \text{ is the cylindrical } Z,
```

- The integer k=0,Nz-1 labels toroidal planes, so that  $\phi=(2\pi/{\rm Nfp})(k/{\rm Nz}),$
- The integer j=1,nPpts labels toroidal iterations.
- Usually (if no fieldline integration errors are encountered) the number of fieldlines followed in volume lvol is given by N+1, where the radial resolution,  $N \equiv Ni \ (lvol)$ , is given on input. This will be over-ruled by if  $nPtrj \ (lvol)$ , given on input, is non-negative.
- The starting location for the fieldline integrations are equally spaced in the radial coordinate  $s_i = s_{l-1} + i(s_l s_{l-1})/N$  for i = 0, N, along the line  $\theta = 0, \zeta = 0$ .

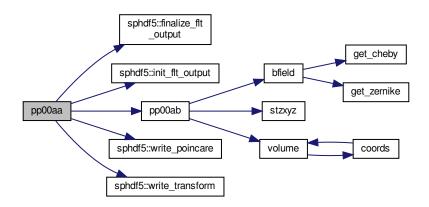
# format of output: rotational-transform

• The rotational-transform data is written to .ext.transform:xxxx , where xxxx is an integer indicating the volume. The format of this file is as follows:

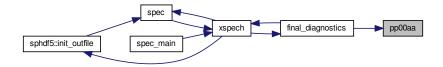
References allglobal::cpus, allglobal::diotadxup, sphdf5::finalize\_flt\_output(), constants::half, inputlist::igeometry, sphdf5::init\_flt\_output(), inputlist::iota, allglobal::ivol, inputlist::lconstraint, allglobal::lcoordinatesingularity, allglobal::lplasmaregion, inputlist::lrad, allglobal::lvacuumregion, allglobal::mpi\_comm\_spec, allglobal::myid, allglobal::ncpu, inputlist::nppts, inputlist::nptrj, inputlist::nvol, allglobal::nz, inputlist::odetol, inputlist::oita, constants::one, fileunits::ounit, constants::pi, pp00ab(), inputlist::ppts, constants::two, inputlist::wmacros, sphdf5::write\_poincare(), sphdf5::write\_transform(), and constants::zero.

Referenced by final diagnostics().

Here is the call graph for this function:



Here is the caller graph for this function:



```
5.1.2.5 pp00ab() subroutine pp00ab (
    integer, intent(in) lvol,
    real, dimension(1:2) sti,
    integer, intent(in) Nz,
    integer, intent(in) nPpts,
    real, dimension(1:4,0:nz-1,1:nppts) poincaredata,
    real, dimension(1:2) fittedtransform,
    integer, intent(out) utflag)
```

Constructs Poincaré plot and "approximate" rotational-transform (for single field line).

# relevant input variables

- · The resolution of Poincaré plot is controlled by
  - nPpts iterations per trajectory;
  - odetol o.d.e. integration tolerance;

The magnetic field is given by bfield().

# rotational-transform

• The approximate rotational transform is determined by field line integration. This is constructed by fitting a least squares fit to the field line trajectory.

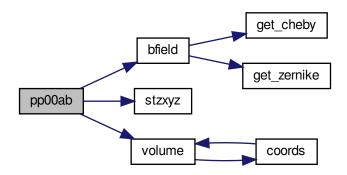
### **Parameters**

in	Ivol	
	sti	
in	Nz	
in	nPpts	
	poincaredata	
	fittedtransform	
out	utflag	

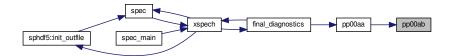
References bfield(), allglobal::cpus, allglobal::ivol, allglobal::mpi\_comm\_spec, allglobal::myid, allglobal::ncpu, allglobal::node, inputlist::nvol, inputlist::odetol, constants::one, fileunits::ounit, constants::pi2, numerical::small, stzxyz(), constants::two, volume(), and constants::zero.

Referenced by pp00aa().

Here is the call graph for this function:



Here is the caller graph for this function:



Calculates coordinates,  $\mathbf{x}(s, \theta, \zeta) \equiv R \mathbf{e}_R + Z \mathbf{e}_Z$ , and metrics, at given  $(s, \theta, \zeta)$ .

- This routine is a "copy" of co01aa(), which calculates the coordinate information on a regular, discrete grid in  $\theta$  and  $\zeta$  at given s whereas stzxyz() calculates the coordinate information at a single point  $(s, \theta, \zeta)$ .
- Todo Please see co01aa() for documentation.

#### **Parameters**

in	Ivol
in	stz
out	RpZ

References allglobal::cpus, constants::half, allglobal::halfmm, inputlist::igeometry, allglobal::im, allglobal::in, allglobal::irbc, allglobal::irbc, allglobal::izbc, allglobal::izbc, allglobal::icoordinatesingularity, allglobal::mn, allglobal::mpi\_comm\_spec, allglobal::myid, allglobal::notstellsym, inputlist::ntor, inputlist::nvol, constants::one, fileunits ::ounit, numerical::vsmall, and constants::zero.

Referenced by pp00ab().

Here is the caller graph for this function:



# 5.2 Free-Boundary Computation

### **Functions/Subroutines**

- subroutine bnorml (mn, Ntz, efmn, ofmn)
  - Computes  $\mathbf{B}_{Plasma}\cdot\mathbf{e}_{\theta} imes\mathbf{e}_{\zeta}$  on the computational boundary,  $\partial\mathcal{D}$ .
- subroutine casing (teta, zeta, gBn, icasing)

Constructs the field created by the plasma currents, at an arbitrary, external location using virtual casing.

• subroutine dvcfield (Ndim, tz, Nfun, vcintegrand)

Differential virtual casing integrand.

### 5.2.1 Detailed Description

### 5.2.2 Function/Subroutine Documentation

Computes  $\mathbf{B}_{Plasma} \cdot \mathbf{e}_{\theta} \times \mathbf{e}_{\zeta}$  on the computational boundary,  $\partial \mathcal{D}$ .

### free-boundary constraint

- The normal field at the computational boundary,  $\partial \mathcal{D}$ , should be equal to  $(\mathbf{B}_P + \mathbf{B}_C) \cdot \mathbf{e}_\theta \times \mathbf{e}_\zeta$ , where  $\mathbf{B}_P$  is the "plasma" field (produced by internal plasma currents) and is computed using virtual casing, and  $\mathbf{B}_C$  is the "vacuum" field (produced by the external coils) and is given on input.
- The plasma field,  $\mathbf{B}_P$ , can only be computed after the equilibrium is determined, but this information is required to compute the equilibrium to begin with; and so there is an iteration involved.
- · Suggested values of the vacuum field can be self generated; see xspech() for more documentation on this.

#### compute the normal field on a regular grid on the computational boundary

- For each point on the computational boundary, casing() is called to compute the normal field produced by the plasma currents.
- Todo There is a very clumsy attempt to parallelize this which could be greatly improved.
- · An FFT gives the required Fourier harmonics.

#### See also

# casing.f90

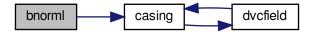
### **Parameters**

in	mn	total number of Fourier harmonics	
in	Ntz	total number of grid points in $\theta$ and $zeta$	
out	efmn	even Fourier coefficients	
out ofmn odd Fouier coefficients			

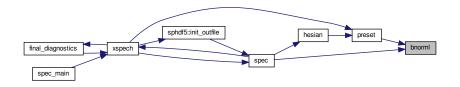
References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, casing(), allglobal::cfmn, allglobal::cpus, allglobal::dxyz, allglobal::global; allglobal::gteta, allglobal::guvij, allglobal::gzeta, constants::half, inputlist::igeometry, allglobal::ijimag, allglobal::ijireal, allglobal::im, allglobal::jiimag, allglobal::jireal, inputlist::lcheck, allglobal::lcoordinatesingularity, inputlist::lrad, fileunits::lunit, allglobal::mpi\_comm\_spec, allglobal::myid, allglobal::ncpu, allglobal::notstellsym, allglobal::nt, allglobal::nxyz, allglobal::nz, constants::one, fileunits::ounit, constants::pi, constants::pi2, allglobal::rij, allglobal::sfmn, allglobal::sg, numerical::small, constants::ten, allglobal::tetazeta, allglobal::tt, constants::two, inputlist::vcasingper, inputlist::vcasingtol, allglobal::virtualcasingfactor, inputlist::wmacros, constants::zero, and allglobal::zij.

Referenced by preset(), and spec().

Here is the call graph for this function:



Here is the caller graph for this function:



Constructs the field created by the plasma currents, at an arbitrary, external location using virtual casing.

Compute the external magnetic field using virtual casing.

# Theory and numerics

· Required inputs to this subroutine are the geometry of the plasma boundary,

$$\mathbf{x}(\theta,\zeta) \equiv x(\theta,\zeta)\mathbf{i} + y(\theta,\zeta)\mathbf{j} + z(\theta,\zeta)\mathbf{k},\tag{18}$$

and the tangential field on this boundary,

$$\mathbf{B}_s = B^{\theta} \mathbf{e}_{\theta} + B^{\zeta} \mathbf{e}_{\zeta},\tag{19}$$

where  $\theta$  and  $\zeta$  are arbitrary poloidal and toroidal angles, and  $\mathbf{e}_{\theta} \equiv \partial \mathbf{x}/\partial \theta$ ,  $\mathbf{e}_{\zeta} \equiv \partial \mathbf{x}/\partial \zeta$ . This routine assumes that the plasma boundary is a flux surface, i.e.  $\mathbf{B} \cdot \mathbf{e}_{\theta} \times \mathbf{e}_{\zeta} = 0$ .

• The virtual casing principle (Shafranov & Zakharov (1972) [7], Lazerson (2012) [5] and Hanson (2015) [1]) shows that the field outside/inside the plasma arising from plasma currents inside/outside the boundary is equivalent to the field generated by a surface current,

$$\mathbf{j} = \mathbf{B}_s \times \mathbf{n},\tag{20}$$

where  ${\bf n}$  is normal to the surface.

• The field at some arbitrary point,  $\bar{\mathbf{x}}$ , created by this surface current is given by

$$\mathbf{B}(\bar{\mathbf{x}}) = -\frac{1}{4\pi} \int_{S} \frac{(\mathbf{B}_s \times d\mathbf{s}) \times \hat{\mathbf{r}}}{r^2},\tag{21}$$

where  $d\mathbf{s} \equiv \mathbf{e}_{\theta} \times \mathbf{e}_{\zeta} \ d\theta d\zeta$ .

· For ease of notation introduce

$$\mathbf{J} \equiv \mathbf{B}_{\mathbf{s}} \times d\mathbf{s} = \alpha \, \mathbf{e}_{\theta} - \beta \, \mathbf{e}_{\zeta}, \tag{22}$$

where  $\alpha \equiv B_{\zeta} = B^{\theta}g_{\theta\zeta} + B^{\zeta}g_{\zeta\zeta}$  and  $\beta \equiv B_{\theta} = B^{\theta}g_{\theta\theta} + B^{\zeta}g_{\theta\zeta}$ .

• We may write in Cartesian coordinates  ${f J}=j_x\ {f i}+j_y\ {f j}+j_z\ {f k},$  where

$$j_x = \alpha x_\theta - \beta x_\zeta \tag{23}$$

$$j_y = \alpha y_\theta - \beta y_\zeta \tag{24}$$

$$j_z = \alpha z_\theta - \beta z_\zeta. \tag{25}$$

· Requiring that the current,

$$\mathbf{j} \quad \equiv \quad \nabla \times \mathbf{B} = \sqrt{g}^{-1} (\partial_{\theta} B_{\zeta} - \partial_{\zeta} B_{\theta}) \ \mathbf{e}_{s} + \sqrt{g}^{-1} (\partial_{\zeta} B_{s} - \partial_{s} B_{\zeta}) \ \mathbf{e}_{\theta} + \sqrt{g}^{-1} (\partial_{s} B_{\theta} - \partial_{\theta} B_{s}) \ \mathbf{e}_{\zeta} \tag{26}$$

has no normal component to the surface, i.e.  $\mathbf{j}\cdot\nabla s=0$ , we obtain the condition  $\partial_{\theta}B_{\zeta}=\partial_{\zeta}B_{\theta}$ , or  $\partial_{\theta}\alpha=\partial_{\zeta}\beta$ . In axisymmetric configurations, where  $\partial_{\zeta}\beta=0$ , we must have  $\partial_{\theta}\alpha=0$ .

• The displacement from an arbitrary point, (X, Y, Z), to a point, (x, y, z), that lies on the surface is given

$$\mathbf{r} \equiv r_x \,\mathbf{i} + r_y \,\mathbf{j} + r_z \,\mathbf{k} = (X - x) \,\mathbf{i} + (Y - y) \,\mathbf{j} + (Z - z) \,\mathbf{k}. \tag{27}$$

· The components of the magnetic field produced by the surface current are then

$$B^{x} = \oint \!\! \int \!\! d\theta d\zeta \ (j_{y}r_{z} - j_{z}r_{y})/r^{3}, \tag{28}$$

$$B^{y} = \oint \!\! \oint \! d\theta d\zeta \ (j_{z}r_{x} - j_{x}r_{z})/r^{3}, \tag{29}$$

$$B^{z} = \oint \!\! \oint \! d\theta d\zeta \ (j_{x}r_{y} - j_{y}r_{x})/r^{3} \tag{30}$$

up to a scaling factor virtualcasing factor  $= -1/4\pi$  that is taken into account at the end.

· When all is said and done, this routine calculates

$$\int_0^{2\pi} \int_0^{2\pi} \text{vcintegrand } d\theta d\zeta \tag{31}$$

for a given (X, Y, Z), where vcintegrand is given in Eqn. (33).

The surface integral is performed using DCUHRE, which uses an adaptive subdivision strategy and also computes absolute error estimates. The absolute and relative accuracy required are provided by the inputvar vcasingtol. The minimum number of function evaluations is provided by the inputvar vcasingits.

## Calculation of integrand

• An adaptive integration is used to compute the integrals. Consequently, the magnetic field tangential to the plasma boundary is required at an arbitrary point. This is computed, as always, from  $\mathbf{B} = \nabla \times \mathbf{A}$ , and this provides  $\mathbf{B} = B^{\theta} \mathbf{e}_{\theta} + B^{\zeta} \mathbf{e}_{\zeta}$ . Recall that  $B^{s} = 0$  by construction on the plasma boundary.

Todo It would be MUCH faster to only require the tangential field on a regular grid!!!

• Then, the metric elements  $g_{\theta\theta}$ ,  $g_{\theta\zeta}$  and  $g_{\zeta\zeta}$  are computed. These are used to "lower" the components of the magnetic field,  $\mathbf{B} = B_{\theta} \nabla \theta + B_{\zeta} \nabla \zeta$ .

**Todo** Please check why  $B_s$  is not computed. Is it because  $B_s \nabla s \times \mathbf{n} = 0$ ?

- The distance between the "evaluate" point, (X,Y,Z), and the given point on the surface, (x,y,z) is computed.
- If the computational boundary becomes too close to the plasma boundary, the distance is small and this causes problems for the numerics. I have tried to regularize this problem by introducing  $\epsilon$  =inputvar vcasingeps. Let the "distance" be

$$D \equiv \sqrt{(X-x)^2 + (Y-y)^2 + (Z-Z)^2} + \epsilon^2.$$
 (32)

• On taking the limit that  $\epsilon \to 0$ , the virtual casing integrand is

$$vcintegrand \equiv (B_x n_x + B_y n_y + B_z n_z)(1 + 3\epsilon^2/D^2)/D^3, \tag{33}$$

where the normal vector is  $\mathbf{n} \equiv n_x \mathbf{i} + n_y \mathbf{j} + n_z \mathbf{k}$ . The normal vector, Nxyz, to the computational boundary (which does not change) is computed in preset().

**Todo** This needs to be revised.

#### **Parameters**

in	teta	$\theta$
in	zeta	ζ
out	gBn	$\sqrt{g}\mathbf{B}\cdot\mathbf{n}$
out	icasing	return flag from dcuhre()

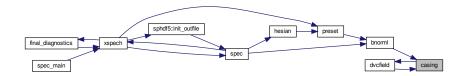
References allglobal::cpus, dvcfield(), allglobal::dxyz, allglobal::globaljk, allglobal::mpi\_comm\_spec, allglobal::myid, allglobal::ncpu, allglobal::nxyz, fileunits::ounit, constants::pi, constants::pi2, inputlist::vcasingits, inputlist::vcasingper, inputlist::vcasingtol, fileunits::vunit, inputlist::wmacros, and constants::zero.

Referenced by bnorml(), and dvcfield().

Here is the call graph for this function:



Here is the caller graph for this function:



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Differential virtual casing integrand.

Differential virtual casing integrand

#### **Parameters**

in	Ndim	number of parameters (==2)
in	tz	$ heta$ and $\zeta$
in	Nfun	number of function values (==3)
out	vcintegrand	cartesian components of magnetic field

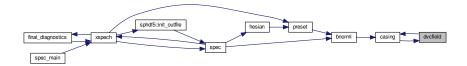
References allglobal::ate, allglobal::ate, allglobal::aze, allglobal::aze, casing(), allglobal::cpus, allglobal::dxyz, allglobal::first\_free\_bound, constants::four, allglobal::global; constants::half, inputlist::igeometry, allglobal::im, allglobal::irbc, allglobal::irbc, allglobal::izbc, allglobal::izbs, inputlist::lrad, allglobal::mn, allglobal::mpi comm\_spec, allglobal::myid, allglobal::ncpu, allglobal::notstellsym, inputlist::nvol, allglobal::nxyz, constants::one, fileunits::ounit, numerical::small, constants::three, allglobal::tt, inputlist::vcasingeps, fileunits::vunit, allglobal::yesstellsym, and constants::zero.

Referenced by casing().

Here is the call graph for this function:



Here is the caller graph for this function:



# 5.3 Parallelization

### **Functions/Subroutines**

subroutine brcast (Ivol)

Broadcasts Beltrami fields, profiles, . . .

# 5.3.1 Detailed Description

#### 5.3.2 Function/Subroutine Documentation

Broadcasts Beltrami fields, profiles, . . .

### broadcasting

- The construction of the Beltrami fields is distributed on separate cpus.
- All "local" information needs to be broadcast so that the "global" force vector,

$$\mathbf{F}_i \equiv [[p + B^2/2]]_i = (p + B^2/2)_{v,i} - (p + B^2/2)_{v-1,i}$$
(34)

can be constructed, and so that restart and output files can be saved to file.

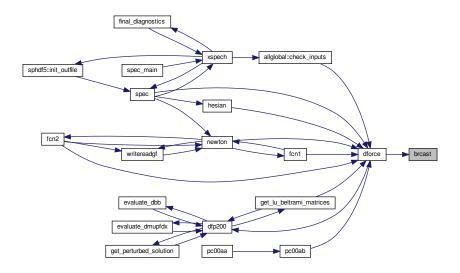
#### **Parameters**

in	Ivol	index of nested volume
----	------	------------------------

References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::bemn, allglobal::bomn, allglobal::bomn, allglobal::cpus, inputlist::curpol, inputlist::curror, allglobal::diotadxup, allglobal::ditgpdxtp, allglobal::dpflux, allglobal::dtflux, inputlist::helicity, allglobal::iemn, allglobal::imagneticok, allglobal::iomn, inputlist::lconstraint, inputlist::lfindzero, inputlist::lrad, allglobal::mn, inputlist::mnvol, allglobal::mpi\_comm\_spec, inputlist::mu, allglobal::myid, allglobal::ncpu, allglobal::ntz, inputlist::nvol, fileunits::ounit, allglobal::pemn, allglobal::pomn, allglobal::semn, allglobal::semn, allglobal::semn, inputlist::wmacros, and constants::zero.

Referenced by dforce().

Here is the caller graph for this function:



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# 5.4 Geometry

#### **Functions/Subroutines**

• subroutine coords (Ivol, Iss, Lcurvature, Ntz, mn) Calculates coordinates,  $\mathbf{x}(s, \theta, \zeta) \equiv R \mathbf{e}_R + Z \mathbf{e}_Z$ , and metrics, using FFTs.

# 5.4.1 Detailed Description

#### 5.4.2 Function/Subroutine Documentation

```
5.4.2.1 coords() subroutine coords (
    integer, intent(in) lvol,
    real, intent(in) lss,
    integer, intent(in), value Lcurvature,
    integer, intent(in) Ntz,
    integer, intent(in) mn)
```

Calculates coordinates,  $\mathbf{x}(s, \theta, \zeta) \equiv R \mathbf{e}_R + Z \mathbf{e}_Z$ , and metrics, using FFTs.

#### Coordinates

- We work in coordinates,  $(s, \theta, \zeta)$ , which are be defined *inversely* via a transformation *to* Cartesian coordinates, (x, y, z).
- The toroidal angle,  $\zeta$ , is identical to the cylindrical angle,  $\zeta \equiv \phi$ .
- The radial coordinate, s, is *not* a global variable: it only needs to be defined in each volume, and in each volume  $s \in [-1, 1]$ .
- The choice of poloidal angle,  $\theta$ , does not affect the following.

# Geometry

- The geometry of the "ideal"-interfaces,  $\mathbf{x}_v(\theta,\zeta)$ , is given by  $R(\theta,\zeta)$  and  $Z(\theta,\zeta)$  as follows:
  - Igeometry=1: Cartesian

$$\mathbf{x} \equiv r_{pol}\theta \,\hat{\mathbf{i}} + r_{tor}\zeta \,\hat{\mathbf{j}} + R \,\hat{\mathbf{k}} \tag{35}$$

where  $r_{pol}$  and  $r_{tor}$  are inputs and  $r_{pol}=r_{tor}=1$  by default.

- Igeometry=2: Cylindrical

$$\mathbf{x} = R \cos \theta \, \hat{\mathbf{i}} + R \sin \theta \, \hat{\mathbf{j}} + \zeta \, \hat{\mathbf{k}} \tag{36}$$

- Igeometry=3: Toroidal

$$\mathbf{x} \equiv R \,\hat{\mathbf{r}} + Z \,\hat{\mathbf{k}} \tag{37}$$

where  $\hat{\mathbf{r}} \equiv \cos \phi \, \hat{\mathbf{i}} + \sin \phi \, \hat{\mathbf{j}}$  and  $\hat{\phi} \equiv -\sin \phi \, \hat{\mathbf{i}} + \cos \phi \, \hat{\mathbf{j}}$ .

The geometry of the ideal interfaces is given as Fourier summation: e.g., for stellarator-symmetry

$$R_v(\theta,\zeta) \equiv \sum_j R_{j,v} \cos \alpha_j,$$
 (38)

$$Z_v(\theta,\zeta) \equiv \sum_j Z_{j,v} \sin \alpha_j,$$
 (39)

where  $\alpha_j \equiv m_j \theta - n_j \zeta$ .

# interpolation between interfaces

- The "coordinate" functions,  $R(s,\theta,\zeta)$  and  $Z(s,\theta,\zeta)$ , are constructed by radially interpolating the Fourier representations of the ideal-interfaces.
- The v-th volume is bounded by  $\mathbf{x}_{v-1}$  and  $\mathbf{x}_{v}$ .
- In each annular volume, the coordinates are constructed by linear interpolation:

$$R(s,\theta,\zeta) \equiv \sum_{j} \left[ \frac{(1-s)}{2} R_{j,v-1} + \frac{(1+s)}{2} R_{j,v} \right] \cos \alpha_{j},$$

$$Z(s,\theta,\zeta) \equiv \sum_{j} \left[ \frac{(1-s)}{2} Z_{j,v-1} + \frac{(1+s)}{2} Z_{j,v} \right] \sin \alpha_{j},$$

$$(40)$$

#### coordinate singularity: regularized extrapolation

- · For cylindrical or toroidal geometry, in the innermost, "simple-torus" volume, the coordinates are constructed by an interpolation that "encourages" the interpolated coordinate surfaces to not intersect.
- Introduce  $\bar{s} \equiv (s+1)/2$ , so that in each volume  $\bar{s} \in [0,1]$ , then

$$R_j(s) = R_{j,0} + (R_{j,1} - R_{j,0})f_j,$$
 (41)

$$Z_j(s) = Z_{j,0} + (Z_{j,1} - Z_{j,0})f_j,$$
 (42)

where, in toroidal geometry,

$$f_j \equiv \left\{ \begin{array}{ll} \bar{s} & , & \text{for } m_j = 0, \\ \bar{s}^{m_j} & , & \text{otherwise.} \end{array} \right\}. \tag{43}$$

• Note: The location of the coordinate axis, i.e. the  $R_{j,0}$  and  $Z_{j,0}$ , is set in the coordinate "packing" and "unpacking" routine, packxi().

## Jacobian

- The coordinate Jacobian (and some other metric information) is given by
  - Igeometry=1: Cartesian

$$\mathbf{e}_{\theta} \times \mathbf{e}_{\zeta} = -r_{tor} R_{\theta} \, \hat{\mathbf{i}} - r_{pol} R_{\zeta} \, \hat{\mathbf{j}} + r_{pol} r_{tor} \hat{\mathbf{k}}$$

$$\boldsymbol{\xi} \cdot \mathbf{e}_{\theta} \times \mathbf{e}_{\zeta} = \delta R$$
(44)

$$\boldsymbol{\xi} \cdot \mathbf{e}_{\theta} \times \mathbf{e}_{\zeta} = \delta R \tag{45}$$

$$\sqrt{g} = R_s \, r_{pol} \, r_{tor} \tag{45}$$

- Igeometry=2: Cylindrical

$$\mathbf{e}_{\theta} \times \mathbf{e}_{\zeta} = (R_{\theta} \sin \theta + R \cos \theta) \, \hat{\mathbf{i}} + (R \sin \theta - R_{\theta} \cos \theta) \, \hat{\mathbf{j}} - RR_{\zeta} \, \hat{\mathbf{k}}$$
 (47)

$$\boldsymbol{\xi} \cdot \mathbf{e}_{\theta} \times \mathbf{e}_{\zeta} = \delta R R \tag{48}$$

$$\sqrt{g} = R_s R \tag{49}$$

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- Igeometry=3: Toroidal

$$\mathbf{e}_{\theta} \times \mathbf{e}_{\zeta} = -R Z_{\theta} \,\hat{r} + (Z_{\theta} R_{\zeta} - R_{\theta} Z_{\zeta}) \hat{\phi} + R R_{\theta} \,\hat{z} \tag{50}$$

$$\boldsymbol{\xi} \cdot \mathbf{e}_{\theta} \times \mathbf{e}_{\zeta} = R(\delta Z R_{\theta} - \delta R Z_{\theta}) \tag{51}$$

$$\sqrt{g} = R(Z_s R_\theta - R_s Z_\theta) \tag{52}$$

#### cartesian metrics

· The cartesian metrics are

$$g_{ss}=R_sR_s,\quad g_{s\theta}=R_sR_{\theta},\quad g_{s\zeta}=R_sR_{\zeta},\quad g_{\theta\theta}=R_{\theta}R_{\theta}+r_{pol}^2,\quad g_{\theta\zeta}=R_{\theta}R_{\zeta},\quad g_{\zeta\zeta}=R_{\zeta}R_{\zeta}+r_{tor}^2 \quad \mbox{(53)}$$

### cylindrical metrics

· The cylindrical metrics are

$$g_{ss} = R_s R_s, \quad g_{s\theta} = R_s R_{\theta}, \quad g_{s\zeta} = R_s R_{\zeta}, \quad g_{\theta\theta} = R_{\theta} R_{\theta} + R^2, \quad g_{\theta\zeta} = R_{\theta} R_{\zeta}, \quad g_{\zeta\zeta} = R_{\zeta} R_{\zeta} + 1 \quad (54)$$

## logical control

- The logical control is provided by Lcurvature as follows:
  - Lcurvature=0 : only the coordinate transformation is computed, i.e. only R and Z are calculated, e.g. global()
  - Lcurvature=1 : the Jacobian,  $\sqrt{g}$ , and "lower" metrics,  $g_{\mu,\nu}$ , are calculated, e.g. bnorml(), lforce(), curent(), metrix(), sc00aa()
  - Lcurvature=2: the "curvature" terms are calculated, by which I mean the second derivatives of the position vector; this information is required for computing the current,  $\mathbf{j} = \nabla \times \nabla \times \mathbf{A}$ , e.g. jo00aa()
  - Lcurvature=3 : the derivative of the  $g_{\mu,\nu}/\sqrt{g}$  w.r.t. the interface boundary geometry is calculated, e.g. metrix(), curent()
  - Lcurvature=4: the derivative of the  $g_{\mu,\nu}$  w.r.t. the interface boundary geometry is calculated, e.g. dforce()
  - Lcurvature=5 : the derivative of  $\sqrt{g}$  w.r.t. the interface boundary geometry is calculated, e.g. rzaxis()

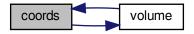
#### **Parameters**

in	specified in which volume to compute coordinate		
in	in Iss radial coordinate s		
in	Lcurvature	logical control flag	
in	Ntz	number of points in $\theta$ and $\zeta$	
in	mn	number of Fourier harmonics	

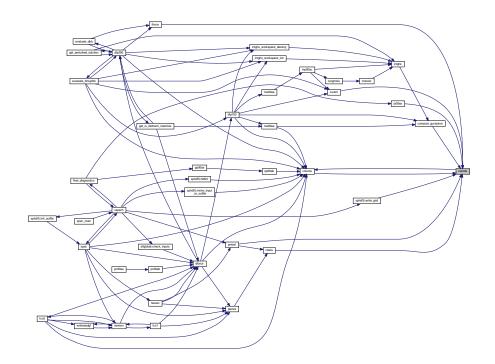
References allglobal::cosi, allglobal::cpus, allglobal::dbdx, allglobal::drodr, allglobal::drodz, allglobal::dzodr, allglobal::dzodr, allglobal::dzodz, allglobal::guvij, constants::half, allglobal::halfmm, inputlist::igeometry, allglobal::im, allglobal::in, allglobal::irbc, allglobal::irbs, allglobal::izbc, allglobal::izbs, allglobal::lcoordinatesingularity, allglobal::mpi\_comm\_ cosec, allglobal::myid, allglobal::notstellsym, allglobal::nt, inputlist::ntor, allglobal::nz, constants::one, fileunits::ounit, constants::pi2, allglobal::rij, inputlist::rtor, allglobal::sg, allglobal::sini, numerical::small, constants::two, volume(), numerical::vsmall, constants::zero, and allglobal::zij.

Referenced by compute\_guvijsave(), curent(), jo00aa(), lforce(), preset(), rzaxis(), volume(), and sphdf5::write\_ $\leftarrow$  grid().

Here is the call graph for this function:



Here is the caller graph for this function:



# 5.5 Plasma Currents

# **Functions/Subroutines**

• subroutine curent (Ivol, mn, Nt, Nz, iflag, IdItGp) Computes the plasma current,  $I\equiv\int B_{\theta}\,d\theta$ , and the "linking" current,  $G\equiv\int B_{\zeta}\,d\zeta$ .

# 5.5.1 Detailed Description

# 5.5.2 Function/Subroutine Documentation

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```
5.5.2.1 curent() subroutine curent (
    integer, intent(in) lvol,
    integer, intent(in) mn,
    integer, intent(in) Nt,
    integer, intent(in) Nz,
    integer, intent(in) iflag,
    real, dimension(0:1,-1:2), intent(out) ldItGp )
```

Computes the plasma current,  $I\equiv\int B_{\theta}\,d\theta$ , and the "linking" current,  $G\equiv\int B_{\zeta}\,d\zeta$ .

#### enclosed currents

In the vacuum region, the enclosed currents are given by either surface integrals of the current density or line
integrals of the magnetic field,

$$\int_{\mathcal{S}} \mathbf{j} \cdot d\mathbf{s} = \int_{\partial \mathcal{S}} \mathbf{B} \cdot d\mathbf{l},\tag{55}$$

and line integrals are usually easier to compute than surface integrals.

- The magnetic field is given by the curl of the magnetic vector potential, as described in e.g. bfield().
- The toroidal, plasma current is obtained by taking a "poloidal" loop,  $d\mathbf{l}=\mathbf{e}_{\theta}\,d\theta$ , on the plasma boundary, where  $B^s=0$ , to obtain

$$I \equiv \int_0^{2\pi} \mathbf{B} \cdot \mathbf{e}_{\theta} \, d\theta = \int_0^{2\pi} (-\partial_s A_{\zeta} \, \bar{g}_{\theta\theta} + \partial_s A_{\theta} \, \bar{g}_{\theta\zeta}) \, d\theta, \tag{56}$$

where  $\bar{g}_{\mu\nu} \equiv g_{\mu\nu}/\sqrt{g}$ .

• The poloidal, "linking" current through the torus is obtained by taking a "toroidal" loop,  $d\mathbf{l}=\mathbf{e}_{\zeta}\,d\zeta$ , on the plasma boundary to obtain

$$G \equiv \int_0^{2\pi} \mathbf{B} \cdot \mathbf{e}_{\zeta} \, d\zeta = \int_0^{2\pi} \left( -\partial_s A_{\zeta} \, \bar{g}_{\theta\zeta} + \partial_s A_{\theta} \, \bar{g}_{\zeta\zeta} \right) \, d\zeta. \tag{57}$$

### Fourier integration

• Using  $f\equiv -\partial_s A_\zeta \; \bar{g}_{\theta\theta} + \partial_s A_\theta \; \bar{g}_{\theta\zeta}$ , the integral for the plasma current is

$$I = \sum_{i}' f_i \cos(n_i \zeta) 2\pi, \tag{58}$$

where  $\sum'$  includes only the  $m_i = 0$  harmonics.

• Using  $g\equiv -\partial_s A_\zeta \; \bar{g}_{\theta\zeta} + \partial_s A_\theta \; \bar{g}_{\zeta\zeta}$ , the integral for the linking current is

$$G = \sum_{i}' g_i \cos(m_i \zeta) 2\pi, \tag{59}$$

where  $\sum'$  includes only the  $n_i=0$  harmonics.

• The plasma current, Eqn. (58), should be independent of  $\zeta$ , and the linking current, Eqn. (59), should be independent of  $\theta$ .

Todo Perhaps this can be proved analytically; in any case it should be confirmed numerically.

# **Parameters**

in	Ivol	index of volume
in	mn	number of Fourier harmonics
in	Nt	number of grid points along $\theta$
in	Nz	number of grid points along $\zeta$
in	iflag	some integer flag
out	ldltGp	plasma and linking current

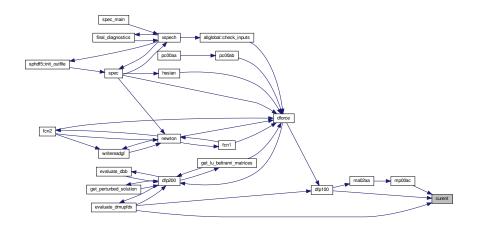
References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::cfmn, allglobal::comn, coords(), allglobal::cpus, allglobal::efmn, allglobal::evmn, allglobal::guvij, allglobal::jiimag, allglobal::jiimag, allglobal::jiimag, allglobal::jiimag, allglobal::jiimag, allglobal::jiimag, allglobal::jiimag, allglobal::jiimag, allglobal::jiimag, allglobal::mne, allglobal::mne, allglobal::mne, allglobal::mne, allglobal::ntz, allglobal::odmn, allglobal::odmn, allglobal::odmn, allglobal::simn, allglobal::simn, allglobal::tt, constants::two, inputlist::wmacros, allglobal::yesstellsym, and constants::zero.

Referenced by dfp100(), evaluate\_dmupfdx(), and mp00ac().

Here is the call graph for this function:



Here is the caller graph for this function:



# 5.6 "global" force

# Functions/Subroutines

• subroutine dforce (NGdof, position, force, LComputeDerivatives, LComputeAxis)  $\textit{Calculates } \mathbf{F}(\mathbf{x}), \textit{where } \mathbf{x} \equiv \{\textit{geometry}\} \equiv \{\textit{R}_{i,v}, \textit{Z}_{i,v}\} \textit{ and } \mathbf{F} \equiv [[p+B^2/2]] + \{\textit{spectral constraints}\}, \textit{and } \nabla \mathbf{F}.$ 

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#### 5.6.1 Detailed Description

#### 5.6.2 Function/Subroutine Documentation

Calculates  $\mathbf{F}(\mathbf{x})$ , where  $\mathbf{x} \equiv \{\text{geometry}\} \equiv \{R_{i,v}, Z_{i,v}\}$  and  $\mathbf{F} \equiv [[p+B^2/2]] + \{\text{spectral constraints}\}$ , and  $\nabla \mathbf{F}$ .

### unpacking

• The geometrical degrees of freedom are represented as a vector,  $\mathbf{x} \equiv \{R_{i,v}, Z_{i,v}\}$ , where i=1, mn labels the Fourier harmonic and v=1, Mvol -1 is the interface label. This vector is "unpacked" using packxi(). (Note that packxi() also sets the coordinate axis, i.e. the  $R_{i,0}$  and  $Z_{i,0}$ .)

### **Matrices computation**

- the volume-integrated metric arrays, DToocc, etc. are evaluated in each volume by calling ma00aa()
- the energy and helicity matrices, dMA (0:NN, 0:NN), dMB (0:NN, 0:2), etc. are evaluated in each volume by calling matrix()

#### parallelization over volumes

Two different cases emerge: either a local constraint or a global constraint is considered. This condition is determined by the flag LocalConstraint.

- · Local constraint
  - In each volume, vvol=1,Mvol,
    - \* the logical array ImagneticOK(vvol) is set to .false.
    - \* The MPI node associated to the volume calls dfp100(). This routine calls ma02aa() (and might iterate on mp00ac()) and computes the field solution in each volume consistent with the constraint.
    - \* The MPI node associated to the volume calls dfp200(). This computes  $p + B^2/2$  (and the spectral constraints if required) at the interfaces in each volumes, as well as the derivatives of the force-balance if LComputeDerivatives=1.
  - After the parallelization loop over the volumes, brcast() is called to broadcast the required information.
- · Global constraint

The MPI node 0 minimizes the constraint with HYBRID1() by iterating on dfp100() until the field matches the constraint. Other MPI nodes enter the subroutine loop dfp100(). In loop dfp100(), each MPI node

- calls dfp100(),
- solves the field in its associated volumes,
- communicates the field to the node 0 and
- repeats this loop until the node 0 sends a flag <code>iflag=5</code>.

## broadcasting

• The required quantities are broadcast by brcast().

## construction of force

• The force vector,  $\mathbf{F}(\mathbf{x})$ , is a combination of the pressure-imbalance Fourier harmonics,  $[[p+B^2/2]]_{i,v}$ , where i labels Fourier harmonic and v is the interface label:

$$F_{i,v} \equiv \left[ (p_{v+1} + B_{i,v+1}^2/2) - (p_v + B_{i,v}^2/2) \right] \times \text{BBweight}_i, \tag{60}$$

where BBweight\_i is defined in preset(); and the spectral condensation constraints,

$$F_{i,v} \equiv I_{i,v} \times \text{epsilon} + S_{i,v,1} \times \text{sweight}_v - S_{i,v+1,0} \times \text{sweight}_{v+1},$$
 (61)

where the spectral condensation constraints,  $I_{i,v}$ , and the "star-like" poloidal angle constraints,  $S_{i,v,\pm 1}$ , are calculated and defined in Iforce(); and the <code>sweight</code>  $_v$  are defined in <code>preset()</code>. All quantities local to a volume are computed in <code>dfp200()</code>, information is then broadcasted to the MPI node 0 in <code>dforce()</code> and the global force is evaluated.

## construct derivatives of matrix equation

• Matrix perturbation theory is used to compute the derivatives of the solution, i.e. the Beltrami fields, as the geometry of the interfaces changes:

#### **Parameters**

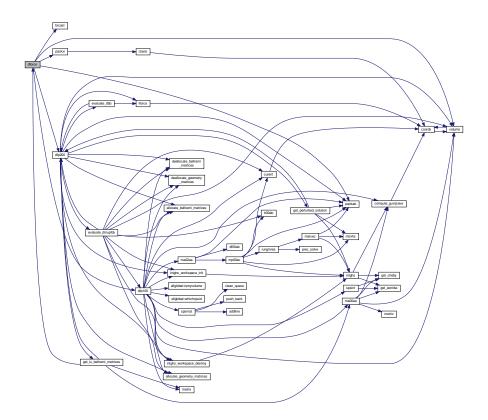
in	NGdof	number of global degrees of freedom
in	position	
out	force	
in	<i>LComputeDerivatives</i>	
in,out	LComputeAxis	

References brcast(), allglobal::cpus, allglobal::dbdx, dfp100(), dfp200(), inputlist::drz, inputlist::epsilon, constants:::half, allglobal::hessian, inputlist::igeometry, allglobal::im, allglobal::in, allglobal::iquad, allglobal::irbc, allglobal::irbc, allglobal::irbc, allglobal::icbc, allglobal::icbc, allglobal::ilconstraint, inputlist::lextrap, inputlist::lfreebound, allglobal::lgdof, numerical::logtolerance, inputlist::lrad, allglobal::mn, allglobal::mpi\_comm\_spec, inputlist::mupftol, allglobal::myid, allglobal::nadof, allglobal::ncpu, allglobal::notstellsym, inputlist::ntor, inputlist::nvol, constants::one, fileunits::ounit, packab(), packxi(), constants::pi, constants::pi2, allglobal::psifactor, constants::two, volume(), inputlist::wmacros, allglobal::yesstellsym, and constants::zero.

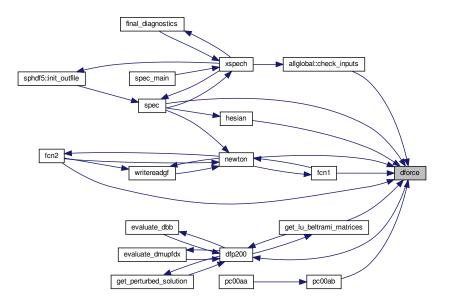
Referenced by allglobal::check\_inputs(), fcn1(), fcn2(), get\_lu\_beltrami\_matrices(), hesian(), newton(), pc00ab(), and spec().

5.6 "global" force

Here is the call graph for this function:

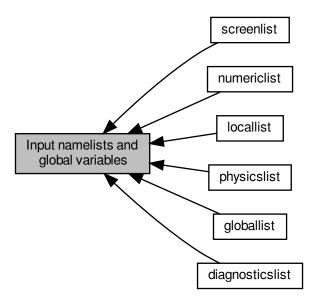


Here is the caller graph for this function:



# 5.7 Input namelists and global variables

Collaboration diagram for Input namelists and global variables:



### **Modules**

· physicslist

The namelist physicslist controls the geometry, profiles, and numerical resolution.

· numericlist

The namelist numericlist controls internal resolution parameters that the user rarely needs to consider.

locallist

The namelist locallist controls the construction of the Beltrami fields in each volume.

· globallist

The namelist globallist controls the search for global force-balance.

diagnosticslist

The namelist diagnosticslist controls post-processor diagnostics, such as Poincaré plot resolution, etc.

· screenlist

The namelist screenlist controls screen output. Every subroutine, e.g. xy00aa.h, has its own write flag, Wxy00aa.h

### **Functions/Subroutines**

• subroutine inputlist::initialize\_inputs

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#### **Variables**

```
• integer, parameter inputlist::mnvol = 256
```

The maximum value of Nvol is MNvol=256.

• integer, parameter inputlist::mmpol = 64

The maximum value of Mpol is MNpol=64.

• integer, parameter inputlist::mntor = 64

The maximum value of Ntor is MNtor=64.

## 5.7.1 Detailed Description

Input namelists.

## 5.8 "local" force

### **Functions/Subroutines**

subroutine Iforce (Ivol, iocons, ideriv, Ntz, dBB, XX, YY, length, DDI, MMI, iflag)
 Computes B<sup>2</sup>, and the spectral condensation constraints if required, on the interfaces, \( \mathcal{I}\_i \).

## 5.8.1 Detailed Description

## 5.8.2 Function/Subroutine Documentation

```
5.8.2.1 Iforce() subroutine lforce (
    integer, intent(in) lvol,
    integer, intent(in) iocons,
    integer, intent(in) ideriv,
    integer, intent(in) Ntz,
    real, dimension(1:ntz, -1:2) dBB,
    real, dimension(1:ntz) XX,
    real, dimension(1:ntz) YY,
    real, dimension(1:ntz) length,
    real DDl,
    real MM1,
    integer, intent(in) iflag)
```

Computes  $B^2$ , and the spectral condensation constraints if required, on the interfaces,  $\mathcal{I}_i$ .

## field strength

- The field strength is given by  $B^2=B^sB_s+B^\theta B_\theta+B^\zeta B_\zeta$ , and on the interfaces  $B^s=0$  by construction.
- The magnetic field is  $\sqrt{g} \mathbf{B} = (\partial_{\theta} A_{\zeta} \partial_{\zeta} A_{\theta}) \mathbf{e}_s \partial_s A_{\zeta} \mathbf{e}_{\theta} + \partial_s A_{\theta} \mathbf{e}_{\zeta}.$
- The covariant components of the field are computed via  $B_{\theta}=B^{\theta}g_{\theta\theta}+B^{\zeta}g_{\theta\zeta}$  and  $B_{\zeta}=B^{\theta}g_{\theta\zeta}+B^{\zeta}g_{\zeta\zeta}$ .

• The expression for  $B^2$  is

$$(\sqrt{g})^2 B^2 = A'_{\zeta} A'_{\zeta} g_{\theta\theta} - 2 A'_{\zeta} A'_{\theta} g_{\theta\zeta} + A'_{\theta} A'_{\theta} g_{\zeta\zeta}, \tag{62}$$

where the " $\prime$ " denotes derivative with respect to s.

· The quantity returned is

$$F \equiv \text{pscale} \times \frac{P}{V^{\gamma}} + \frac{B^2}{2},\tag{63}$$

where  $P \equiv \text{adiabatic}$  and  $V \equiv \text{volume}$ .

## spectral constraints

- In addition to the physical-force-balance constraints, namely that  $[[p + B^2/2]] = 0$  across the interfaces, additional angle constraints are required to obtain a unique Fourier representation of the interface geometry.
- Introducing the angle functional: a weighted combination of the "polar" constraint; the normalized, poloidal, spectral width (Hirshman & Meier (1985) [3], Hirshman & Breslau (1998) [2]) the poloidal-angle origin constraint; and the "length" of the angle curves

where i labels the interfaces, and

$$\Theta_{i,\theta} \equiv \frac{x y_{\theta} - x_{\theta} y}{x^2 + y^2},\tag{65}$$

$$M_i \equiv \frac{\sum_j m_j^p (R_{j,i}^2 + Z_{j,i}^2)}{\sum_j (R_{j,i}^2 + Z_{j,i}^2)},$$
(66)

$$L_i \equiv \sqrt{[R_i(\theta,\zeta) - R_{i-1}(\theta,\zeta)]^2 + [Z_i(\theta,\zeta) - Z_{i-1}(\theta,\zeta)]^2},$$
(67)

and where j labels the Fourier harmonics. The  $\alpha_i$ ,  $\beta_i$ ,  $\gamma_i$  and  $\delta_i \equiv \text{sweight}$  are user-supplied weight factors.

• The polar constraint is derived from defining  $\tan\Theta\equiv y/x$ , where

$$x(\theta,\zeta) \equiv R_i(\theta,\zeta) - R_{i,0}(\zeta),$$
 (68)

$$y(\theta,\zeta) \equiv Z_i(\theta,\zeta) - Z_{i,0}(\zeta), \tag{69}$$

and where the geometric center of each interface is given by the arc-length weighted integrals, see rzaxis(),

$$R_{i,0} \equiv \int_0^{2\pi} d\theta \, R_i(\theta,\zeta) \sqrt{R_{i,\theta}(\theta,\zeta)^2 + Z_{i,\theta}(\theta,\zeta)^2}, \tag{70}$$

$$Z_{i,0} \equiv \int_0^{2\pi} d\theta \ Z_i(\theta,\zeta) \sqrt{R_{i,\theta}(\theta,\zeta)^2 + Z_{i,\theta}(\theta,\zeta)^2}, \tag{71}$$

and  $\cos\Theta=x/\sqrt{x^2+y^2}$  has been used to simplify the expressions and to avoid divide-by-zero.

Only "poloidal tangential" variations will be allowed to find the extremum of F, which are described by

$$\delta R_i(\theta, \zeta) \equiv R_{i,\theta}(\theta, \zeta) \, \delta u_i(\theta, \zeta),$$
 (72)

$$\delta Z_i(\theta,\zeta) \equiv Z_{i,\theta}(\theta,\zeta) \,\delta u_i(\theta,\zeta),\tag{73}$$

from which it follows that the variation in each Fourier harmonic is

$$\delta R_{j,i} = \oint \!\! \int \!\! d\theta d\zeta \ R_{i,\theta}(\theta,\zeta) \, \delta u_i(\theta,\zeta) \, \cos(m_j \theta - n_j \zeta), \tag{74}$$

$$\delta Z_{j,i} = \oint \!\! \int \!\! d\theta d\zeta \ Z_{i,\theta}(\theta,\zeta) \, \delta u_i(\theta,\zeta) \, \sin(m_j \theta - n_j \zeta), \tag{75}$$

and

$$\delta R_{i,\theta}(\theta,\zeta) \equiv R_{i,\theta\theta}(\theta,\zeta) \,\delta u_i(\theta,\zeta) + R_{i,\theta}(\theta,\zeta) \,\delta u_{i,\theta}(\theta,\zeta) \tag{76}$$

$$\delta Z_{i,\theta}(\theta,\zeta) \equiv Z_{i,\theta\theta}(\theta,\zeta) \,\delta u_i(\theta,\zeta) + Z_{i,\theta}(\theta,\zeta) \,\delta u_{i,\theta}(\theta,\zeta) \tag{77}$$

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• The variation in F is

$$\delta F = \sum_{i=1}^{N-1} \alpha_{i} \oint d\theta d\zeta \left(\frac{-2\Theta_{i,\theta\theta}}{\Theta_{i,\theta}^{2}}\right) \delta u_{i} 
+ \sum_{i=1}^{N-1} \beta_{i} \oint d\theta d\zeta \left(R_{i,\theta}X_{i} + Z_{i,\theta}Y_{i}\right) \delta u_{i} 
+ \sum_{i=1}^{N-1} \gamma_{i} \int d\zeta \left(Z_{i}(0,\zeta) - Z_{i,0}\right) Z_{i,\theta} \delta u_{i} 
+ \sum_{i=1}^{N-1} \delta_{i} \oint d\theta d\zeta \left(\frac{\Delta R_{i}R_{i,\theta} + \Delta Z_{i}Z_{i,\theta}}{L_{i}}\right) \delta u_{i} 
- \sum_{i=1}^{N-1} \delta_{i+1} \oint d\theta d\zeta \left(\frac{\Delta R_{i+1}R_{i,\theta} + \Delta Z_{i+1}Z_{i,\theta}}{L_{i+1}}\right) \delta u_{i}$$
(78)

where, for the stellarator symmetric case.

$$X_i \equiv \sum_{j} (m_j^p - M_i) R_{j,i} \cos(m_j \theta - n_j \zeta), \tag{79}$$

$$Y_i \equiv \sum_{j} (m_j^p - M_i) Z_{j,i} \sin(m_j \theta - n_j \zeta), \tag{80}$$

and

$$\Delta R_i \equiv R_i(\theta, \zeta) - R_{i-1}(\theta, \zeta), \tag{81}$$

$$\Delta Z_i \equiv Z_i(\theta, \zeta) - Z_{i-1}(\theta, \zeta), \tag{82}$$

• The spectral constraints derived from Eqn. (78) are

$$I_{i}(\theta,\zeta) \equiv -2\alpha_{i}\frac{\Theta_{i,\theta\theta}}{\Theta_{i,\theta}^{2}} + \beta_{i}\left(R_{i,\theta}X_{i} + Z_{i,\theta}Y_{i}\right) + \gamma_{i}\left(Z_{i}(0,\zeta) - Z_{i,0}\right)Z_{i,\theta}(0,\zeta)$$

$$+ \delta_{i}\frac{\Delta R_{i}R_{i,\theta} + \Delta Z_{i}Z_{i,\theta}}{L_{i}} - \delta_{i+1}\frac{\Delta R_{i+1}R_{i,\theta} + \Delta Z_{i+1}Z_{i,\theta}}{L_{i+1}}$$
(83)

- Note that choosing p=2 gives  $X=-R_{\theta\theta}$  and  $Y=-Z_{\theta\theta}$ , and the spectrally condensed angle constraint,  $R_{\theta}X+Z_{\theta}Y=0$ , becomes  $\partial_{\theta}(R_{\theta}^2+Z_{\theta}^2)=0$ , which defines the equal arc length angle.
- The poloidal-angle origin term, namely  $\gamma_i\left(Z_i(0,\zeta)-Z_{i,0}\right)Z_{i,\theta}(0,\zeta)$  is only used to constrain the  $m_j=0$  harmonics.
- The construction of the angle functional was influenced by the following considerations:
  - The minimal spectral width constraint is very desirable as it reduces the required Fourier resolution, but it does not constrain the m=0 harmonics and the minimizing spectral-width poloidal-angle may not be consistent with the poloidal angle used on adjacent interfaces.
  - The regularization of the vector potential and the coordinate interpolation near the coordinate origin (see elsewhere) assumes that the poloidal angle is the polar angle.
  - The user will provide the Fourier harmonics of the boundary, and thus the user will implicitly define the
    poloidal angle used on the boundary.
  - Minimizing the length term will ensure that the poloidal angle used on each interface is smoothly connected to the poloidal angle used on adjacent interfaces.
- A suitable choice of the weight factors,  $\alpha_i$ ,  $\beta_i$ ,  $\gamma_i$  and  $\delta_i$ , will ensure that the polar constraint dominates for the innermost surfaces and that this constraint rapidly becomes insignificant away from the origin; that the minimal spectral constraint dominates in the "middle"; and that the minimizing length constraint will be significant near the origin and dominant near the edge, so that the minimizing spectral width angle will be continuously connected to the polar angle on the innermost surfaces and the user-implied angle at the plasma boundary. The length constraint should not be insignificant where the spectral constraint is dominant (so that the m=0 harmonics are constrained).

- The polar constraint does not need normalization. The spectral width constraint has already been normalized. The length constraint is not yet normalized, but perhaps it should be.
- The spectral constraints given in Eqn. (83) need to be differentiated with respect to the interface Fourier harmonics,  $R_{j,i}$  and  $Z_{j,i}$ . The first and second terms lead to a block diagonal hessian, and the length term leads to a block tri-diagonal hessian.
- Including the poloidal-angle origin constraint means that the polar angle constraint can probably be ignored, i.e.  $\alpha_i=0$ .

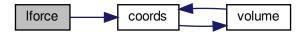
#### **Parameters**

in	Ivol	
in	iocons	
in	ideriv	
in	Ntz	
	dBB	
	XX	
	YY	
	length	
	DDI	
	MMI	
in	iflag	

References inputlist::adiabatic, allglobal::ate, allglobal::ato, allglobal::aze, allglobal::aze, allglobal::aze, allglobal::bemn, allglobal::bemn, allglobal::comn, coords(), allglobal::cpus, allglobal::drij, allglobal::dzij, allglobal::efmn, allglobal::efmn, inputlist::gamma, allglobal::guvij, constants::half, allglobal::iemn, inputlist::igeometry, allglobal-:ijimag, allglobal::irij, allglobal::mmj\_comm\_spec, allglobal::myid, allglobal::ncpu, allglobal::notstellsym, allglobal::nt, inputlist::nvol, allglobal::mz, allglobal::odmn, allglobal::odmn, allglobal::odmn, allglobal::regumm, allglobal::rett, allglobal::semn, allglobal::sfmn, allglobal::sg, allglobal::simn, allglobal::somn, allglobal::trij, allglobal::trij, allglobal::ttij, allglobal::ttij, allglobal::ttij, allglobal::ttij, allglobal::ttij, allglobal::ttij, allglobal::ttij, allglobal::yesstellsym, and constants::zero.

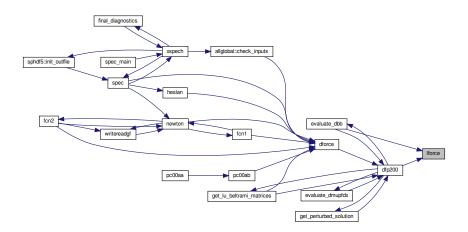
Referenced by dfp200(), and evaluate\_dbb().

Here is the call graph for this function:



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Here is the caller graph for this function:



# 5.9 Integrals

## **Functions/Subroutines**

- subroutine df00ab (pNN, xi, Fxi, DFxi, Ldfjac, iflag)

  Evaluates volume integrals, and their derivatives w.r.t. interface geometry, using "packed" format.
- subroutine ma00aa (Iquad, mn, Ivol, Irad)

Calculates volume integrals of Chebyshev polynomials and metric element products.

• subroutine spsint (Iquad, mn, Ivol, Irad)

Calculates volume integrals of Chebyshev-polynomials and metric elements for preconditioner.

## 5.9.1 Detailed Description

## 5.9.2 Function/Subroutine Documentation

Evaluates volume integrals, and their derivatives w.r.t. interface geometry, using "packed" format.

## **Parameters**

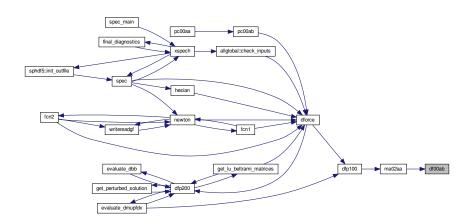
in	pNN	
in	хi	
out	Fxi	
out	DFxi	

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in	iflag		

References allglobal::cpus, allglobal::dma, allglobal::dmd, constants::half, inputlist::helicity, allglobal::mpi\_comm\_spec, allglobal::myid, inputlist::nvol, constants::one, fileunits::ounit, numerical::small, constants::two, and constants::zero.

Referenced by ma02aa().

Here is the caller graph for this function:



# **5.9.2.2 ma00aa()** subroutine ma00aa (

integer, intent(in) lquad,
integer, intent(in) mn,
integer, intent(in) lvol,
integer, intent(in) lrad )

Calculates volume integrals of Chebyshev polynomials and metric element products.

## Chebyshev-metric information

· The following quantities are calculated:

$$\mathsf{DToocc}(\mathsf{l},\mathsf{p},\mathsf{i},\mathsf{j}) \equiv \int ds \, \overline{T}'_{l,i} \, \overline{T}_{p,j} \, \oint \!\!\!\!\! \oint \!\!\! d\theta d\zeta \, \cos\alpha_i \cos\alpha_j \tag{84}$$

$$\mathsf{DToosc}(\mathsf{l},\mathsf{p},\mathsf{i},\mathsf{j}) \equiv \int ds \, \overline{T}'_{l,i} \, \overline{T}_{p,j} \, \oint \!\!\!\!\! \oint \!\!\! d\theta d\zeta \, \sin\alpha_i \cos\alpha_j \tag{86}$$

DTooss(l,p,i,j) 
$$\equiv \int ds \, \overline{T}'_{l,i} \, \overline{T}_{p,j} \, \oint \!\!\!\! \oint \!\!\! d\theta d\zeta \, \sin \alpha_i \sin \alpha_j$$
 (87)

$$\mathsf{TTsscc}(\mathsf{l},\mathsf{p},\mathsf{i},\mathsf{j}) \equiv \int ds \, \overline{T}_{l,i} \, \overline{T}_{p,j} \, \oint \!\!\!\!\! \oint \!\!\! d\theta d\zeta \, \cos\alpha_i \cos\alpha_j \, \bar{g}_{ss} \tag{88}$$

TTsscs(l,p,i,j) 
$$\equiv \int ds \, \overline{T}_{l,i} \, \overline{T}_{p,j} \, \oint \!\!\!\! \oint \!\!\! d\theta d\zeta \, \cos \alpha_i \sin \alpha_j \, \overline{g}_{ss}$$
 (89)

$$\text{TTsssc}(l,p,i,j) \equiv \int ds \, \overline{T}_{l,i} \, \overline{T}_{p,j} \, \oint \!\!\!\! \oint \!\!\! d\theta d\zeta \, \sin\alpha_i \cos\alpha_j \, \bar{g}_{ss} \tag{90}$$

TTssss(l,p,i,j) 
$$\equiv \int ds \, \overline{T}_{l,i} \, \overline{T}_{p,j} \, \oint \!\!\!\! \oint \!\!\! d\theta d\zeta \, \sin \alpha_i \sin \alpha_j \, \bar{g}_{ss}$$
 (91)

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$$\mathsf{TDstcc}(\mathsf{l},\mathsf{p},\mathsf{i},\mathsf{j}) \ \equiv \ \int ds \ \overline{T}_{l,i} \ \overline{T}'_{p,j} \ \phi \phi \, d\theta d\zeta \ \cos\alpha_i \cos\alpha_j \ \overline{g}_{s\theta} \tag{92}$$

TDstcs(l,p,i,j) 
$$\equiv \int ds \, \overline{T}_{l,i} \, \overline{T}'_{p,j} \, \oint \!\!\!\!\! \oint d\theta d\zeta \, \cos \alpha_i \sin \alpha_j \, \bar{g}_{s\theta}$$
 (93)

TDstsc(l,p,i,j) 
$$\equiv \int ds \, \overline{T}_{l,i} \, \overline{T}'_{p,j} \, \oint \!\!\!\! \oint \!\!\! d\theta d\zeta \, \sin \alpha_i \cos \alpha_j \, \overline{g}_{s\theta}$$
 (94)

TDstss(l,p,i,j) 
$$\equiv \int ds \, \overline{T}_{l,i} \, \overline{T}'_{p,j} \, \oint \!\!\!\! \oint \!\!\! d\theta d\zeta \, \sin \alpha_i \sin \alpha_j \, \overline{g}_{s\theta}$$
 (95)

$$\mathsf{TDstcc}(\mathsf{l},\mathsf{p},\mathsf{i},\mathsf{j}) \equiv \int ds \, \overline{T}_{l,i} \, \overline{T}'_{p,j} \, \oint \!\!\!\!\! \oint \!\!\! d\theta d\zeta \, \cos\alpha_i \cos\alpha_j \, \bar{g}_{s\zeta} \tag{96}$$

TDstsc(l,p,i,j) 
$$\equiv \int ds \, \overline{T}_{l,i} \, \overline{T}'_{p,j} \, \phi \!\!\!\!/ \, d\theta d\zeta \, \sin \alpha_i \cos \alpha_j \, \overline{g}_{s\zeta}$$
 (98)

TDstss(l,p,i,j) 
$$\equiv \int ds \, \overline{T}_{l,i} \, \overline{T}'_{p,j} \, \oint \!\!\!\! \int \!\!\!\! d\theta \, d\zeta \, \sin \alpha_i \sin \alpha_j \, \bar{g}_{s\zeta}$$
 (99)

$$\mathrm{DDstcc}(1,\mathbf{p},\mathbf{i},\mathbf{j}) \equiv \int ds \, \overline{T}'_{l,i} \, \overline{T}'_{p,j} \, \oint \!\!\!\!\! \oint \!\!\! d\theta d\zeta \, \cos\alpha_i \cos\alpha_j \, \overline{g}_{\theta\theta} \tag{100}$$

$$\text{DDstcc}(l,p,i,j) \equiv \int ds \, \overline{T}'_{l,i} \, \overline{T}'_{p,j} \, \phi \!\!\!\!/ \, d\theta d\zeta \, \cos \alpha_i \cos \alpha_j \, \overline{g}_{\theta\zeta} \tag{104}$$

$$\text{DDstsc}(1,p,i,j) \equiv \int ds \, \overline{T}'_{l,i} \, \overline{T}'_{p,j} \, \oint \!\!\!\! \oint d\theta d\zeta \, \sin \alpha_i \cos \alpha_j \, \overline{g}_{\theta\zeta} \tag{106}$$

DDstss(l,p,i,j) 
$$\equiv \int ds \, \overline{T}'_{l,i} \, \overline{T}'_{p,j} \, \oint \!\!\!\!\! \oint \!\!\!\! d\theta d\zeta \, \sin \alpha_i \sin \alpha_j \, \bar{g}_{\theta\zeta}$$
 (107)

DDstcs(l,p,i,j) 
$$\equiv \int ds \, \overline{T}'_{l,i} \, \overline{T}'_{p,j} \, \oint \!\!\!\! \oint \!\!\! d\theta d\zeta \, \cos \alpha_i \sin \alpha_j \, \bar{g}_{\zeta\zeta}$$
 (109)

$$\text{DDstsc}(1,p,i,j) \equiv \int ds \, \overline{T}'_{l,i} \, \overline{T}'_{p,j} \, \oint \!\!\!\! \oint \!\! d\theta d\zeta \, \sin \alpha_i \cos \alpha_j \, \overline{g}_{\zeta\zeta} \tag{110}$$

where  $\overline{T}_{l,i} \equiv T_l \, \overline{s}^{m_i/2}$  if the domain includes the coordinate singularity, and  $\overline{T}_{l,i} \equiv T_l$  if not; and  $\overline{g}_{\mu\nu} \equiv g_{\mu\nu}/\sqrt{g}$ .

• The double-angle formulae are used to reduce the above expressions to the Fourier harmonics of  $\bar{g}_{\mu\nu}$ : see kija and kijs, which are defined in preset.f90 .

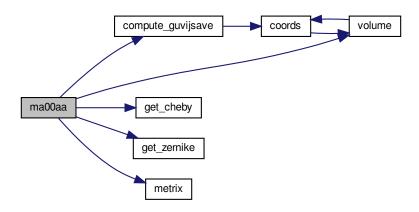
#### **Parameters**

in	Iquad	degree of quadrature
in	mn	number of Fourier harmonics
in	Ivol	index of nested volume
in	Irad	order of Chebychev polynomials

References compute\_guvijsave(), allglobal::cpus, allglobal::dbtx, allglobal::ddttcc, allglobal::ddttcs, allglobal::dtoocc, allglobal::gstmno, allglobal::gstmno, allglobal::gstmno, allglobal::gstmno, allglobal::gstmno, allglobal::gstmno, allglobal::gttmno, allglobal::gttmno, allglobal::gttmno, allglobal::dtoocc, allglobal::dtoocc, allglobal::mne, allglobal::mne

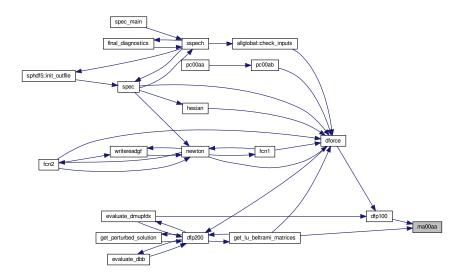
Referenced by dfp100(), and get\_lu\_beltrami\_matrices().

Here is the call graph for this function:



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Here is the caller graph for this function:



Calculates volume integrals of Chebyshev-polynomials and metric elements for preconditioner.

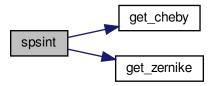
Computes the integrals needed for spsmat.f90. Same as ma00aa.f90, but only compute the relevant terms that are non-zero.

## **Parameters**

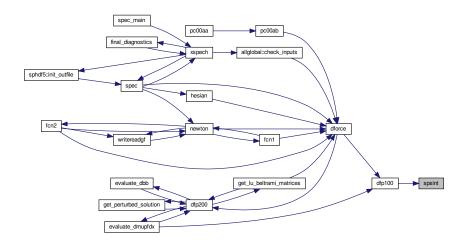
Iquad	
mn	
Ivol	
Irad	

Referenced by dfp100().

Here is the call graph for this function:



Here is the caller graph for this function:



## 5.10 Solver/Driver

## **Functions/Subroutines**

• subroutine ma02aa (Ivol, NN)

Constructs Beltrami field in given volume consistent with flux, helicity, rotational-transform and/or parallel-current constraints.

## 5.10.1 Detailed Description

## 5.10.2 Function/Subroutine Documentation

Constructs Beltrami field in given volume consistent with flux, helicity, rotational-transform and/or parallel-current constraints.

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#### **Parameters**

in	Ivol	index of nested volume for which to run this
in	NN	number of degrees of freedom in the (packed format) vector potential;

# sequential quadratic programming

- Only relevant if LBsequad=T . See LBeltrami for details.
- Documentation on the implementation of E04UFF is under construction.

#### **Newton method**

• Only relevant if LBnewton=T . See LBeltrami for details.

#### linear method

- Only relevant if LBlinear=T . See LBeltrami for details.
- The quantity  $\mu$  is *not* not treated as a "magnetic" degree-of-freedom equivalent to in the degrees-of-freedom in the magnetic vector potential (as it strictly should be, because it is a Lagrange multiplier introduced to enforce the helicity constraint).
- In this case, the Beltrami equation,  $\nabla \times \mathbf{B} = \mu \mathbf{B}$ , is *linear* in the magnetic degrees-of-freedom.
- · The algorithm proceeds as follows:

#### plasma volumes

- In addition to the enclosed toroidal flux,  $\Delta\psi_t$ , which is held constant in the plasma volumes, the Beltrami field in a given volume is assumed to be parameterized by  $\mu$  and  $\Delta\psi_p$ . (Note that  $\Delta\psi_p$  is not defined in a torus.)
- These are "packed" into an array, e.g.  $\mu \equiv (\mu, \Delta \psi_p)^T$ , so that standard library routines , e.g. C05PCF, can be used to (iteratively) find the appropriately-constrained Beltrami solution, i.e.  $\mathbf{f}(\mu) = 0$ .
- The function  $f(\mu)$ , which is computed by mp00ac(), is defined by the input parameter Lconstraint:
  - \* If Lconstraint = -1, 0, then  $\mu$  is not varied and Nxdof=0.
  - \* If Lconstraint = 1, then  $\mu$  is varied to satisfy the transform constraints; and Nxdof=1 in the simple torus and Nxdof=2 in the annular regions. (Note that in the "simple-torus" region, the enclosed poloidal flux  $\Delta \psi_p$  is not well-defined, and only  $\mu=\mu_1$  is varied in order to satisfy the transform constraint on the "outer" interface of that volume.)
  - \* Todo If Lconstraint = 2, then  $\mu=\mu_1$  is varied in order to satisfy the helicity constraint, and  $\Delta\psi_p=\mu_2$  is *not* varied, and Nxdof=1. (under re-construction)

## vacuum volume

- In the vacuum,  $\mu=0$ , and the enclosed fluxes,  $\Delta\psi_t$  and  $\Delta\psi_p$ , are considered to parameterize the family of solutions. (These quantities may not be well-defined if  ${\bf B}\cdot{\bf n}\neq 0$  on the computational boundary.)
- These are "packed" into an array,  $\mu \equiv (\Delta \psi_t, \Delta \psi_p)^T$ , so that, as above, standard routines can be used to iteratively find the appropriately constrained solution, i.e.  $\mathbf{f}(\mu) = 0$ .
- The function  $f(\mu)$ , which is computed by mp00ac(), is defined by the input parameter Lconstraint:
  - \* If Lconstraint = -1, then  $\mu$  is not varied and Nxdof=0.
  - \* If Lconstraint = 0,2, then  $\mu$  is varied to satisfy the enclosed current constraints, and Nxdof=2.

- \* If Lconstraint = 1, then  $\mu$  is varied to satisfy the constraint on the transform on the inner boundary  $\equiv$  plasma boundary and the "linking" current, and Nxdof=2.
- The Beltrami fields, and the rotational-transform and helicity etc. as required to determine the function  $f(\mu)$  are calculated in mp00ac().
- This routine, mp00ac(), is called iteratively if Nxdof>1 via C05PCF to determine the appropriately constrained Beltrami field,  $\mathbf{B}_{\mu}$ , so that  $\mathbf{f}(\mu)=0$ .
- The input variables mupftol and mupfits control the required accuracy and maximum number of iterations.
- If Nxdof=1, then mp00ac() is called only once to provide the Beltrami fields with the given value of  $\mu$ .

## debugging: finite-difference confirmation of the derivatives of the rotational-transform

- Note that the rotational-transform (if required) is calculated by tr00ab(), which is called by mp00ac().
- If Lconstraint=1, then mp00ac() will ask tr00ab() to compute the derivatives of the transform with respect to variations in the helicity-multiplier,  $\mu$ , and the enclosed poloidal-flux,  $\Delta\psi_p$ , so that C05PCF may more efficiently find the solution.
- · The required derivatives are

$$\frac{\partial t}{\partial \mu}$$
 (112)

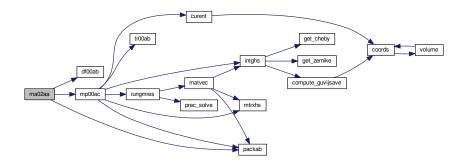
$$\frac{\partial \, \iota}{\partial \Delta \psi_{\nu}} \tag{113}$$

to improve the efficiency of the iterative search. A finite difference estimate of these derivatives is available; need DEBUG, Lcheck=2 and Lconstraint=1.

References allglobal::cpus, df00ab(), constants::half, inputlist::helicity, allglobal::im, allglobal::in, allglobal::lblinear, allglobal::lbsequad, inputlist::lcheck, inputlist::lconstraint, inputlist::lrad, allglobal::mn, mp00ac(), allglobal::mpi\_comm\_spec, inputlist::mu, inputlist::mupfits, inputlist::mupftol, allglobal::myid, allglobal::ncpu, constants::one, fileunits::ounit, packab(), numerical::small, constants::ten, numerical::vsmall, inputlist::wmacros, and constants::zero.

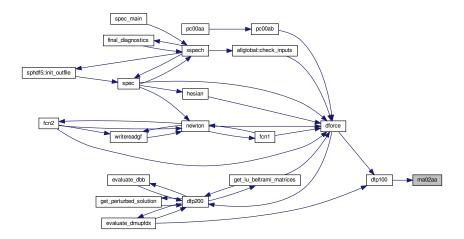
Referenced by dfp100().

Here is the call graph for this function:



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Here is the caller graph for this function:



## 5.11 Build matrices

#### **Functions/Subroutines**

- subroutine matrix (Ivol, mn, Irad)
   Constructs energy and helicity matrices that represent the Beltrami linear system.
   gauge conditions
- subroutine mtrxhs (Ivol, mn, Irad, resultA, resultD, idx)
   Constructs matrices that represent the Beltrami linear system, matrix-free.
- subroutine spsmat (Ivol, mn, Irad)

Constructs matrices for the precondtioner.

# 5.11.1 Detailed Description

## 5.11.2 Function/Subroutine Documentation

Constructs energy and helicity matrices that represent the Beltrami linear system.

## gauge conditions

• In the v-th annulus, bounded by the (v-1)-th and v-th interfaces, a general covariant representation of the magnetic vector-potential is written

$$\bar{\mathbf{A}} = \bar{A}_s \nabla s + \bar{A}_\theta \nabla \theta + \bar{A}_\zeta \nabla \zeta eta. \tag{114}$$

• To this add  $\nabla g(s, \theta, \zeta)$ , where g satisfies

$$\begin{array}{lcl} \partial_s g(s,\theta,\zeta) & = & - & \bar{A}_s(s,\theta,\zeta) \\ \partial_\theta g(-1,\theta,\zeta) & = & - & \bar{A}_\theta(-1,\theta,\zeta) \\ \partial_\zeta g(-1,0,\zeta) & = & - & \bar{A}_\zeta(-1,0,\zeta). \end{array} \tag{115}$$

• Then  $\mathbf{A} = \bar{\mathbf{A}} + \nabla g$  is given by  $\mathbf{A} = A_{\theta} \nabla \theta + A_{\zeta} \nabla \zeta$  with

$$A_{\theta}(-1,\theta,\zeta) = 0 \tag{116}$$

$$A_{\zeta}(-1,0,\zeta) = 0 \tag{117}$$

- This specifies the gauge: to see this, notice that no gauge term can be added without violating the conditions in Eqn. (116) or Eqn. (117).
- · Note that the gauge employed in each volume is distinct.

## boundary conditions

- The magnetic field is  $\sqrt{g} \mathbf{B} = (\partial_{\theta} A_{\zeta} \partial_{\zeta} A_{\theta}) \mathbf{e}_{s} \partial_{s} A_{\zeta} \mathbf{e}_{\theta} + \partial_{s} A_{\theta} \mathbf{e}_{\zeta}$ .
- In the annular volumes, the condition that the field is tangential to the inner interface,  $\sqrt{g}\mathbf{B}\cdot\nabla s=0$  at s=-1, gives  $\partial_{\theta}A_{\zeta}-\partial_{\zeta}A_{\theta}=0$ . With the above condition on  $A_{\theta}$  given in Eqn. (116), this gives  $\partial_{\theta}A_{\zeta}=0$ , which with Eqn. (117) gives

$$A_{\zeta}(-1,\theta,\zeta) = 0. \tag{118}$$

• The condition at the outer interface, s=+1, is that the field is  $\sqrt{g}\,\mathbf{B}\cdot\nabla s=\partial_{\theta}A_{\zeta}-\partial_{\zeta}A_{\theta}=b$ , where b is supplied by the user. For each of the plasma regions, b=0. For the vacuum region, generally  $b\neq 0$ .

### enclosed fluxes

- In the plasma regions, the enclosed fluxes must be constrained.
- · The toroidal and poloidal fluxes enclosed in each volume are determined using

$$\int_{S} \mathbf{B} \cdot \mathbf{ds} = \int_{\partial S} \mathbf{A} \cdot \mathbf{dl}.$$
 (119)

## Fourier-Chebyshev representation

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

$$A_{\theta}(s,\theta,\zeta) = \sum_{i,l} A_{\theta,e,i,l} \, \overline{T}_{l,i}(s) \cos \alpha_i + \sum_{i,l} A_{\theta,o,i,l} \, \overline{T}_{l,i}(s) \sin \alpha_i, \tag{120}$$

$$A_{\zeta}(s,\theta,\zeta) = \sum_{i,l} A_{\zeta,e,i,l} \, \overline{T}_{l,i}(s) \cos \alpha_i + \sum_{i,l} A_{\zeta,o,i,l} \, \overline{T}_{l,i}(s) \sin \alpha_i, \tag{121}$$

where  $\overline{T}_{l,i}(s)$  is the **recombined** Chebyshev polynomial in a volume without an axis, or **modified** Zernike polynomial in a volume with an axis (i.e. only in the innermost volume, and only in cylindrical and toroidal geometry.), and  $\alpha_j \equiv m_j \theta - n_j \zeta$ .

• 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

$$\sqrt{g} \mathbf{B} = \mathbf{e}_{s} \sum_{i,l} \left[ ( -m_{i} A_{\zeta,e,i,l} - n_{i} A_{\theta,e,i,l} ) \overline{T}_{l,i} \sin \alpha_{i} + ( +m_{i} A_{\zeta,o,i,l} + n_{i} A_{\theta,o,i,l} ) \overline{T}_{l,i} \cos \alpha_{i} \right] 
+ \mathbf{e}_{\theta} \sum_{i,l} \left[ ( -A_{\theta,e,i,l} ) \overline{T}'_{l,i} \cos \alpha_{i} + ( -A_{\zeta,o,i,l} ) \overline{T}'_{l,i} \sin \alpha_{i} \right] (122) 
+ \mathbf{e}_{\zeta} \sum_{i,l} \left[ ( -A_{\theta,e,i,l} ) \overline{T}'_{l,i} \cos \alpha_{i} + ( -A_{\theta,o,i,l} ) \overline{T}'_{l,i} \sin \alpha_{i} \right]$$

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• The components of the velocity,  $\mathbf{v} \equiv v_s \nabla s + v_\theta \nabla \theta + v_\zeta \nabla \zeta eta$ , are

$$v_s(s,\theta,\zeta) = \sum_{i,l} \frac{v_{s,e,i,l}}{T_{l,i}(s)} \cos \alpha_i + \sum_{i,l} \frac{v_{s,o,i,l}}{T_{l,i}(s)} \sin \alpha_i, \tag{123}$$

$$v_{\theta}(s,\theta,\zeta) = \sum_{i,l} v_{\theta,e,i,l} \, \overline{T}_{l,i}(s) \cos \alpha_i + \sum_{i,l} v_{\theta,o,i,l} \, \overline{T}_{l,i}(s) \sin \alpha_i, \tag{124}$$

$$v_{\zeta}(s,\theta,\zeta) = \sum_{i,l} v_{\zeta,e,i,l} \, \overline{T}_{l,i}(s) \cos \alpha_i + \sum_{i,l} v_{\zeta,o,i,l} \, \overline{T}_{l,i}(s) \sin \alpha_i. \tag{125}$$

#### constrained energy functional

 The constrained energy functional in each volume depends on the vector potential and the Lagrange multipliers,

$$\mathcal{F} \equiv \mathcal{F}[A_{\theta,e,i,l},A_{\zeta,e,i,l},A_{\theta,o,i,l},A_{\zeta,o,i,l},v_{s,e,i,l},v_{s,o,i,l},v_{\theta,e,i,l},v_{\theta,o,i,l},v_{\zeta,e,i,l},v_{\zeta,o,i,l},\mu,a_i,b_i,c_i,d_i,e_i,f_i,g_1,h_1], (126)$$
 and is given by:

$$\mathcal{F} \equiv \int \mathbf{B} \cdot \mathbf{B} \, dv + \int \mathbf{v} \cdot \mathbf{v} \, dv - \mu \left[ \int \mathbf{A} \cdot \mathbf{B} \, dv - K \right]$$

$$+ \sum_{i=1}^{n} a_{i} \left[ \sum_{l} A_{\theta,e,i,l} T_{l}(-1) - 0 \right]$$

$$+ \sum_{i=1}^{n} b_{i} \left[ \sum_{l} A_{\zeta,e,i,l} T_{l}(-1) - 0 \right]$$

$$+ \sum_{i=2}^{n} c_{i} \left[ \sum_{l} A_{\theta,o,i,l} T_{l}(-1) - 0 \right]$$

$$+ \sum_{i=2}^{n} d_{i} \left[ \sum_{l} A_{\zeta,o,i,l} T_{l}(-1) - 0 \right]$$

$$+ \sum_{i=2}^{n} d_{i} \left[ \sum_{l} (-m_{i}A_{\zeta,e,i,l} - n_{i}A_{\theta,e,i,l}) T_{l}(+1) - b_{s,i} \right]$$

$$+ \sum_{i=2}^{n} f_{i} \left[ \sum_{l} (+m_{i}A_{\zeta,o,i,l} + n_{i}A_{\theta,o,i,l}) T_{l}(+1) - b_{c,i} \right]$$

$$+ \sum_{l=2}^{n} A_{\theta,e,1,l} T_{l}(+1) - \Delta \psi_{t}$$

$$+ \sum_{l} A_{\xi,e,1,l} T_{l}(+1) + \Delta \psi_{p}$$

where

- $-a_i, b_i, c_i$  and  $d_i$  are Lagrange multipliers used to enforce the combined gauge and interface boundary condition on the inner interface,
- $e_i$  and  $f_i$  are Lagrange multipliers used to enforce the interface boundary condition on the outer interface, namely  $\sqrt{g}\,{f B}\cdot\nabla s=b$ ; and
- $g_1$  and  $h_1$  are Lagrange multipliers used to enforce the constraints on the enclosed fluxes.
- In each plasma volume the boundary condition on the outer interface is b=0.
- In the vacuum volume (only for free-boundary), we may set  $\mu = 0$ .
- **Note:** in SPEC version >3.00, the basis recombination method is used to ensure the boundary condition on the inner side of an interface. The lagrange multipliers  $a_i, b_i, c_i, d_i$  are no longer used in volumes without a coordinate singularity. In a volume with a coordinate singularity, they are used only  $a_i, c_i$  with \$m=0,1\$ are excluded also due to Zernike basis recombination.

#### derivatives of magnetic energy integrals

• The first derivatives of  $\int dv \ \mathbf{B} \cdot \mathbf{B}$  with respect to  $A_{\theta,e,i,l}, A_{\theta,o,i,l}, A_{\zeta,e,i,l}$  and  $A_{\zeta,o,i,l}$  are

$$\begin{split} &\frac{\partial}{\partial A_{\theta,e,i,l}} \int\!\! dv \; \mathbf{B} \cdot \mathbf{B} &= 2 \int\!\! dv \; \mathbf{B} \cdot \frac{\partial \mathbf{B}}{\partial A_{\theta,e,i,l}} = 2 \int\!\! dv \; \mathbf{B} \cdot \left[ -n_i \overline{T}_{l,i} \sin \alpha_i \, \mathbf{e}_s + \overline{T}'_{l,i} \cos \alpha_i \, \mathbf{e}_\zeta \right] / \sqrt{N_c} \mathbf{B}) \\ &\frac{\partial}{\partial A_{\theta,o,i,l}} \int\!\! dv \; \mathbf{B} \cdot \mathbf{B} &= 2 \int\!\! dv \; \mathbf{B} \cdot \frac{\partial \mathbf{B}}{\partial A_{\theta,o,i,l}} = 2 \int\!\! dv \; \mathbf{B} \cdot \left[ +n_i \overline{T}_{l,i} \cos \alpha_i \, \mathbf{e}_s + \overline{T}'_{l,i} \sin \alpha_i \, \mathbf{e}_\zeta \right] / \sqrt{N_c} \mathbf{P}) \\ &\frac{\partial}{\partial A_{\zeta,e,i,l}} \int\!\! dv \; \mathbf{B} \cdot \mathbf{B} &= 2 \int\!\! dv \; \mathbf{B} \cdot \frac{\partial \mathbf{B}}{\partial A_{\zeta,e,i,l}} = 2 \int\!\! dv \; \mathbf{B} \cdot \left[ -m_i \overline{T}_{l,i} \sin \alpha_i \, \mathbf{e}_s - \overline{T}'_{l,i} \cos \alpha_i \, \mathbf{e}_\theta \right] / \sqrt{N_c} \mathbf{P}) \\ &\frac{\partial}{\partial A_{\zeta,o,i,l}} \int\!\! dv \; \mathbf{B} \cdot \mathbf{B} &= 2 \int\!\! dv \; \mathbf{B} \cdot \frac{\partial \mathbf{B}}{\partial A_{\zeta,o,i,l}} = 2 \int\!\! dv \; \mathbf{B} \cdot \left[ +m_i \overline{T}_{l,i} \cos \alpha_i \, \mathbf{e}_s - \overline{T}'_{l,i} \sin \alpha_i \, \mathbf{e}_\theta \right] / \sqrt{N_c} \mathbf{P}) \end{split}$$

• The second derivatives of  $\int dv \, \mathbf{B} \cdot \mathbf{B}$  with respect to  $A_{\theta,e,i,l}$ ,  $A_{\theta,o,i,l}$ ,  $A_{\zeta,e,i,l}$  and  $A_{\zeta,o,i,l}$  are

$$\frac{\partial}{\partial A_{\theta,e,j,p}} \frac{\partial}{\partial A_{\theta,e,i,l}} \int dv \ \mathbf{B} \cdot \mathbf{B} = 2 \int dv \ (+n_j n_i \overline{T}_{p,j} \overline{T}_{l,i} s_j s_i g_{ss} - n_j \overline{T}_{p,j} \overline{T}'_{l,i} s_j c_i g_{s\zeta} - n_i \overline{T}_{l,i} \overline{T}'_{p,j} s_i c_j g_{s\zeta} + \overline{T}'_{p,j} \overline{T}'_{l,i} c_j c_i g_{\zeta\zeta}) / \sqrt{\partial \partial A_{\theta,e,i,l}} \int dv \ \mathbf{B} \cdot \mathbf{B} = 2 \int dv \ (-n_j n_i \overline{T}_{p,j} \overline{T}_{l,i} c_j s_i g_{ss} + n_j \overline{T}_{p,j} \overline{T}'_{l,i} c_j c_i g_{s\zeta} - n_i \overline{T}_{l,i} \overline{T}'_{p,j} s_i s_j g_{s\zeta} + \overline{T}'_{p,j} \overline{T}'_{l,i} s_j c_i g_{\zeta\zeta}) / \sqrt{\partial \partial A_{\theta,e,i,l}} \int dv \ \mathbf{B} \cdot \mathbf{B} = 2 \int dv \ (+m_j n_i \overline{T}_{p,j} \overline{T}_{l,i} s_j s_i g_{ss} - m_j \overline{T}_{p,j} \overline{T}'_{l,i} s_j c_i g_{s\zeta} + n_i \overline{T}_{l,i} \overline{T}'_{p,j} s_i c_j g_{s\theta} - \overline{T}'_{p,j} \overline{T}'_{l,i} c_j c_i g_{\theta\zeta}) / \sqrt{\partial \partial A_{\theta,e,i,l}} \int dv \ \mathbf{B} \cdot \mathbf{B} = 2 \int dv \ (-m_j n_i \overline{T}_{p,j} \overline{T}_{l,i} c_j s_i g_{ss} + m_j \overline{T}_{p,j} \overline{T}'_{l,i} c_j c_i g_{s\zeta} + n_i \overline{T}_{l,i} \overline{T}'_{p,j} s_i s_j g_{s\theta} - \overline{T}'_{p,j} \overline{T}'_{l,i} s_j c_i g_{\theta\zeta}) / \sqrt{\partial \partial A_{\theta,e,i,l}} \int dv \ \mathbf{B} \cdot \mathbf{B} = 2 \int dv \ (-n_j n_i \overline{T}_{p,j} \overline{T}_{l,i} s_j c_i g_{ss} - n_j \overline{T}_{p,j} \overline{T}'_{l,i} s_j s_i g_{s\zeta} + n_i \overline{T}_{l,i} \overline{T}'_{p,j} c_i c_j g_{s\zeta} + \overline{T}'_{p,j} \overline{T}'_{l,i} c_j s_i g_{\zeta\zeta}) / \sqrt{\partial \partial A_{\theta,e,i,l}} \int dv \ \mathbf{B} \cdot \mathbf{B} = 2 \int dv \ (-n_j n_i \overline{T}_{p,j} \overline{T}_{l,i} s_j c_i g_{ss} - n_j \overline{T}_{p,j} \overline{T}'_{l,i} s_j s_i g_{s\zeta} + n_i \overline{T}_{l,i} \overline{T}'_{p,j} c_i c_j g_{s\zeta} + \overline{T}'_{p,j} \overline{T}'_{l,i} c_j s_i g_{\zeta\zeta}) / \sqrt{\partial \partial A_{\theta,e,i,l}} \int dv \ \mathbf{B} \cdot \mathbf{B} = 2 \int dv \ (-n_j n_i \overline{T}_{p,j} \overline{T}_{l,i} c_j c_i g_{ss} + n_j \overline{T}_{p,j} \overline{T}'_{l,i} c_j s_i g_{s\zeta} + n_i \overline{T}_{l,i} \overline{T}'_{p,j} c_i c_j g_{s\zeta} + \overline{T}'_{p,j} \overline{T}'_{l,i} c_j s_i g_{\zeta\zeta}) / \sqrt{\partial \partial A_{\theta,e,i,l}} \int dv \ \mathbf{B} \cdot \mathbf{B} = 2 \int dv \ (-n_j n_i \overline{T}_{p,j} \overline{T}_{l,i} c_j c_i g_{ss} - m_j \overline{T}_{p,j} \overline{T}'_{l,i} c_j s_i g_{s\zeta} - n_i \overline{T}_{l,i} \overline{T}'_{p,j} c_i c_j g_{s\theta} - \overline{T}'_{p,j} \overline{T}'_{l,i} c_j s_i g_{\theta\zeta}) / \sqrt{\partial \partial A_{\theta,e,i,l}} \int dv \ \mathbf{B} \cdot \mathbf{B} = 2 \int dv \ (-n_j n_i \overline{T}_{p,j} \overline{T}_{l,i} c_j c_i g_{ss} - m_j \overline{T}_{p,j} \overline{T}'_{l,i} c_j s_i g_{s\zeta} - n_i \overline{T}_{l,i} \overline{T}'_{p,j} c_i c_j g_{s\theta} - \overline{T}'_{p,j} \overline$$

$$\frac{\partial}{\partial A_{\theta,e,j,p}} \frac{\partial}{\partial A_{\zeta,e,i,l}} \int dv \ \mathbf{B} \cdot \mathbf{B} = 2 \int dv \left( +n_j m_i \overline{T}_{p,j} \overline{T}_{l,i} s_j s_i g_{ss} + n_j \overline{T}_{p,j} \overline{T}'_{l,i} s_j c_i g_{s\theta} - m_i \overline{T}_{l,i} \overline{T}'_{p,j} s_i c_j g_{s\zeta} - \overline{T}'_{p,j} \overline{T}'_{l,i} c_j c_i g_{\theta\zeta} \right) / dv$$

$$\frac{\partial}{\partial A_{\theta,o,j,p}} \frac{\partial}{\partial A_{\zeta,e,i,l}} \int dv \ \mathbf{B} \cdot \mathbf{B} = 2 \int dv \left( -n_j m_i \overline{T}_{p,j} \overline{T}_{l,i} c_j s_i g_{ss} - n_j \overline{T}_{p,j} \overline{T}'_{l,i} c_j c_i g_{s\theta} - m_i \overline{T}_{l,i} \overline{T}'_{p,j} s_i s_j g_{s\zeta} - \overline{T}'_{p,j} \overline{T}'_{l,i} s_j c_i g_{\theta\zeta} \right) / dv$$

$$\frac{\partial}{\partial A_{\zeta,e,j,p}} \frac{\partial}{\partial A_{\zeta,e,i,l}} \int dv \ \mathbf{B} \cdot \mathbf{B} = 2 \int dv \left( +m_j m_i \overline{T}_{p,j} \overline{T}_{l,i} s_j s_i g_{ss} + m_j \overline{T}_{p,j} \overline{T}'_{l,i} s_j c_i g_{s\theta} + m_i \overline{T}_{l,i} \overline{T}'_{p,j} s_i c_j g_{s\theta} + \overline{T}'_{p,j} \overline{T}'_{l,i} c_j c_i g_{\theta\theta} \right) / dv$$

$$\frac{\partial}{\partial A_{\zeta,e,i,l}} \frac{\partial}{\partial A_{\zeta,e,i,l}} \int dv \ \mathbf{B} \cdot \mathbf{B} = 2 \int dv \left( -m_j m_i \overline{T}_{p,j} \overline{T}_{l,i} c_j s_i g_{ss} - m_j \overline{T}_{p,j} \overline{T}'_{l,i} c_j c_i g_{s\theta} + m_i \overline{T}_{l,i} \overline{T}'_{p,j} s_i s_j g_{s\theta} + \overline{T}'_{p,j} \overline{T}'_{l,i} s_j c_i g_{\theta\theta} \right) / dv$$

$$\frac{\partial}{\partial A_{\theta,e,j,p}} \frac{\partial}{\partial A_{\zeta,o,i,l}} \int dv \, \mathbf{B} \cdot \mathbf{B} = 2 \int dv \, (-n_j m_i \overline{T}_{p,j} \overline{T}_{l,i} s_j c_i g_{ss} + n_j \overline{T}_{p,j} \overline{T}'_{l,i} s_j s_i g_{s\theta} + m_i \overline{T}_{l,i} \overline{T}'_{p,j} c_i c_j g_{s\zeta} - \overline{T}'_{p,j} \overline{T}'_{l,i} c_j s_i g_{\theta\zeta}) / \frac{\partial}{\partial A_{\theta,o,j,p}} \frac{\partial}{\partial A_{\zeta,o,i,l}} \int dv \, \mathbf{B} \cdot \mathbf{B} = 2 \int dv \, (+n_j m_i \overline{T}_{p,j} \overline{T}_{l,i} c_j c_i g_{ss} - n_j \overline{T}_{p,j} \overline{T}'_{l,i} c_j s_i g_{s\theta} + m_i \overline{T}_{l,i} \overline{T}'_{p,j} c_i s_j g_{s\zeta} - \overline{T}'_{p,j} \overline{T}'_{l,i} s_j s_i g_{\theta\zeta}) / \frac{\partial}{\partial A_{\zeta,o,i,l}} \int dv \, \mathbf{B} \cdot \mathbf{B} = 2 \int dv \, (-m_j m_i \overline{T}_{p,j} \overline{T}_{l,i} s_j c_i g_{ss} + m_j \overline{T}_{p,j} \overline{T}'_{l,i} s_j s_i g_{s\theta} - m_i \overline{T}_{l,i} \overline{T}'_{p,j} c_i c_j g_{s\theta} + \overline{T}'_{p,j} \overline{T}'_{l,i} c_j s_i g_{\theta\theta}) / \frac{\partial}{\partial A_{\zeta,o,i,l}} \int dv \, \mathbf{B} \cdot \mathbf{B} = 2 \int dv \, (+m_j m_i \overline{T}_{p,j} \overline{T}_{l,i} c_j c_i g_{ss} - m_j \overline{T}_{p,j} \overline{T}'_{l,i} c_j s_i g_{s\theta} - m_i \overline{T}_{l,i} \overline{T}'_{p,j} c_i s_j g_{s\theta} + \overline{T}'_{p,j} \overline{T}'_{l,i} s_j s_i g_{\theta\theta}) / \frac{\partial}{\partial A_{\zeta,o,i,l}} \int dv \, \mathbf{B} \cdot \mathbf{B} = 2 \int dv \, (+m_j m_i \overline{T}_{p,j} \overline{T}_{l,i} c_j c_i g_{ss} - m_j \overline{T}_{p,j} \overline{T}'_{l,i} c_j s_i g_{s\theta} - m_i \overline{T}_{l,i} \overline{T}'_{p,j} c_i s_j g_{s\theta} + \overline{T}'_{p,j} \overline{T}'_{l,i} s_j s_i g_{\theta\theta}) / \frac{\partial}{\partial A_{\zeta,o,i,l}} \int dv \, \mathbf{B} \cdot \mathbf{B} = 2 \int dv \, (+m_j m_i \overline{T}_{p,j} \overline{T}_{l,i} c_j c_i g_{ss} - m_j \overline{T}_{p,j} \overline{T}'_{l,i} c_j s_i g_{s\theta} - m_i \overline{T}_{l,i} \overline{T}'_{p,j} c_i s_j g_{s\theta} + \overline{T}'_{p,j} \overline{T}'_{l,i} s_j s_i g_{\theta\theta}) / \frac{\partial}{\partial A_{\zeta,o,i,l}} \int dv \, \mathbf{B} \cdot \mathbf{B} = 2 \int dv \, (+m_j m_i \overline{T}_{p,j} \overline{T}_{l,i} c_j c_i g_{ss} - m_j \overline{T}_{p,j} \overline{T}'_{l,i} c_j s_i g_{s\theta} - m_i \overline{T}_{l,i} \overline{T}'_{p,j} c_i s_j g_{s\theta} + \overline{T}'_{p,j} \overline{T}'_{l,i} s_j s_i g_{\theta\theta}) / \frac{\partial}{\partial A_{\zeta,o,i,l}} \int dv \, \mathbf{B} \cdot \mathbf{B} = 2 \int dv \, (+m_j m_i \overline{T}_{p,j} \overline{T}_{l,i} c_j c_i g_{ss} - m_j \overline{T}_{p,j} \overline{T}'_{l,i} c_j s_i g_{s\theta} - m_i \overline{T}_{l,i} \overline{T}'_{p,j} c_i s_j g_{s\theta} + \overline{T}'_{p,j} \overline{T}'_{l,i} s_j s_i g_{\theta\theta}) / \frac{\partial}{\partial A_{\zeta,o,i,l}} \int dv \, \mathbf{B} \cdot \mathbf{B} + \mathbf{B} \cdot \mathbf{B} + \mathbf{B} \cdot \mathbf{B} + \mathbf{B} \cdot \mathbf{B} \cdot \mathbf{B} \cdot \mathbf{B} + \mathbf{B} \cdot \mathbf{B} \cdot \mathbf{B} \cdot \mathbf{B} \cdot \mathbf{B} \cdot \mathbf{B} + \mathbf{B} \cdot \mathbf{B} \cdot \mathbf{B} \cdot \mathbf{B} \cdot \mathbf{B}$$

# derivatives of helicity integrals

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• The first derivatives of  $\int dv \ \mathbf{A} \cdot \mathbf{B}$  with respect to  $A_{\theta,e,i,l}$ ,  $A_{\theta,o,i,l}$ ,  $A_{\zeta,e,i,l}$  and  $A_{\zeta,o,i,l}$  are

$$\frac{\partial}{\partial A_{\theta,e,i,l}} \int dv \, \mathbf{A} \cdot \mathbf{B} = \int dv \, \left( \frac{\partial \mathbf{A}}{\partial A_{\theta,e,i,l}} \cdot \mathbf{B} + \mathbf{A} \cdot \frac{\partial \mathbf{B}}{\partial A_{\theta,e,i,l}} \right) = \int dv \, \left( \overline{T}_{l,i} \cos \alpha_i \nabla \theta \cdot \mathbf{B} + \mathbf{A} \cdot \overline{T}'_{l,i} \cos \alpha_i \, \mathbf{e}_{\zeta} \right) \left( \sqrt{3} \right) dv \, \mathbf{A} \cdot \mathbf{B} = \int dv \, \left( \frac{\partial \mathbf{A}}{\partial A_{\theta,o,i,l}} \cdot \mathbf{B} + \mathbf{A} \cdot \frac{\partial \mathbf{B}}{\partial A_{\theta,o,i,l}} \right) = \int dv \, \left( \overline{T}_{l,i} \sin \alpha_i \nabla \theta \cdot \mathbf{B} + \mathbf{A} \cdot \overline{T}'_{l,i} \sin \alpha_i \, \mathbf{e}_{\zeta} \right) \left( \sqrt{3} \right) dv \, \mathbf{A} \cdot \mathbf{B} = \int dv \, \left( \frac{\partial \mathbf{A}}{\partial A_{\zeta,e,i,l}} \cdot \mathbf{B} + \mathbf{A} \cdot \frac{\partial \mathbf{B}}{\partial A_{\zeta,e,i,l}} \right) = \int dv \, \left( \overline{T}_{l,i} \cos \alpha_i \nabla \zeta \cdot \mathbf{B} - \mathbf{A} \cdot \overline{T}'_{l,i} \cos \alpha_i \, \mathbf{e}_{\theta} \right) \left( \sqrt{3} \right) dv \, \mathbf{A} \cdot \mathbf{B} = \int dv \, \left( \frac{\partial \mathbf{A}}{\partial A_{\zeta,o,i,l}} \cdot \mathbf{B} + \mathbf{A} \cdot \frac{\partial \mathbf{B}}{\partial A_{\zeta,o,i,l}} \right) = \int dv \, \left( \overline{T}_{l,i} \sin \alpha_i \nabla \zeta \cdot \mathbf{B} - \mathbf{A} \cdot \overline{T}'_{l,i} \sin \alpha_i \, \mathbf{e}_{\theta} \right) \left( \sqrt{3} \right) dv \, \mathbf{A} \cdot \mathbf{B} = \int dv \, \left( \frac{\partial \mathbf{A}}{\partial A_{\zeta,o,i,l}} \cdot \mathbf{B} + \mathbf{A} \cdot \frac{\partial \mathbf{B}}{\partial A_{\zeta,o,i,l}} \right) = \int dv \, \left( \overline{T}_{l,i} \sin \alpha_i \nabla \zeta \cdot \mathbf{B} - \mathbf{A} \cdot \overline{T}'_{l,i} \sin \alpha_i \, \mathbf{e}_{\theta} \right) \left( \sqrt{3} \right) dv \, \mathbf{A} \cdot \mathbf{B} = \int dv \, \left( \frac{\partial \mathbf{A}}{\partial A_{\zeta,o,i,l}} \cdot \mathbf{B} + \mathbf{A} \cdot \frac{\partial \mathbf{B}}{\partial A_{\zeta,o,i,l}} \right) = \int dv \, \left( \overline{T}_{l,i} \sin \alpha_i \nabla \zeta \cdot \mathbf{B} - \mathbf{A} \cdot \overline{T}'_{l,i} \sin \alpha_i \, \mathbf{e}_{\theta} \right) \left( \sqrt{3} \right) dv \, \mathbf{A} \cdot \mathbf{B} = \int dv \, \left( \frac{\partial \mathbf{A}}{\partial A_{\zeta,o,i,l}} \cdot \mathbf{B} + \mathbf{A} \cdot \frac{\partial \mathbf{B}}{\partial A_{\zeta,o,i,l}} \right) = \int dv \, \left( \overline{T}_{l,i} \sin \alpha_i \nabla \zeta \cdot \mathbf{B} - \mathbf{A} \cdot \overline{T}'_{l,i} \sin \alpha_i \, \mathbf{e}_{\theta} \right) \left( \sqrt{3} \right) dv \, \mathbf{A} \cdot \mathbf{B} = \int dv \, \left( \frac{\partial \mathbf{A}}{\partial A_{\zeta,o,i,l}} \cdot \mathbf{B} + \mathbf{A} \cdot \frac{\partial \mathbf{B}}{\partial A_{\zeta,o,i,l}} \right) = \int dv \, \left( \overline{T}_{l,i} \sin \alpha_i \nabla \zeta \cdot \mathbf{B} - \mathbf{A} \cdot \overline{T}'_{l,i} \sin \alpha_i \, \mathbf{e}_{\theta} \right) \left( \sqrt{3} \right) dv \, \mathbf{A} \cdot \mathbf{B} = \int dv \, \left( \overline{T}_{l,i} \sin \alpha_i \nabla \zeta \cdot \mathbf{B} - \mathbf{A} \cdot \overline{T}'_{l,i} \sin \alpha_i \nabla \zeta \cdot \mathbf{B} \right) dv \, \mathbf{A} \cdot \mathbf{B} + \mathbf{A} \cdot \overline{T}'_{l,i} \sin \alpha_i \nabla \zeta \cdot \mathbf{B} \right) dv \, \mathbf{A} \cdot \mathbf{B} = \int dv \, \left( \overline{T}_{l,i} \sin \alpha_i \nabla \zeta \cdot \mathbf{B} \right) dv \, \mathbf{A} \cdot \mathbf{B} + \mathbf{A} \cdot \overline{T}_{l,i} \sin \alpha_i \nabla \zeta \cdot \mathbf{B} + \mathbf{A} \cdot \overline{T}'_{l,i} \sin \alpha_i \nabla \zeta \cdot \mathbf{B} \right) dv \, \mathbf{A} \cdot \mathbf{B} + \mathbf{A} \cdot \overline{T}_{l,i} \sin \alpha_i \nabla \zeta \cdot \mathbf{B} + \mathbf{A} \cdot \overline{T}_{l,i} \sin \alpha_i \nabla \zeta \cdot \mathbf{B} \right) dv \, \mathbf{A} \cdot \mathbf{B} + \mathbf{A} \cdot \mathbf{A} \cdot \mathbf{B} + \mathbf{A} \cdot \mathbf{A} \cdot \mathbf{B} \cdot \mathbf{B} + \mathbf{A} \cdot \mathbf{A} \cdot \mathbf{B} + \mathbf{A} \cdot$$

- Note that in the above expressions,  $\mathbf{A} \cdot \mathbf{e}_s = 0$  has been used.
- The second derivatives of  $\int dv \ \mathbf{A} \cdot \mathbf{B}$  with respect to  $A_{\theta,e,i,l}$ ,  $A_{\theta,o,i,l}$ ,  $A_{\zeta,e,i,l}$  and  $A_{\zeta,o,i,l}$  are

• In these expressions the terms  $\nabla \theta \cdot \mathbf{e}_{\theta} = \nabla \zeta \cdot \mathbf{e}_{\zeta} = 1$ , and  $\nabla \theta \cdot \mathbf{e}_{\zeta} = \nabla \zeta \cdot \mathbf{e}_{\theta} = 0$  have been included to show the structure of the derivation.

## derivatives of kinetic energy integrals

• The first derivatives of  $\int dv \ v^2$  with respect to  $v_{s.e.i.l}$  etc. are

$$\frac{\partial}{\partial v_{s,e,i,l}} \int dv \, \mathbf{v} \cdot \mathbf{v} = 2 \int dv \, \mathbf{v} \cdot \overline{T}_{l,i} \cos \alpha_i \nabla s \tag{152}$$

$$\frac{\partial}{\partial v_{s,o,i,l}} \int dv \, \mathbf{v} \cdot \mathbf{v} = 2 \int dv \, \mathbf{v} \cdot \overline{T}_{l,i} \sin \alpha_i \nabla s$$
 (153)

$$\frac{\partial}{\partial v_{\theta,e,i,l}} \int dv \, \mathbf{v} \cdot \mathbf{v} = 2 \int dv \, \mathbf{v} \cdot \overline{T}_{l,i} \cos \alpha_i \nabla \theta$$
 (154)

$$\frac{\partial}{\partial v_{\theta,o,i,l}} \int dv \, \mathbf{v} \cdot \mathbf{v} = 2 \int dv \, \mathbf{v} \cdot \overline{T}_{l,i} \sin \alpha_i \nabla \theta$$
 (155)

$$\frac{\partial}{\partial v_{\zeta,e,i,l}} \int dv \, \mathbf{v} \cdot \mathbf{v} = 2 \int dv \, \mathbf{v} \cdot \overline{T}_{l,i} \cos \alpha_i \nabla \zeta$$
 (156)

$$\frac{\partial}{\partial v_{\zeta, 0, i, l}} \int dv \, \mathbf{v} \cdot \mathbf{v} = 2 \int dv \, \mathbf{v} \cdot \overline{T}_{l, i} \sin \alpha_i \nabla \zeta \tag{157}$$

(158)

## calculation of volume-integrated basis-function-weighted metric information

• The required geometric information is calculated in ma00aa().

#### **Parameters**

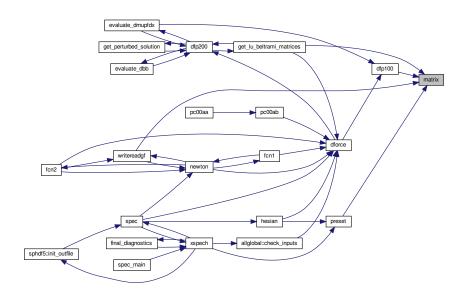
in	Ivol	
in	mn	
in	Irad	

References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::cpus, allglobal::dbdx, allglobal::ddttcc, allglobal::ddttccc, allglobal::ddttccc, allglobal::ddttccc, allglobal::ddttccc, allglobal::ddtcccc, allglobal::inc, allglobal::inc, allglobal::inc, allglobal::inc, allglobal::me, a

Referenced by dfp100(), get lu beltrami matrices(), preset(), and writereadgf().

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Here is the caller graph for this function:



Constructs matrices that represent the Beltrami linear system, matrix-free.

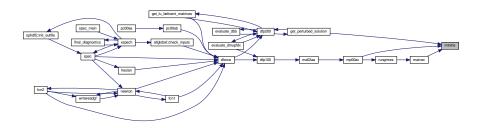
## **Parameters**

Ivol	
mn	
Irad	
resultA	
resultD	
idx	

References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::aze, allglobal::aze, allglobal::cpus, allglobal::dbdx, allglobal::dtc, allglobal::dts, allglobal::dzs, constants::half, allglobal::im, allglobal::in, allglobal::lcoordinatesingularity, allglobal::lma, allglobal::lmavalue, allglobal::lmbvalue, allglobal::lmc, allglobal::lmcvalue, allglobal::lmcvalue, allglobal::lmf, allglobal::lmf, allglobal::lmfvalue, allglobal::lmg, allglobal::lmg, allglobal::lmgvalue, allglobal::lmg, allglobal::lmg, allglobal::lmpvalue, allglobal::mpi\_comm\_spec, inputlist::mpol, allglobal::myid, allglobal::nadof, allglobal::ncpu, allglobal::ntstellsym, constants::one, fileunits::ounit, allglobal::rtm, allglobal::rtm, numerical::small, allglobal::tsc, allglobal::tsc, allglobal::ttc, allglobal::ttc, allglobal::ttc, allglobal::ttc, allglobal::tzc, allglobal::tzs, inputlist::wmacros, allglobal::yesstellsym, and constants::zero.

Referenced by get\_perturbed\_solution(), matvec(), and mp00ac().

Here is the caller graph for this function:



Constructs matrices for the precondtioner.

#### Preconditioner

GMRES iteratively looks for  $\mathbf{a}_n$  that minimises the residual  $\epsilon_{\text{GMRES}} = \|\hat{A} \cdot \mathbf{a}_n - \mathbf{b}\|$ , where  $\|.\|$  is the Euclidean norm. Instead of solving the original problem which is usually ill-conditioned, a left preconditioner matrix  $\mathcal{M}$  is applied on both side of  $\mathcal{A} \cdot \mathbf{a} = \mathbf{b}$  so that the transformed problem is well conditioned. The convergence speed of (the preconditioned) GMRES depends highly on the quality of  $\mathcal{M}$ . A good preconditioner will require the matrix product  $\mathcal{M}^{-1}\hat{\mathcal{A}}$  to be as close as possible to an identity matrix. Also, inverting the preconditioner  $\mathcal{M}$  should be considerably cheaper than inverting  $\hat{\mathcal{A}}$  itself.

If the i-th and j-th unknowns in a correspond to  $A_{\theta,m_i,n_i,l_i}$  and  $A_{\theta,m_j,n_j,l_j}$ , respectively, then the matrix element  $\hat{\mathcal{A}}_{i,j}$  describes the coupling strength between harmonics  $(m_i,n_i)$  and  $(m_j,n_j)$ . Noting that if the Fourier series of the boundary  $R_{m,n}$  and  $Z_{m,n}$  have spectral convergence, then the coupling terms between  $A_{\theta,m_i,n_i,l_i}$  and  $A_{\theta,m_j,n_j,l_j}$ , formed by the  $(|m_i-m_j|,|n_i-n_j|)$  harmonics of the coordinate metrics, should also decay exponentially with  $|m_i-m_j|$  and  $|n_i-n_j|$  and are thus small compared to the 'diagonals"  $m_i=m_j$  and  $n_i=n_j$ . Therefore, we can construct  $\mathcal M$  from the elements of  $\hat{\mathcal A}$  by eliminating all the coupling terms with  $m_i\neq m_j$  or  $n_i\neq n_j$ , and keeping the rest ('diagonals" and terms related to Lagrange mulitpliers). Physically, the matrix  $\mathcal M$  is equivalent to the  $\hat{\mathcal A}$  matrix of a tokamak with similar major radius and minor radius to the stellarator we are solving for. The preconditioning matrix  $\mathcal M$  is sparse, with the number of nonzero elements  $\sim O(MNL^2)$ , while the total number of elements in  $\mathcal M$  is  $O(M^2N^2L^2)$ . After the construction of  $\mathcal M$ , the approximate inverse  $\mathcal M$  is computed by an incomplete LU factorisation.

This subroutine constructs such a preconditioner matrix  $\mathcal{M}$  and store it inside a sparse matrix. The matrix elements are the same as **matrix.f90**, however, only the aforementioned terms are kept. The sparse matrix uses the storage structure of **Compact Sparse Row (CSR)**.

#### **Parameters**

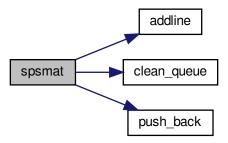
Ivol	
mn	
Irad	

References addline(), clean\_queue(), allglobal::cpus, allglobal::dma, allglobal::dmas, allglobal::dmb, allglobal::dmb, allglobal::dmb, allglobal::dmb, allglobal::dmas, allglobal::im, allglobal::jdmas, allgloba

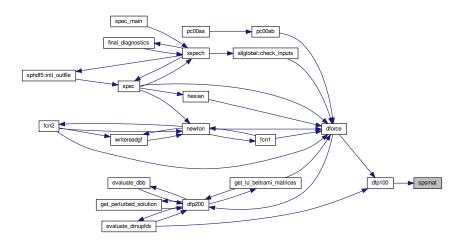
::liluprecond, allglobal::mpi\_comm\_spec, inputlist::mpol, allglobal::myid, allglobal::nadof, allglobal::ncpu, allglobal::ndmas, allglobal::ndmas, allglobal::notstellsym, constants::one, fileunits::ounit, push\_back(), numerical::small, constants::two, inputlist::wmacros, allglobal::yesstellsym, and constants::zero.

Referenced by dfp100().

Here is the call graph for this function:



Here is the caller graph for this function:



# 5.12 Metric quantities

## **Functions/Subroutines**

• subroutine metrix (Iquad, IvoI) Calculates the metric quantities,  $\sqrt{g} \ g^{\mu\nu}$ , which are required for the energy and helicity integrals.

# 5.12.1 Detailed Description

# 5.12.2 Function/Subroutine Documentation

Calculates the metric quantities,  $\sqrt{g}\,g^{\mu\nu}$ , which are required for the energy and helicity integrals.

#### metrics

• The Jacobian,  $\sqrt{g}$ , and the "lower" metric elements,  $g_{\mu\nu}$ , are calculated by coords(), and are provided on a regular grid in "real-space", i.e.  $(\theta, \zeta)$ , at a given radial location, i.e. where s is input.

## plasma region

• In the plasma region, the required terms are  $\bar{g}_{\mu\nu} \equiv g_{\mu\nu}/\sqrt{g}$ .

$$\sqrt{g} g^{ss} = (g_{\theta\theta}g_{\zeta\zeta} - g_{\theta\zeta}g_{\theta\zeta})/\sqrt{g}$$

$$\sqrt{g} g^{s\theta} = (g_{\theta\zeta}g_{s\zeta} - g_{s\theta}g_{\zeta\zeta})/\sqrt{g}$$

$$\sqrt{g} g^{s\zeta} = (g_{s\theta}g_{\theta\zeta} - g_{\theta\theta}g_{s\zeta})/\sqrt{g}$$

$$\sqrt{g} g^{\theta\theta} = (g_{\zeta\zeta}g_{ss} - g_{s\zeta}g_{s\zeta})/\sqrt{g}$$

$$\sqrt{g} g^{\theta\zeta} = (g_{s\zeta}g_{s\theta} - g_{\theta\zeta}g_{ss})/\sqrt{g}$$

$$\sqrt{g} g^{\zeta\zeta} = (g_{ss}g_{\theta\theta} - g_{s\theta}g_{s\theta})/\sqrt{g}$$
(159)

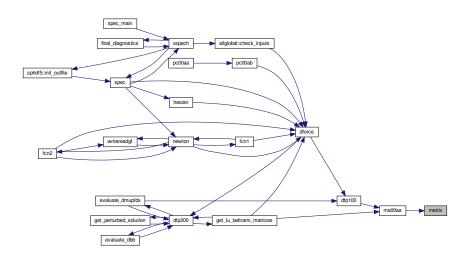
#### **FFTs**

• After constructing the required quantities in real space, FFTs provided the required Fourier harmonics, which are returned through global.f90. (The "extended" Fourier resolution is used.)

References allglobal::cfmn, allglobal::cpus, allglobal::dbdx, allglobal::efmn, allglobal::im, allglobal::ime, allglobal::ine, allglobal::mn, allglobal::mn, allglobal::mt, allglobal::nt, allglobal::nt,

Referenced by ma00aa().

Here is the caller graph for this function:



# 5.13 Solver for Beltrami (linear) system

#### **Functions/Subroutines**

subroutine mp00ac (Ndof, Xdof, Fdof, Ddof, Ldfjac, iflag)
 Solves Beltrami/vacuum (linear) system, given matrices.
 unpacking fluxes, helicity multiplier

## 5.13.1 Detailed Description

### 5.13.2 Function/Subroutine Documentation

Solves Beltrami/vacuum (linear) system, given matrices.

## unpacking fluxes, helicity multiplier

• The vector of "parameters",  $\mu$ , is unpacked. (Recall that  $\mu$  was "packed" in ma02aa() .) In the following,  $\psi \equiv (\Delta \psi_t, \Delta \psi_p)^T$ .

## construction of linear system

• The equation  $\nabla \times \mathbf{B} = \mu \mathbf{B}$  is cast as a matrix equation,

$$\mathcal{M} \cdot \mathbf{a} = \mathcal{R},\tag{160}$$

where a represents the degrees-of-freedom in the magnetic vector potential,  $\mathbf{a} \equiv \{A_{\theta,e,i,l}, A_{\zeta,e,i,l}, \ldots\}$ .

• The matrix  $\mathcal M$  is constructed from  $\mathcal A\equiv \text{dMA}$  and  $\mathcal D\equiv \text{dMD}$ , which were constructed in matrix(), according to

$$\mathcal{M} \equiv \mathcal{A} - \mu \mathcal{D}. \tag{161}$$

Note that in the vacuum region,  $\mu=0$ , so  $\mathcal{M}$  reduces to  $\mathcal{M}\equiv\mathcal{A}.$ 

- The construction of the vector  $\mathcal R$  is as follows:
  - if Lcoordinatesingularity=T, then

$$\mathcal{R} \equiv -\left(\mathcal{B} - \mu \mathcal{E}\right) \cdot \boldsymbol{\psi} \tag{162}$$

- if Lcoordinatesingularity=F and Lplasmaregion=T, then

$$\mathcal{R} \equiv -\mathcal{B} \cdot \psi \tag{163}$$

- if Lcoordinatesingularity=F and Lvacuumregion=T, then

$$\mathcal{R} \equiv -\mathcal{G} - \mathcal{B} \cdot \psi \tag{164}$$

The quantities  $\mathcal{B} \equiv \text{dMB}$ ,  $\mathcal{E} \equiv \text{dME}$  and  $\mathcal{G} \equiv \text{dMG}$  are constructed in matrix().

## solving linear system

It is *not* assumed that the linear system is positive definite. The LAPACK routine DSYSVX is used to solve the linear system.

## unpacking, ...

- The magnetic degrees-of-freedom are unpacked by packab() .
- The error flag, ImagneticOK, is set that indicates if the Beltrami fields were successfully constructed.

#### construction of "constraint" function

• The construction of the function  $f(\mu)$  is required so that iterative methods can be used to construct the Beltrami field consistent with the required constraints (e.g. on the enclosed fluxes, helicity, rotational-transform, ...).

#### See also

ma02aa() for additional details.

## plasma region

- For Lcoordinatesingularity=T, the returned function is:

$$\mathbf{f}(\mu, \Delta \psi_p) \equiv \begin{cases} ( & 0 & , & 0 )^T, & \text{if Lconstraint} = -1 \\ ( & 0 & , & 0 )^T, & \text{if Lconstraint} = 0 \\ ( & \pounds(+1) - \text{iota (lvol )} & , & 0 )^T, & \text{if Lconstraint} = 1 \\ ( & ? & , & ? )^T, & \text{if Lconstraint} = 2 \end{cases}$$
 (165)

- For Lcoordinatesingularity=F, the returned function is:

$$\mathbf{f}(\mu,\Delta\psi_p) \equiv \left\{ \begin{array}{lll} (&0&,&0&\\ (&0&,&0&\\ (&\pm(-1)-\mathrm{oita}\,(\mathrm{lvol-1})&,&\pm(+1)-\mathrm{iota}\,(\mathrm{lvol})&)^T,&\mathrm{if}\,\,\mathrm{Lconstraint}&=&-1\\ (&?&,&?&)^T,&\mathrm{if}\,\,\mathrm{Lconstraint}&=&1\\ (&?&,&?&)^T,&\mathrm{if}\,\,\mathrm{Lconstraint}&=&2 \end{array} \right.$$

### vacuum region

- For the vacuum region, the returned function is:

$$\mathbf{f}(\Delta\psi_t,\Delta\psi_p) \equiv \begin{cases} \begin{pmatrix} 0 & , & 0 & \end{pmatrix}^T, & \text{if Lconstraint} = -1\\ (I-\text{curtor} & , & G-\text{curpol} & \end{pmatrix}^T, & \text{if Lconstraint} = 0\\ (t-1)-\text{oita(lvol-1)} & , & G-\text{curpol} & \end{pmatrix}^T, & \text{if Lconstraint} = 1\\ (t-1)-\text{oita(lvol-1)} & , & G-\text{curpol} & \end{pmatrix}^T, & \text{if Lconstraint} = 1\\ (t-1)-\text{oita(lvol-1)} & , & G-\text{curpol} & \end{pmatrix}^T, & \text{if Lconstraint} = 1 \end{cases}$$

• The rotational-transform,  $\pm$ , is computed by tr00ab(); and the enclosed currents, I and G, are computed by curent().

# early termination

• If  $|\mathbf{f}| < \text{mupftol}$ , then early termination is enforced (i.e., iflag is set to a negative integer). (See ma02aa() for details of how mp00ac() is called iteratively.)

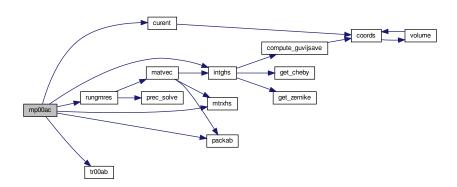
## **Parameters**

in	Ndof	
in	Xdof	
	Fdof	
	Ddof	
in	Ldfjac	
	iflag	indicates whether (i) iflag=1: "function" values are required; or (ii) iflag=2: "derivative" values are required

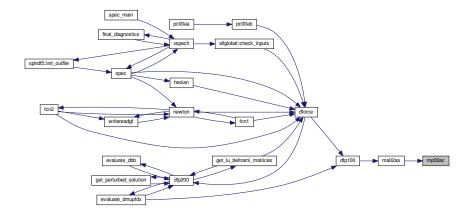
References allglobal::cpus, curent(), inputlist::currol, inputlist::curtor, constants::half, inputlist::helicity, allglobal::im, allglobal::in, intghs(), inputlist::iota, allglobal::ivol, allglobal::lcoordinatesingularity, allglobal::lplasmaregion, inputlist::lrad, allglobal::lvacuumregion, numerical::machprec, allglobal::mn, allglobal::mns, allglobal::mpi\_commc\_spec, mtrxhs(), inputlist::mu, allglobal::myid, allglobal::ncpu, allglobal::notstellsym, allglobal::nt, inputlist::ntor, allglobal::nz, inputlist::oita, constants::one, fileunits::ounit, packab(), rungmres(), numerical::small, tr00ab(), inputlist::wmacros, allglobal::yesstellsym, and constants::zero.

Referenced by ma02aa().

Here is the call graph for this function:



Here is the caller graph for this function:



## 5.14 Force-driver

#### **Functions/Subroutines**

```
    subroutine newton (NGdof, position, ihybrd)
        Employs Newton method to find F(x) = 0, where x ≡ {geometry} and F is defined in dforce() .
    subroutine writereadgf (readorwrite, NGdof, ireadhessian)
        read or write force-derivative matrix
    subroutine fcn1 (NGdof, xx, fvec, irevcm)
        fcn1
    subroutine fcn2 (NGdof, xx, fvec, fjac, Ldfjac, irevcm)
        fcn2
```

#### 5.14.1 Detailed Description

#### 5.14.2 Function/Subroutine Documentation

```
Solves \mathbf{F}(\xi) = 0, where \mathbf{F} \equiv \{[[p + B^2/2]]_{i,l}, I_{i,l}\} and \xi \equiv \{R_{i,l}, Z_{i,l}\}.
```

## iterative, reverse communication loop

- The iterative, Newton search to find  $\mathbf{x} \equiv \{\text{geometry}\} \equiv \{R_{i,l}, Z_{i,l}\}$  such that  $\mathbf{F}(\mathbf{x}) = 0$ , where  $\mathbf{F}$  and its derivatives,  $\nabla_{\mathbf{x}} \mathbf{F}$ , are calculated by dforce(), is provided by either
  - C05NDF if Lfindzero=1, which only uses function values; or
  - C05PDF if Lfindzero=2, which uses user-provided derivatives.
- The iterative search will terminate when the solution is within c05xtol of the true solution (see NAG documentation).
- The input variable c05factor is provided to determine the initial step bound (see NAG documentation).

## logic, writing/reading from file

- Before proceeding with iterative search, dforce() is called to determine the magnitude of the initial force imbalance, and if this is less than forcetol then the iterative search will not be performed.
- As the iterations proceed, wrtend() will be called to save itermediate information (also see xspech()).
- If the derivative matrix,  $\nabla_{\mathbf{x}} \mathbf{F}$ , is required, i.e. if Lfindzero=2, and if LreadGF=T then the derivative matrix will initially be read from .ext.sp.DF, if it exists, or from .sp.DF.
- As the iterations proceed, the derivative matrix will be written to .ext.sp.DF.

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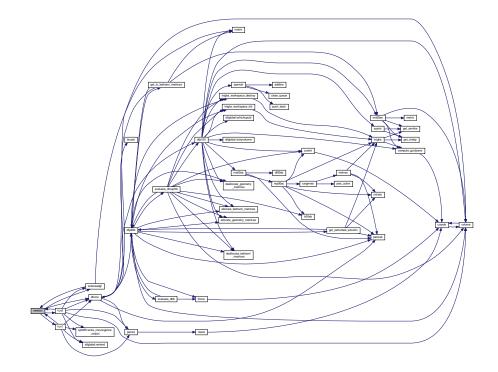
#### **Parameters**

in	NGdof	
in,out	position	
out	ihybrd	

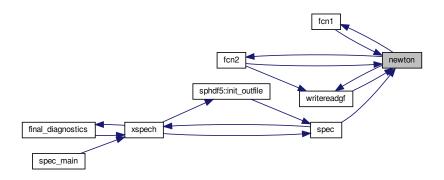
References allglobal::bbe, allglobal::bbo, allglobal::cpus, allglobal::dbdmp, allglobal::dessian, allglobal::dffdrz, dforce(), allglobal::dmupfdx, allglobal::energy, fcn1(), fcn2(), allglobal::forceerr, allglobal::hessian, inputlist ::igeometry, allglobal::iie, allglobal::iio, allglobal::im, allglobal::irbc, allglobal::irbs, allglobal::irbs, allglobal::localconstraint, allglobal::mn, allglobal::mpi\_comm\_spec, allglobal::myid, allglobal::ncpu, newtontime::ndcalls, newtontime::nfcalls, allglobal::nfreeboundaryiterations, allglobal::notstellsym, constants::one, fileunits::ounit, numerical::sqrtmachprec, constants::ten, constants::two, inputlist::wmacros, writereadgf(), and constants::zero.

Referenced by fcn1(), fcn2(), spec(), and writereadgf().

Here is the call graph for this function:



Here is the caller graph for this function:



read or write force-derivative matrix

## **Parameters**

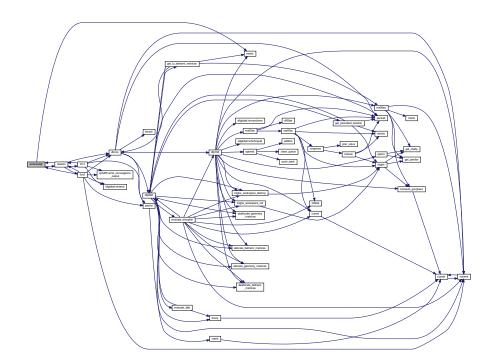
in	readorwrite	
in	NGdof	
out	ireadhessian	

References allglobal::cpus, fileunits::dunit, allglobal::hessian, inputlist::igeometry, allglobal::im, allglobal::in, inputlist::istellsym, inputlist::lfreebound, allglobal::lhessianallocated, matrix(), allglobal::mn, allglobal::mpi\_comm \_ spec, inputlist::mpol, allglobal::myid, newton(), inputlist::ntor, inputlist::nvol, fileunits::ounit, and constants::zero.

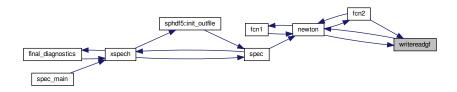
Referenced by fcn2(), and newton().

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Here is the call graph for this function:



Here is the caller graph for this function:



# fcn1

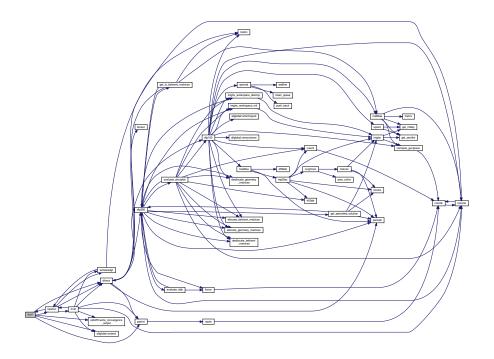
# **Parameters**

in	NGdof	
in	XX	
out	fvec	
in	irevcm	

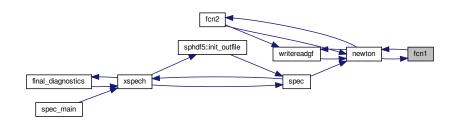
References allglobal::bbe, allglobal::cpus, allglobal::cpus, allglobal::dbdmp, allglobal::dessian, allglobal:-dfdrz, dforce(), allglobal::dmupfdx, allglobal::energy, allglobal::forceerr, allglobal::hessian, inputlist::igeometry, allglobal::iie, allglobal::iio, allglobal::im, allglobal::irbc, allglobal::irbs, allglobal::irbs, allglobal::izbc, allglobal::izbc, allglobal::irbs, allglobal::mn, allglobal::mpi\_comm\_spec, allglobal::myid, allglobal::ncpu, newtontime::ndcalls, newton(), newtontime::nfcalls, allglobal::nfreeboundaryiterations, allglobal::notstellsym, constants::one, fileunits::ounit, packxi(), numerical::sqrtmachprec, constants::ten, constants::two, inputlist::wmacros, sphdf5::write\_convergence\_output(), allglobal::wrtend(), and constants::zero.

Referenced by newton().

Here is the call graph for this function:



Here is the caller graph for this function:



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```
real, dimension(1:ngdof), intent(out) fvec,
real, dimension(1:ldfjac,1:ngdof), intent(out) fjac,
integer, intent(in) Ldfjac,
integer, intent(in) irevcm )
```

#### fcn2

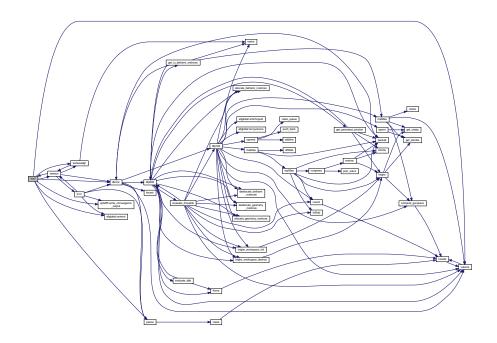
#### **Parameters**

in	NGdof	
in	XX	
out	fvec	
out	fjac	
in	Ldfjac	
in	irevcm	

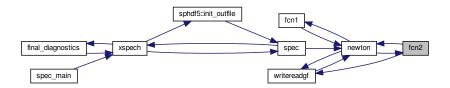
References allglobal::bbe, allglobal::cpus, allglobal::cpus, allglobal::dbbdmp, allglobal::dessian, allglobal:-cffdrz, dforce(), allglobal::dmupfdx, allglobal::energy, allglobal::forceerr, allglobal::hessian, inputlist::igeometry, allglobal::iie, allglobal::iio, allglobal::im, allglobal::irbc, allglobal::irbs, allglobal::izbc, allglobal::izbc, allglobal::izbc, allglobal::izbc, allglobal::irbs, allglobal::mpi\_comm\_spec, allglobal::myid, allglobal::ncpu, newtontime::ndcalls, newton(), newtontime::nfcalls, allglobal::nfreeboundaryiterations, allglobal::notstellsym, constants::one, fileunits::ounit, packxi(), numerical::sqrtmachprec, constants::ten, constants::two, volume(), inputlist::wmacros, sphdf5::write\_convergence\_output(), writereadgf(), allglobal::wrtend(), and constants::zero.

Referenced by newton().

Here is the call graph for this function:



Here is the caller graph for this function:



# 5.15 "packing" of Beltrami field solution vector

## **Functions/Subroutines**

- subroutine packab (packorunpack, Ivol, NN, solution, ideriv)

  Packs and unpacks Beltrami field solution vector.
- subroutine packxi (NGdof, position, Mvol, mn, iRbc, iZbs, iRbs, iZbc, packorunpack, LComputeDerivatives, LComputeAxis)

Packs, and unpacks, geometrical degrees of freedom; and sets coordinate axis.

## 5.15.1 Detailed Description

## 5.15.2 Function/Subroutine Documentation

Packs and unpacks Beltrami field solution vector.

# construction of "vector" of independent degrees of freedom

- Numerical routines for solving linear equations typically require the unknown, independent degrees of freedom to be "packed" into a vector,  $\mathbf{x}$ .
- The magnetic field is defined by the independent degrees of freedom in the Chebyshev-Fourier representation of the vector potential,  $A_{\theta,e,i,l}$  and  $A_{\zeta,e,i,l}$ ; and the non-stellarator-symmetric terms if relevant,  $A_{\theta,o,i,l}$  and  $A_{\zeta,o,i,l}$ ; and the Lagrange multipliers,  $a_i$ ,  $b_i$ ,  $c_i$ ,  $d_i$ ,  $e_i$ , etc. as required to enforce the constraints:

$$\mathbf{x} \equiv \{ A_{\theta,e,i,l}, A_{\zeta,e,i,l}, A_{\theta,o,i,l}, A_{\zeta,o,i,l}, a_i, b_i, c_i, d_i, e_i, f_i, g_1, h_1 \}.$$
(168)

• The "packing" index is assigned in preset() .

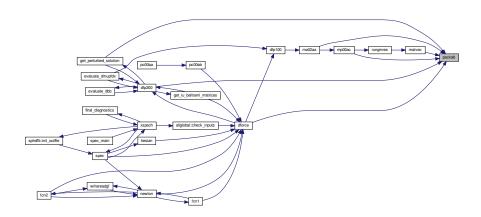
#### **Parameters**

packorunpack	
Ivol	
NN	
solution	
ideriv	

References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::cpus, allglobal::im, allglobal::im, allglobal::im, allglobal::lmb, allglobal::lmbvalue, allglobal::lmc, allglobal::lmcvalue, allglobal::lmcvalue, allglobal::lmcvalue, allglobal::lmf, allglobal::lmfvalue, allglobal::lmg, allglobal::lmf, allglobal::lmfvalue, allglobal::lmg, allglobal::lmg, allglobal::mn, allglobal::mn, allglobal::mpi\_comm\_spec, allglobal::myid, allglobal::ncpu, allglobal::notstellsym, fileunits::ounit, numerical::small, allglobal::tt, allglobal::yesstellsym, and constants::zero.

Referenced by dforce(), dfp200(), get perturbed solution(), ma02aa(), matvec(), and mp00ac().

Here is the caller graph for this function:



```
5.15.2.2 packxi() subroutine packxi (
    integer, intent(in) NGdof,
    real, dimension(0:ngdof) position,
    integer, intent(in) Mvol,
    integer, intent(in) mn,
    real, dimension(1:mn,0:mvol) iRbc,
    real, dimension(1:mn,0:mvol) iRbs,
    real, dimension(1:mn,0:mvol) iZbs,
    real, dimension(1:mn,0:mvol) iZbc,
    character packorunpack,
    logical, intent(in) LComputeDerivatives,
    logical, intent(in) LComputeAxis)
```

Packs, and unpacks, geometrical degrees of freedom; and sets coordinate axis.

## geometrical degrees of freedom

- The geometrical degrees-of-freedom, namely the  $R_{j,v}$  and  $Z_{j,v}$  where v labels the interface and j labels the Fourier harmonic, must be "packxi", and "unpackxi", into a single vector,  $\xi$ , so that standard numerical routines can be called to find solutions to force-balance, i.e.  $\mathbf{F}[\xi] = 0$ .
- A coordinate "pre-conditioning" factor is included:

$$\boldsymbol{\xi}_k \equiv \frac{R_{j,v}}{\Psi_{j,v}},\tag{169}$$

where  $\Psi_{j,v} \equiv exttt{psifactor}$  (j,v), which is defined in global.f90.

#### coordinate axis

- The coordinate axis is not an independent degree-of-freedom of the geometry. It is constructed by extrapolating the geometry of the innermost interface down to a line.
- Note that if the coordinate axis depends only on the geometry of the innermost interface then the block tridiagonal structure of the the force-derivative matrix is preserved.
- · Define the arc-length weighted averages,

$$R_0(\zeta) \equiv \frac{\int_0^{2\pi} R_1(\theta, \zeta) dl}{L(\zeta)}, \qquad Z_0(\zeta) \equiv \frac{\int_0^{2\pi} Z_1(\theta, \zeta) dl}{L(\zeta)}, \tag{170}$$

where  $L(\zeta) \equiv \int_0^{2\pi} dl$  and  $dl \equiv \sqrt{\partial_\theta R_1(\theta,\zeta)^2 + \partial_\theta Z_1(\theta,\zeta)^2} \, d\theta$ .

- Note that if dl does not depend on  $\theta$ , i.e. if  $\theta$  is the equal arc-length angle, then the expressions simplify.
- Note that the geometry of the coordinate axis thus constructed only depends on the geometry of the innermost interface, by which I mean that the geometry of the coordinate axis is independent of the angle parameterization.

## some numerical comments

- First, the differential poloidal length,  $dl \equiv \sqrt{R_{\theta}^2 + Z_{\theta}^2}$ , is computed in real space using an inverse FFT from the Fourier harmonics of R and Z.
- Second, the Fourier harmonics of the dl are computed using an FFT. The integration over  $\theta$  to construct  $L \equiv \int dl$  is now trivial: just multiply the m=0 harmonics of dl by  $2\pi$ . The ajk (1:mn) variable is used.
- Next, the weighted R dl and Z dl are computed in real space, and the poloidal integral is similarly taken.
- · Lastly, the Fourier harmonics are constructed using an FFT after dividing in real space.

### **Parameters**

in	NGdof	
	position	
in	Mvol	
in	mn	
	iRbc	
	iZbs	
	iRbs	
	iZbc	
	packorunpack	
in	LComputeDerivatives	
in	LComputeAxis	

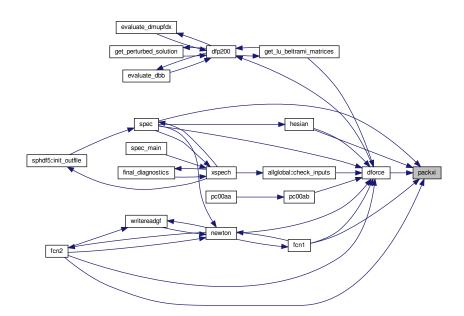
References allglobal::ajk, allglobal::cfmn, allglobal::comn, allglobal::cpus, allglobal::efmn, allglobal::evmn, inputlist::igeometry, allglobal::ijimag, allglobal::ijimag, allglobal::ijimag, allglobal::ijimag, allglobal::ijimag, allglobal::ijimag, allglobal::ijimag, allglobal::mpi\_comm\_spec, allglobal::myid, allglobal::ncpu, allglobal::ncpu, allglobal::ncpu, allglobal::ncpu, allglobal::ntz, inputlist::nvol, allglobal::nz, allglobal::odmn, allglobal::ofmn, fileunits::ounit, allglobal::psifactor, allglobal::rscale, rzaxis(), allglobal::sfmn, allglobal::simn, allglobal::trij, allglobal::trij, allglobal::trij, allglobal::yesstellsym, and constants::zero.

Referenced by dforce(), fcn1(), fcn2(), hesian(), and spec().

Here is the call graph for this function:



Here is the caller graph for this function:



# 5.16 Conjugate-Gradient method

# Functions/Subroutines

- subroutine pc00aa (NGdof, position, Nvol, mn, ie04dgf)
  - Use preconditioned conjugate gradient method to find minimum of energy functional.
- subroutine pc00ab (mode, NGdof, Position, Energy, Gradient, nstate, iuser, ruser)

Returns the energy functional and it's derivatives with respect to geometry.

## 5.16.1 Detailed Description

### 5.16.2 Function/Subroutine Documentation

```
5.16.2.1 pc00aa() subroutine pc00aa (
    integer, intent(in) NGdof,
    real, dimension(0:ngdof), intent(inout) position,
    integer, intent(in) Nvol,
    integer, intent(in) mn,
    integer ie04dgf)
```

Use preconditioned conjugate gradient method to find minimum of energy functional.

## energy functional

The energy functional is described in pc00ab().

## relevant input variables

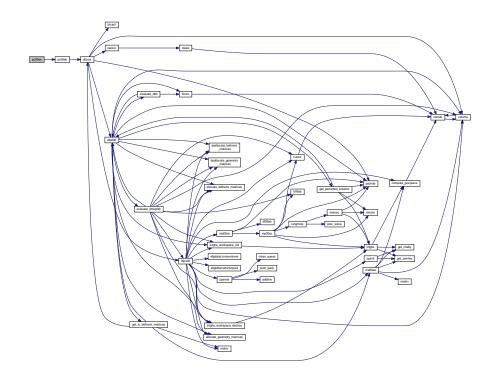
- The following input variables control the operation of E04DGF:
  - epsilon: weighting of "spectral energy"; see pc00ab()maxstep: this is given to E04DGF for the Maximum Step Length
  - maxiter: upper limit on derivative calculations used in the conjugate gradient iterations
  - verify: if verify=1, then E04DGF will confirm user supplied gradients (provided by pc00ab()) are correct;
- Todo Unfortunately,  $\verb"E04DGF"$  seems to require approximately 3N function evaluations before proceeding to minimize the energy functional, where there are N degrees of freedom. I don't know how to turn this off!

### **Parameters**

in	NGdof
in,out	position
in	Nvol
in	mn
	ie04dgf

References allglobal::cpus, allglobal::energy, allglobal::forceerr, inputlist::forcetol, allglobal::myid, allglobal::ncpu, fileunits::ounit, pc00ab(), constants::ten, and constants::zero.

Here is the call graph for this function:



```
5.16.2.2 pc00ab() subroutine pc00ab (
    integer mode,
    integer NGdof,
    real, dimension(1:ngdof) Position,
    real Energy,
    real, dimension(1:ngdof) Gradient,
    integer nstate,
    integer, dimension(1:2) iuser,
    real, dimension(1:1) ruser)
```

Returns the energy functional and it's derivatives with respect to geometry.

# **Energy functional**

· The energy functional is

$$F \equiv \sum_{l=1}^{N} \int_{\mathcal{V}} \left( \frac{p}{\gamma - 1} + \frac{B^2}{2} \right) dv, \tag{171}$$

where  $N \equiv \mathtt{Nvol}$  is the number of interfaces.

• Assuming that the toroidal and poloidal fluxes,  $\psi_t$  and  $\psi_p$ , the helicity,  $\mathcal{K}$ , the helicity multiplier,  $\mu$ , and/or the interface rotational-transforms,  $\epsilon$ , are appropriately constrained, the Beltrami fields in each volume depend only the geometry of the adjacent interfaces. So, the energy functional is assumed to be a function of "position", i.e.  $F = F(R_{l,j}, Z_{l,j})$ .

Introducing a ficitious time, t, the position may be advanced according to

$$\frac{\partial R_{j}}{\partial t} \equiv -\frac{\partial}{\partial R_{j}} \sum_{l=1}^{N} \int \left(\frac{p}{\gamma - 1} + \frac{B^{2}}{2}\right) dv, 
\frac{\partial Z_{j}}{\partial t} \equiv -\frac{\partial}{\partial Z_{j}} \sum_{l=1}^{N} \int \left(\frac{p}{\gamma - 1} + \frac{B^{2}}{2}\right) dv.$$
(172)

· There remain degrees of freedom in the angle representation of the interfaces.

## Spectral energy minimization

· Consider variations which do not affect the geometry of the surfaces,

$$\delta R = R_{\theta} u, \tag{173}$$

$$\delta Z = Z_{\theta} u, \tag{174}$$

where u is a angle variation.

· The corresponding variation in each of the Fourier harmonics is

$$\delta Z_j \equiv \oint \!\! \oint \! d\theta d\zeta \ Z_\theta \ u \ \sin \alpha_j, \tag{176}$$

· Following Hirshman et al., introducing the normalized spectral width

$$M \equiv \frac{\sum_{j} (m_{j}^{p} + n_{j}^{q}) (R_{l,j}^{2} + Z_{l,j}^{2})}{\sum_{j} (R_{l,j}^{2} + Z_{l,j}^{2})},$$
(177)

· Using the notation

$$N \equiv \sum_{j} \lambda_{j} (R_{l,j}^{2} + Z_{l,j}^{2}),$$
 (178)

$$D \equiv \sum_{i} (R_{l,j}^2 + Z_{l,j}^2), \tag{179}$$

where  $\lambda_j \equiv m_j^p + n_j^q$ , the variation in the normalized spectral width is

$$\delta M = (\delta N - M\delta D)/D. \tag{180}$$

· For tangential variations,

$$\delta N = 2 \oint \!\! \int \!\! d\theta d\zeta \ u \left( R_{\theta} \sum_{j} \lambda_{j} R_{j} \cos \alpha_{j} + Z_{\theta} \sum_{j} \lambda_{j} Z_{j} \sin \alpha_{j} \right), \tag{181}$$

$$\delta D = 2 \oint \!\! \int \!\! d\theta d\zeta \ u \left( R_{\theta} \sum_{j} R_{j} \cos \alpha_{j} + Z_{\theta} \sum_{j} Z_{j} \sin \alpha_{j} \right). \tag{182}$$

· The "tangential spectral-width descent direction" is thus

$$\frac{\partial u}{\partial t} = -\left[R_{\theta} \sum_{j} (\lambda_{j} - M) R_{j} \cos \alpha_{j} / D + Z_{\theta} \sum_{j} (\lambda_{j} - M) Z_{j} \sin \alpha_{j} / D\right]. \tag{183}$$

· This suggests that position should be advanced according to

$$\frac{\partial R_j}{\partial t} \equiv -\frac{\partial}{\partial R_j} \sum_{l=1}^N \int \left(\frac{p}{\gamma - 1} + \frac{B^2}{2}\right) dv - [R_\theta (R_\theta X + Z_\theta Y)]_j, \tag{184}$$

$$\frac{\partial Z_j}{\partial t} \equiv -\frac{\partial}{\partial Z_j} \sum_{l=1}^N \int \left(\frac{p}{\gamma - 1} + \frac{B^2}{2}\right) dv - [Z_{\theta}(R_{\theta}X + Z_{\theta}Y)]_j, \tag{185}$$

where  $X \equiv \sum_j (\lambda_j - M) R_j \cos \alpha_j / D$  and  $Y \equiv \sum_j (\lambda_j - M) Z_j \sin \alpha_j / D$ .

## numerical implementation

· The spectral condensation terms,

$$R_{\theta}(R_{\theta}X + Z_{\theta}Y) = \sum_{j,k,l} m_j m_k (\lambda_l - M) R_j (+R_k R_l \sin \alpha_j \sin \alpha_k \cos \alpha_l - Z_k Z_l \sin \alpha_j \cos \alpha_k \sin \alpha_l) (186)$$

$$Z_{\theta}(R_{\theta}X + Z_{\theta}Y) = \sum_{j,k,l} m_j m_k (\lambda_l - M) Z_j (-R_k R_l \cos \alpha_j \sin \alpha_k \cos \alpha_l + Z_k Z_l \cos \alpha_j \cos \alpha_k \sin \alpha_l) (187)$$

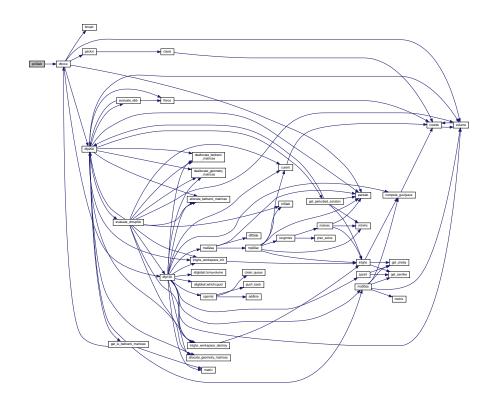
are calculated using triple angle expressions...

Todo IT IS VERY LIKELY THAT FFTs WOULD BE FASTER!!!

References allglobal::cpus, allglobal::dbbdrz, dforce(), allglobal::diidrz, inputlist::epsilon, allglobal::forceerr, inputlist::forcetol, constants::half, inputlist::igeometry, allglobal::lbbintegral, allglobal::mn, allglobal::myid, inputlist::nvol, constants::one, fileunits::ounit, allglobal::yesstellsym, and constants::zero.

Referenced by pc00aa().

Here is the call graph for this function:



Here is the caller graph for this function:



## 5.17 Initialization of the code

### **Functions/Subroutines**

· subroutine preset

Allocates and initializes internal arrays.

# 5.17.1 Detailed Description

## 5.17.2 Function/Subroutine Documentation

# **5.17.2.1 preset()** subroutine preset

Allocates and initializes internal arrays.

## LGdof and NGdof: number of geometrical degrees-of-freedom

- $LGdof \equiv$  the number of degrees-of-freedom in the geometry (i.e. Fourier harmonics) of each interface
- $NGdof \equiv total number of degrees-of-freedom in geometry, i.e. of all interfaces$

## iota and oita: rotational transform on interfaces

- The input variables iota and oita are the rotational transform on "inner-side" and on the "outer-side" of each interface.
- · These quantities are formally inputs.
- Note that if  $q_l + \gamma q_r \neq 0$ , then iota is given by

$$t \equiv \frac{p_l + \gamma p_r}{q_l + \gamma q_r},\tag{188}$$

where  $p_l \equiv {
m pl}$  ,  $q_l \equiv {
m ql}$  , etc.; and similarly for oita .

# dtflux(1:Mvol) and dpflux(1:Mvol): enclosed fluxes

- dtflux  $\equiv \Delta \psi_{tor}/2\pi$  and dpflux  $\equiv \Delta \psi_{pol}/2\pi$  in each volume.
- Note that the total toroidal flux enclosed by the plasma boundary is  $\Phi_{edge} \equiv {\tt phiedge}$  .
- $\psi_{tor} \equiv exttt{tflux}$  and  $\psi_{pol} \equiv exttt{pflux}$  are immediately normalized (in readin() ) according to  $\psi_{tor,i} \to \psi_{tor,i}/\psi_0$ and  $\psi_{pol,i} \to \psi_{pol,i}/\psi_0$ , where  $\psi_0 \equiv \psi_{tor,N}$  on input.

### sweight(1:Mvol): star-like angle constraint weight

• the "star-like" poloidal angle constraint weights (only required for toroidal geometry, i.e. Igeometry=3) are given by

$$sweight_v \equiv upsilon \times (l_v/N_{vol})^w, \tag{189}$$

where  $l_v$  is the volume number, and  $w \equiv wpoloidal$ .

## TT(0:Mrad,0:1,0:1): Chebyshev polynomials at inner/outer interface

- TT (0:Lrad, 0:1, 0:1) gives the Chebyshev polynomials, and their first derivative, evaluated at s=-1
- Precisely, TT (1, i, d)  $\equiv T_I^{(d)}(s_i)$  for  $s_0 = -1$  and  $s_1 = +1$ .
- Note that  $T_l^{(0)}(s)=s^l$  and  $T_l^{(1)}(s)=s^{l+1}l^2$  for  $s=\pm 1.$
- · Note that

$$T_{l}(-1) = \begin{cases} +1, & \text{if } l \text{ is even,} \\ -1, & \text{if } l \text{ is odd;} \end{cases} \qquad T_{l}(+1) = \begin{cases} +1, & \text{if } l \text{ is even,} \\ +1, & \text{if } l \text{ is odd;} \end{cases}$$
(190)  
$$T'_{l}(-1) = \begin{cases} -l^{2}, & \text{if } l \text{ is even,} \\ +l^{2}, & \text{if } l \text{ is odd;} \end{cases} \qquad T'_{l}(+1) = \begin{cases} +l^{2}, & \text{if } l \text{ is even,} \\ +l^{2}, & \text{if } l \text{ is odd.} \end{cases}$$
(191)

$$T'_l(-1) = \begin{cases} -l^2, & \text{if } l \text{ is even,} \\ +l^2, & \text{if } l \text{ is odd;} \end{cases} \qquad T'_l(+1) = \begin{cases} +l^2, & \text{if } l \text{ is even,} \\ +l^2, & \text{if } l \text{ is odd.} \end{cases}$$
(191)

- TT (0:Mrad, 0:1, 0:1) is used in routines that explicity require interface information, such as
  - the interface force-balance routine, Iforce()
  - the virtual casing routine, casing()
  - computing the rotational-transform on the interfaces, tr00ab()
  - computing the covariant components of the interface magnetic field, sc00aa()
  - enforcing the constraints on the Beltrami fields, matrix() and
  - computing the enclosed currents of the vacuum field, curent().

## ImagneticOK(1:Mvol): Beltrami/vacuum error flag

- · error flags that indicate if the magnetic field in each volume has been successfully constructed
- ImagneticOK is initialized to .false. in dforce() before the Beltrami solver routines are called. If the construction of the Beltrami field is successful (in either ma02aa() or mp00ac() ) then ImagneticOK is set to .true. .

### Lhessianallocated

• The internal logical variable, Lhessianallocated, indicates whether the 'Hessian' matrix of secondpartial derivatives (really, the first derivatives of the force-vector) has been allocated, or not!

### ki(1:mn,0:1): Fourier identification

· Consider the "abbreviated" representation for a double Fourier series,

$$\sum_{i} f_{i} \cos(m_{i}\theta - n_{i}\zeta) \equiv \sum_{n=0}^{N_{0}} f_{0,n} \cos(-n\zeta) + \sum_{m=1}^{M_{0}} \sum_{n=-N_{0}}^{N_{0}} f_{m,n} \cos(m\theta - n\zeta),$$
(192)

and the same representation but with enhanced resolution,

$$\sum_{k} \bar{f}_{k} \cos(\bar{m}_{k}\theta - \bar{n}_{k}\zeta) \equiv \sum_{n=0}^{N_{1}} f_{0,n} \cos(-n\zeta) + \sum_{m=1}^{M_{1}} \sum_{n=-N_{1}}^{N_{1}} f_{m,n} \cos(m\theta - n\zeta), \tag{193}$$

with  $M_1 \geq M_0$  and  $N_1 \geq N_0$ ; then  $k_i \equiv \text{ki}$  (i, 0) is defined such that  $\bar{m}_{k_i} = m_i$  and  $\bar{n}_{k_i} = n_i$ .

# kija(1:mn,1:mn,0:1), kijs(1:mn,1:mn,0:1): Fourier identification

• Consider the following quantities, which are computed in ma00aa(), where  $\bar{g}^{\mu\nu}=\sum_k \bar{g}_k^{\mu\nu}\cos\alpha_k$  for  $\alpha_k\equiv m_k\theta-n_k\zeta$ ,

$$\oint \oint d\theta d\zeta \ \bar{g}^{\mu\nu} \cos \alpha_i \ \cos \alpha_j = \frac{1}{2} \oint \oint d\theta d\zeta \ \bar{g}^{\mu\nu} (+\cos \alpha_{k_{ij+}} + \cos \alpha_{k_{ij-}}), \tag{194}$$

$$\oint \!\! \oint d\theta d\zeta \ \bar{g}^{\mu\nu} \cos \alpha_i \sin \alpha_j = \frac{1}{2} \oint \!\! \oint d\theta d\zeta \ \bar{g}^{\mu\nu} (+\sin \alpha_{k_{ij+}} - \sin \alpha_{k_{ij-}}), \tag{195}$$

$$\oint \!\! \oint \! d\theta d\zeta \ \bar{g}^{\mu\nu} \sin \alpha_i \cos \alpha_j = \frac{1}{2} \oint \!\! \oint \! d\theta d\zeta \ \bar{g}^{\mu\nu} (+\sin \alpha_{k_{ij+}} + \sin \alpha_{k_{ij-}}), \tag{196}$$

$$\oint \!\! \oint d\theta d\zeta \ \bar{g}^{\mu\nu} \sin \alpha_i \ \sin \alpha_j = \frac{1}{2} \oint \!\! \oint d\theta d\zeta \ \bar{g}^{\mu\nu} (-\cos \alpha_{k_{ij+}} + \cos \alpha_{k_{ij-}}), \tag{197}$$

where  $(m_{k_{ij+}},n_{k_{ij+}})=(m_i+m_j,n_i+n_j)$  and  $(m_{k_{ij-}},n_{k_{ij-}})=(m_i-m_j,n_i-n_j)$ ; then kija (i, j, 0)  $\equiv k_{ij+}$  and kijs (i, j, 0)  $\equiv k_{ij-}$ .

• Note that Eqn. (193) does not include m<0; so, if  $m_i-m_j<0$  then  $k_{ij-}$  is re-defined such that  $(m_{k_{ij-}},n_{k_{ij-}})=(m_j-m_i,n_j-n_i)$ ; and similarly for the case m=0 and n<0. Also, take care that the sign of the sine harmonics in the above expressions will change for these cases.

## djkp

## iotakki

## cheby(0:Lrad,0:2): Chebyshev polynomial workspace

- cheby (0:Lrad, 0:2) is global workspace for computing the Chebyshev polynomials, and their derivatives, using the recurrence relations  $T_0(s) = 1$ ,  $T_1(s) = s$  and  $T_l(s) = 2sT_{l-1}(s) T_{l-2}(s)$ .
- These are computed as required, i.e. for arbitrary s, in bfield(), jo00aa() and ma00aa().
- Note that the quantities required for ma00aa() are for fixed s, and so these quantities should be precomputed.

### Iquad, gaussianweight, gaussianabscissae: Gauss-Legendre quadrature

- The volume integrals are computed using a "Fourier" integration over the angles and by Gauss-Legendre quadrature over the radial, i.e.  $\int \! f(s) ds = \sum_k \omega_k f(s_k)$ .
- The quadrature resolution in each volume is give by Iquad(1:Mvol) which is determined as follows:

- if Nquad.gt.0, then Iquad(vvol)=Nquad
- if Nquad.le.0 and .not.Lcoordinatesingularity, then Iquad(vvol)=2\*Lrad(vvol)-Nquad
- if Nquad.le.0 and Lcoordinatesingularity , then Iquad(vvol)=2\*Lrad(vvol)Nquad+Mpol
- The Gaussian weights and abscissae are given by gaussianweight (1:maxIquad, 1:Mvol) and gaussianabscissae(1:maxIquad, 1:Mvol), which are computed using modified Numerical Recipes routine gauleg().
- Iquad v is passed through to ma00aa() to compute the volume integrals of the metric elements; also see jo00aa(), where Iquad v is used to compute the volume integrals of  $||\nabla \times \mathbf{B} \mu \mathbf{B}||$ .

### LBsequad, LBnewton and LBlinear

• LBsequad, LBnewton and LBlinear depend simply on LBeltrami, which is described in global.f90 .

## BBweight(1:mn): weighting of force-imbalance harmonics

· weight on force-imbalance harmonics;

$$BBweight_i \equiv opsilon \times exp \left[ -escale \times (m_i^2 + n_i^2) \right]$$
 (198)

this is only used in dforce() in constructing the force-imbalance vector

## mmpp(1:mn): spectral condensation weight factors

· spectral condensation weight factors;

$$mmpp(i) \equiv m_i^p, \tag{199}$$

where  $p \equiv pcondense$ .

# NAdof, Ate, Aze, Ato and Azo: degrees-of-freedom in magnetic vector potential

- NAdof (1:Mvol) = total number of degrees-of-freedom in magnetic vector potential, including Lagrange multipliers, in each volume. This can de deduced from matrix().
- The components of the vector potential,  $\mathbf{A} = A_{\theta} \nabla + A_{\zeta} \nabla \zeta$ , are

$$A_{\theta}(s,\theta,\zeta) = \sum_{i,l} A_{\theta,e,i,l} \overline{T}_{l,i}(s) \cos \alpha_i + \sum_{i,l} A_{\theta,o,i,l} \overline{T}_{l,i}(s) \sin \alpha_i, \qquad (200)$$

$$A_{\zeta}(s,\theta,\zeta) = \sum_{i,l} A_{\zeta,e,i,l} \, \overline{T}_{l,i}(s) \cos \alpha_i + \sum_{i,l} A_{\zeta,o,i,l} \, \overline{T}_{l,i}(s) \sin \alpha_i, \tag{201}$$

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.)

• The Chebyshev-Fourier harmonics of the covariant components of the magnetic vector potential are kept in

$$A_{\theta,e,i,l} \equiv \text{Ate}(v,0,j) \%s(1), \qquad (202)$$

$$A_{\zeta,e,i,l} \equiv \operatorname{Aze}(v,0,j) \%s(1), \tag{203}$$

$$A_{\theta,o,i,l} \equiv \text{Ato}(v,0,j)\%s(1), \text{and}$$
 (204)

$$A_{\zeta,o,i,l} \equiv \text{Azo}(v,0,j)\%s(1); \tag{205}$$

where v=1, Mvol labels volume, j=1, mn labels Fourier harmonic, and l=0, Lrad(v) labels Chebyshev polynomial. (These arrays also contains derivative information.)

- If Linitguess=1, a guess for the initial state for the Beltrami fields is constructed. An initial state is required for iterative solvers of the Beltrami fields, see LBeltrami.
- If Linitguess=2, the initial state for the Beltrami fields is read from file (see ra00aa()). An initial state is required for iterative solvers of the Beltrami fields, see LBeltrami.

## workspace

goomne, goomno: metric information These are defined in metrix(), and used in ma00aa(). gssmne, gssmno: metric information These are defined in metrix(), and used in ma00aa(). gstmne, gstmno: metric information These are defined in metrix(), and used in ma00aa(). gszmne, gszmno: metric information These are defined in metrix(), and used in ma00aa(). gttmne, gttmno: metric information These are defined in metrix(), and used in ma00aa(). gtzmne, gtzmno: metric information These are defined in metrix(), and used in ma00aa(). gzzmne, gzzmno: metric information These are defined in metrix(), and used in ma00aa(). cosi(1:Ntz,1:mn) and sini(1:Ntz,1:mn)

· Trigonometric factors used in various Fast Fourier transforms, where

$$\cos i_{j,i} = \cos(m_i \theta_j - n_i \zeta_j), \tag{206}$$

$$\sin_{i,i} = \sin(m_i \theta_i - n_i \zeta_i). \tag{207}$$

# psifactor(1:mn,1:Mvol): coordinate "pre-conditioning" factor

· In toroidal geometry, the coordinate "pre-conditioning" factor is

$$f_{j,v} \equiv \begin{cases} \psi_{t,v}^0 &, & \text{for } m_j = 0, \\ \psi_{t,v}^{m_j/2} &, & \text{otherwise.} \end{cases}$$
 (208)

where  $\psi_{t,v} \equiv exttt{tflux}$  is the (normalized?) toroidal flux enclosed by the v-th interface.

- psifactor is used in packxi(), dforce() and hesian().
- inifactor is similarly constructed, with

$$f_{j,v} \equiv \left\{ \begin{array}{ll} \psi_{t,v}^{1/2} & , & \text{for } m_j = 0, \\ \psi_{t,v}^{m_j/2} & , & \text{otherwise.} \end{array} \right. \tag{209}$$

and used only for the initialization of the surfaces taking into account axis information if provided.

### **Bsupumn and Bsupvmn**

### diotadxup and glambda: transformation to straight fieldline angle

- Given the Beltrami fields in any volume, the rotational-transform on the adjacent interfaces may be determined (in tr00ab()) by constructing the straight fieldline angle on the interfaces.
- The rotational transform on the inner or outer interface of a given volume depends on the magnetic field in that volume, i.e.  $\pm_{\pm} = \pm(\mathbf{B}_{\pm})$ , so that

$$\delta_{\pm} = \frac{\partial_{\pm}}{\partial \mathbf{B}_{\pm}} \cdot \delta \mathbf{B}_{\pm}. \tag{210}$$

• The magnetic field depends on the Fourier harmonics of both the inner and outer interface geometry (represented here as  $x_j$ ), the helicity multiplier, and the enclosed poloidal flux, i.e.  $\mathbf{B}_{\pm} = \mathbf{B}_{\pm}(x_j, \mu, \Delta \psi_p)$ , so that

$$\delta \mathbf{B}_{\pm} = \frac{\partial \mathbf{B}_{\pm}}{\partial x_{i}} \delta x_{j} + \frac{\partial \mathbf{B}_{\pm}}{\partial \mu} \delta \mu + \frac{\partial \mathbf{B}_{\pm}}{\partial \Delta \psi_{p}} \delta \Delta \psi_{p}. \tag{211}$$

- The rotational-transforms, thus, can be considered to be functions of the geometry, the helicity-multiplier and the enclosed poloidal flux,  $\epsilon_{\pm} = \epsilon_{\pm}(x_j, \mu, \Delta \psi_p)$ .
- The rotational-transform, and its derivatives, on the inner and outer interfaces of each volume is stored in diotadxup(0:1,-1:2,1:Mvol). The indices label:
  - the first index labels the inner or outer interface,
  - the the second one labels derivative, with
    - $\star$  -1 : indicating the derivative with respect to the interface geometry, i.e.  $\frac{\partial +_{\pm}}{\partial x_j},$
    - \* 0 : the rotational-transform itself,
    - \* 1,2 : the derivatives with respec to  $\mu$  and  $\Delta\psi_p$ , i.e.  $\frac{\partial \psi_\pm}{\partial \mu}$  and  $\frac{\partial \psi_\pm}{\partial \Delta\psi_p}$ ;
  - The third index labels volume.
- The values of diotadxup are assigned in mp00aa() after calling tr00ab().

## vvolume, IBBintegral and IABintegral

· volume integrals

$$vvolume(i) = \int_{\mathcal{V}_i} dv$$
 (212)

lBBintegral(i) = 
$$\int_{\mathcal{V}} \mathbf{B} \cdot \mathbf{B} \, dv$$
 (213)

lABintegral(i) = 
$$\int_{\mathcal{V}_i} \mathbf{A} \cdot \mathbf{B} \, dv$$
 (214)

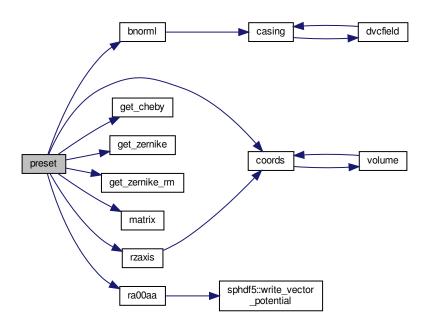
References allglobal::ajk, allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::bbe, allglobal::bbe, allglobal::bbe, allglobal::bbemn, allglobal::bloweremn, allglobal::bloweremn, allglobal::bloweremn, allglobal::bloweremn, allglobal::bloweremn, allglobal::bsupvmn, allglobal::btemn, allglobal::bsupvmn, allglobal::btemn, allglobal::btemn, allglobal::bzemn, allglobal::bzemn, allglobal::cfmn, allglobal::cheby, allglobal::comn, coords(), allglobal::cosi, fftw\_interface::cplxin, fftw\_interface::cplxout, allglobal::cpus, allglobal::diotadxup, allglobal::ditgpdxtp, allglobal::djkm, allglobal::drigh, allglobal::drigh, allglobal::drigh, allglobal::drodz, allglobal::dradz, allglobal::dradz, allglobal::dzadz, allglobal::dzadz, allglobal::dzadz, allglobal::dzadz, allglobal::dzadz, allglobal::dzodz, allglobal::dzodz, allglobal::dzodz, allglobal::efmn, inputlist:-:escale, allglobal::evmn, inputlist::forcetol, allglobal::fse, allglobal::gaussianabscissae, allglobal::gaussiana

allglobal::goomne, allglobal::goomne, allglobal::gssmne, allglobal::gssmne, allglobal::gstmne, allglobal::gstmne, allglobal::gszmne, allglobal::gszmno, allglobal::gteta, allglobal::gttmne, allglobal::gttmne, allglobal::gttmne, allglobal::gtzmno, allglobal::guvij, allglobal::gvuij, allglobal::gzeta, allglobal::gzzmne, allglobal::gzzmno, allglobal: ::halfmm, inputlist::helicity, allglobal::hnt, allglobal::hnz, allglobal::ibnc, allglobal::ibns, allglobal::iemn, inputlist ← ::igeometry, allglobal::iie, allglobal::iio, allglobal::ijimag, allglobal::ijreal, allglobal::im, allglobal::imagneticok, allglobal::ime, inputlist::impol, allglobal::ims, allglobal::in, allglobal::ine, allglobal::inifactor, allglobal::ins, inputlist ::intor, allglobal::iomn, inputlist::iota, allglobal::iotakadd, allglobal::iotakkii, allglobal::iotaksqn, allglobal::iotaksqb, allglobal::ipdtdpf, allglobal::iquad, allglobal::irbc, allglobal::irbs, allglobal::irij, inputlist::istellsym, allglobal::ivnc, allglobal::ivns, inputlist::ivolume, allglobal::izbc, allglobal::izbs, allglobal::izij, allglobal::jiimag, allglobal::jireal, allglobal::jkimag, allglobal::jkreal, allglobal::jxyz, allglobal::ki, allglobal::kija, allglobal::kijs, allglobal::kjimag, allglobal::kjreal, allglobal::labintegral, allglobal::lbbintegral, inputlist::lbeltrami, allglobal::lblinear, allglobal ::lbnewton, allglobal::lbsequad, inputlist::lcheck, inputlist::lconstraint, allglobal::lcoordinatesingularity, inputlist ← ::lfindzero, inputlist::lfreebound, allglobal::lgdof, inputlist::lgmresprec, allglobal::lhessianallocated, inputlist ← ::lhevalues, inputlist::lhevectors, inputlist::lhmatrix, allglobal::liluprecond, inputlist::linitgues, inputlist::linitialize, allglobal::lma, inputlist::lmatsolver, allglobal::lmavalue, allglobal::lmb, allglobal::lmbvalue, allglobal::lmc, allglobal. ::lmcvalue, allglobal::lmd, allglobal::lmdvalue, allglobal::lme, allglobal::lmevalue, allglobal::lmf, allglobal::lmfvalue, allglobal::lmg, allglobal::lmgvalue, allglobal::lmh, allglobal::lmhvalue, allglobal::lmns, allglobal::lmpol, allglobal ::Intor, allglobal::localconstraint, inputlist::lp, inputlist::lperturbed, inputlist::lq, inputlist::lrad, inputlist::lreflect, matrix(), inputlist::maxrndgues, allglobal::mmpp, allglobal::mn, allglobal::mne, allglobal::mns, inputlist::mpol, inputlist::mregular, inputlist::mu, constants::mu0, allglobal::myid, allglobal::nadof, inputlist::ndiscrete, allglobal ::ndmas, allglobal::ndmasmax, allglobal::nfielddof, inputlist::nfp, allglobal::ngdof, allglobal::notmatrixfree, allglobal ::notstellsym, inputlist::nppts, inputlist::nquad, allglobal::nt, inputlist::ntor, allglobal::ntz, inputlist::nvol, allglobal ↔ ::nxyz, allglobal::nz, allglobal::odmn, allglobal::ofmn, inputlist::oita, constants::one, inputlist::opsilon, fileunits::ounit, inputlist::pcondense, allglobal::pemn, inputlist::pflux, inputlist::phiedge, inputlist::pl, fftw interface::planb, fftw ← interface::planf, allglobal::pomn, inputlist::pr, allglobal::psifactor, inputlist::ql, inputlist::qr, ra00aa(), inputlist::rac, inputlist::ras, inputlist::rbc, inputlist::rbs, allglobal::regumm, allglobal::rij, inputlist::rp, inputlist::rq, allglobal::rscale, allglobal::rtm, allglobal::rtt, inputlist::rwc, inputlist::rws, rzaxis(), allglobal::semn, allglobal::sfmn, allglobal::sg, allglobal::simn, allglobal::sini, numerical::small, allglobal::smpol, allglobal::sntor, allglobal::somn, allglobal::sontz, numerical::sgrtmachprec, allglobal::sweight, inputlist::tflux, allglobal::trij, allglobal::tt, allglobal::tzij, inputlist::upsilon, inputlist::vnc, inputlist::vns, numerical::vsmall, allqlobal::vvolume, inputlist::wpoloidal, allqlobal::yesstellsym, inputlist::zac, inputlist::zas, inputlist::zbs, inputlist::zbs, allglobal::zernike, constants::zero, allglobal::zij, inputlist⇔ ::zwc, and inputlist::zws.

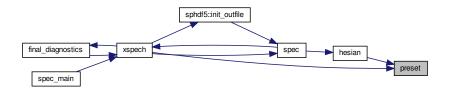
Referenced by hesian(), and xspech().

5.18 Output file(s) 79

Here is the call graph for this function:



Here is the caller graph for this function:



# 5.18 Output file(s)

# **Functions/Subroutines**

- subroutine ra00aa (writeorread)
  - Writes vector potential to .ext.sp.A .
- subroutine sphdf5::init\_outfile

Initialize the interface to the HDF5 library and open the output file.

- subroutine sphdf5::mirror\_input\_to\_outfile
  - Mirror input variables into output file.
- subroutine sphdf5::init\_convergence\_output
  - Prepare convergence evolution output.
- subroutine sphdf5::write\_convergence\_output (nDcalls, ForceErr)

Write convergence output (evolution of interface geometry, force, etc).

· subroutine sphdf5::write\_grid

Write the magnetic field on a grid.

subroutine sphdf5::init flt output (numTrajTotal)

Initialize field line tracing output group and create array datasets.

subroutine sphdf5::write\_poincare (offset, data, success)

Write a hyperslab of Poincare data corresponding to the output of one parallel worker.

- subroutine sphdf5::write\_transform (offset, length, lvol, diotadxup, fiota)
  - Write the rotational transform output from field line following.
- subroutine sphdf5::finalize flt output

Finalize Poincare output.

• subroutine sphdf5::write\_vector\_potential (sumLrad, allAte, allAze, allAto, allAzo)

Write the magnetic vector potential Fourier harmonics to the output file group /vector\_potential.

• subroutine sphdf5::hdfint

Write the final state of the equilibrium to the output file.

subroutine sphdf5::finish\_outfile

Close all open HDF5 objects (we know of) and list any remaining still-open objects.

## 5.18.1 Detailed Description

#### 5.18.2 Function/Subroutine Documentation

```
5.18.2.1 ra00aa() subroutine ra00aa ( character, intent(in) writeorread )
```

Writes vector potential to .ext.sp.A .

## representation of vector potential

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

$$A_{\theta}(s,\theta,\zeta) = \sum_{i,l} A_{\theta,e,i,l} \overline{T}_{l,i}(s) \cos \alpha_i + \sum_{i,l} A_{\theta,o,i,l} \overline{T}_{l,i}(s) \sin \alpha_i, \tag{215}$$

$$A_{\zeta}(s,\theta,\zeta) = \sum_{i,l} A_{\zeta,e,i,l} \, \overline{T}_{l,i}(s) \cos \alpha_i + \sum_{i,l} A_{\zeta,o,i,l} \, \overline{T}_{l,i}(s) \sin \alpha_i, \tag{216}$$

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.)

## file format

• The format of the files containing the vector potential is as follows:

```
open(aunit, file="."//trim(ext)//".sp.A", status="replace", form="unformatted")
write(aunit) mvol, mpol, ntor, mn, nfp ! integers;
write(aunit) im(1:mn) ! integers; poloidal modes;
write(aunit) in(1:mn) ! integers; toroidal modes;
do vvol = 1, mvol ! integers; loop over volumes;
write(aunit) lrad(vvol) ! integers; the radial resolution in each volume may be different;
do ii = 1, mn
write(aunit) ate(vvol,ii)%s(0:lrad(vvol)) ! reals;
write(aunit) aze(vvol,ii)%s(0:lrad(vvol)) ! reals;
write(aunit) ato(vvol,ii)%s(0:lrad(vvol)) ! reals;
write(aunit) azo(vvol,ii)%s(0:lrad(vvol)) ! reals;
enddo ! end of do ii;
enddo ! end of do vvol;
close(aunit)
```

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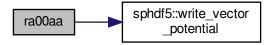
#### **Parameters**

in	writeorread	'W' to write the vector potential; 'R' to read it	
----	-------------	---	--

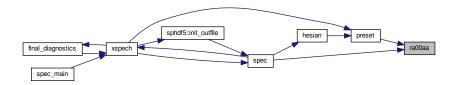
References allglobal::ate, allglobal::ato, fileunits::aunit, allglobal::aze, allglobal::azo, allglobal::cpus, allglobal::im, allglobal::in, inputlist::lrad, allglobal::mn, allglobal::mpi\_comm\_spec, inputlist::mpol, allglobal::myid, allglobal::ncpu, inputlist::nfp, inputlist::ntor, fileunits::ounit, inputlist::wmacros, sphdf5::write vector potential(), and constants::zero.

Referenced by preset(), and spec().

Here is the call graph for this function:



Here is the caller graph for this function:



## **5.18.2.2** mirror\_input\_to\_outfile() subroutine sphdf5::mirror\_input\_to\_outfile

Mirror input variables into output file.

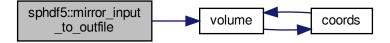
The goal of this routine is to have an exact copy of the input file contents that were used to parameterize a given SPEC run. This also serves to check after the run if SPEC correctly understood the text-based input file.

References inputlist::absacc, inputlist::absreq, inputlist::adiabatic, inputlist::bnc, inputlist::bns, inputlist::bnsblend, inputlist::c05factor, inputlist::c05xmax, inputlist::c05xtol, inputlist::currol, inputlist::curror, inputlist::dpp, inputlist::dqq, inputlist::epsgmres, inputlist::epsilon, inputlist::epsilon, inputlist::epsr, inputlist::escale, sphdf5cotifile\_id, inputlist::forcetol, inputlist::fudge, inputlist::gamma, inputlist::gbnbld, inputlist::gbntol, inputlist::helicity, inputlist::igeometry, inputlist::imethod, inputlist::impol, inputlist::intor, inputlist::iorder, inputlist::iota, inputlist::iotal, inputlist::iotal, inputlist::iotal, inputlist::iotal, inputlist::leadiabatic, inputlist::lellsym, inputlist::lerrortype, inputlist::lextrap, inputlist::lfindzero, inputlist::limitatice, inputlist::limitatice, inputlist::limitatice, inputlist::limitatice, inputlist::limitatice, inputlist::limitatice, inputlist::limitatice, inputlist::lector, inputlist::lector,

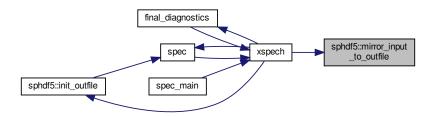
inputlist::Izerovac, inputlist::maxrndgues, inputlist::mcasingcal, inputlist::mfreeits, inputlist::mpol, inputlist::mregular, inputlist::mu, inputlist::mupfits, inputlist::mupftol, inputlist::ndiscrete, inputlist::nfp, inputlist::ngrid, inputlist::nptps, inputlist::nptrj, inputlist::nquad, inputlist::ntor, inputlist::ntoraxis, inputlist::nvol, inputlist::odetol, inputlist::oita, inputlist::psoalen, inputlist::pcondense, inputlist::pflux, inputlist::phiedge, inputlist::pl, inputlist::ppts, inputlist::pr, inputlist::prssure, inputlist::pscale, inputlist::q, inputlist::rac, inputlist::ras, inputlist::rbs, inputlist::relreq, inputlist::rp, inputlist::rpol, inputlist::rtor, inputlist::rwc, inputlist::rws, inputlist::scaling, inputlist::tlux, inputlist::upsilon, inputlist::vcasingeps, inputlist::vcasingits, inputlist::vcasinger, inputlist::vcasingtol, inputlist::vnc, inputlist::vnc, inputlist::vnc, inputlist::vas, inputlist::zbs, inputlist::zws, and inputlist::zws.

Referenced by xspech().

Here is the call graph for this function:



Here is the caller graph for this function:



# **5.18.2.3 init\_convergence\_output()** subroutine sphdf5::init\_convergence\_output

Prepare convergence evolution output.

• The group iterations is created in the output file. This group contains the interface geometry at each iteration, which is useful for constructing movies illustrating the convergence. The data structure in use is an unlimited array of the following compound datatype:

DATATYPE HST COMPOUND {

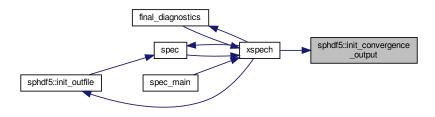
```
H5T_NATIVE_INTEGER "nDcalls";
H5T_NATIVE_DOUBLE "Energy";
H5T_NATIVE_DOUBLE "ForceErr";
H5T_ARRAY { [Mvol+1] [mn] H5T_NATIVE_DOUBLE } "iRbc";
H5T_ARRAY { [Mvol+1] [mn] H5T_NATIVE_DOUBLE } "iZbs";
H5T_ARRAY { [Mvol+1] [mn] H5T_NATIVE_DOUBLE } "iRbs";
H5T_ARRAY { [Mvol+1] [mn] H5T_NATIVE_DOUBLE } "iZbc";
```

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References sphdf5::dt\_energy\_id, sphdf5::dt\_forceerr\_id, sphdf5::dt\_irbc\_id, sphdf5::dt\_irbs\_id, sphdf5::dt\_izbc 
\_id, sphdf5::dt\_izbs\_id, sphdf5::dt\_ndcalls\_id, sphdf5::file\_id, sphdf5::hdfier, sphdf5::iteration\_dset\_id, sphdf5
::memspace, allglobal::mn, and sphdf5::plist\_id.

Referenced by xspech().

Here is the caller graph for this function:



### **5.18.2.4 write grid()** subroutine sphdf5::write\_grid

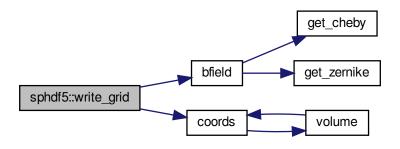
Write the magnetic field on a grid.

The magnetic field is evaluated on a regular grid in  $(s, \theta, \zeta)$  and the corresponding cylindrical coordinates (R, Z) as well as the cylindrical components of the magnetic field  $(B^R, B^{\varphi}, B^Z)$  are written out.

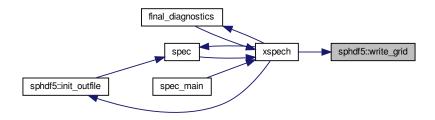
References bfield(), coords(), sphdf5::file\_id, allglobal::gbzeta, inputlist::igeometry, allglobal::jimag, allglobal::jireal, allglobal::lcoordinatesingularity, allglobal::lplasmaregion, inputlist::lrad, allglobal::lvacuumregion, allglobal::mn, allglobal::myid, inputlist::ngrid, allglobal::node, allglobal::nt, allglobal::ntz, inputlist::nvol, allglobal::nz, constants::one, constants::pi2, allglobal::rij, inputlist::rpol, inputlist::rtor, allglobal::sg, constants::two, constants::zero, and allglobal::zij.

Referenced by xspech().

Here is the call graph for this function:



Here is the caller graph for this function:



Initialize field line tracing output group and create array datasets.

The field-line tracing diagnostic is parallelized over volumes, where all threads/ranks produce individual output. This is gathered in the output file, stacked over the radial dimension. The success flag signals if the integrator was successful in following the fieldline for the derired number of toroidal periods.

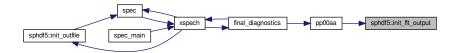
### **Parameters**

i	า	numTrajTotal	total number of Poincare trajectories
---	---	--------------	---------------------------------------

References sphdf5::dset\_id\_diotadxup, sphdf5::dset\_id\_fiota, sphdf5::dset\_id\_r, sphdf5::dset\_id\_s, sphdf5::dset\_id\_s, sphdf5::dset\_id\_s, sphdf5::dset\_id\_s, sphdf5::dset\_id\_s, sphdf5::file\_id, sphdf5::filespace\_diotadxup, sphdf5::filespace = \_\_fiota, sphdf5::filespace\_r, sphdf5::filespace\_s, sphdf5::filespace\_s, sphdf5::filespace\_t, sphdf5::filespace\_t, sphdf5::grptransform, sphdf5::hdfier, sphdf5::memspace\_diotadxup, sphdf5::memspace=c, sphdf5::memspace=c, sphdf5::memspace\_t, sphdf5::memspace\_z, inputlist = ::nppts, allglobal::nz, sphdf5::rankp, and sphdf5::rankt.

Referenced by pp00aa().

Here is the caller graph for this function:



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Write a hyperslab of Poincare data corresponding to the output of one parallel worker.

#### **Parameters**

offset radial offset at which the data belongs	
data	output from field-line tracing
success	flags to indicate if integrator was successful

References sphdf5::dset\_id\_r, sphdf5::dset\_id\_s, sphdf5::dset\_id\_success, sphdf5::dset\_id\_t, sphdf5::dset\_id \_z, sphdf5::filespace\_r, sphdf5::filespace\_s, sphdf5::filespace\_success, sphdf5::filespace\_t, sphdf5::filespace\_c z, sphdf5::memspace\_r, sphdf5::memspace\_s, sphdf5::memspace\_s, sphdf5::memspace\_t, sphdf5::memspace\_t, sphdf5::memspace\_t, sphdf5::memspace\_z, inputlist::nppts, and allglobal::nz.

Referenced by pp00aa().

Here is the caller graph for this function:



Write the rotational transform output from field line following.

## **Parameters**

offset	ffset radial offset at which the data belongs	
length length of dataset to write		
Ivol	nested volume index	
diotadxup	derivative of rotational transform (?)	
fiota	rotational transform	

References sphdf5::dset\_id\_diotadxup, sphdf5::dset\_id\_fiota, sphdf5::filespace\_diotadxup, sphdf5::filespace\_fiota, sphdf5::hdfier, sphdf5::memspace\_diotadxup, sphdf5::memspace\_fiota, and sphdf5::rankt.

Referenced by pp00aa().

Here is the caller graph for this function:



## 5.18.2.8 finalize\_flt\_output() subroutine sphdf5::finalize\_flt\_output

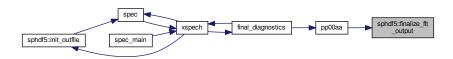
Finalize Poincare output.

This closes the still-open datasets related to field-line tracing, which had to be kept open during the tracing to be able to write the outputs directly when a given worker thread is finished.

References sphdf5::dset\_id\_diotadxup, sphdf5::dset\_id\_fiota, sphdf5::dset\_id\_r, sphdf5::dset\_id\_s, sphdf5::dset id\_s, sphdf5::dset\_id\_s, sphdf5::dset\_id\_s, sphdf5::dset\_id\_z, sphdf5::filespace\_diotadxup, sphdf5::filespace\_fiota, sphdf5::filespace\_fiota, sphdf5::filespace\_r, sphdf5::filespace\_s, sphdf5::filespace\_s, sphdf5::filespace\_t, sphdf5::filespace\_z, sphdf5::grppoincare, sphdf5::grptransform, sphdf5::hdfier, sphdf5::memspace\_diotadxup, sphdf5::memspace\_r, sphdf5::memspace\_r, sphdf5::memspace\_z, sphdf5::memspace\_z.

Referenced by pp00aa().

Here is the caller graph for this function:



```
5.18.2.9 write_vector_potential() subroutine sphdf5::write_vector_potential (
    integer, intent(in) sumLrad,
    real, dimension(:,:), intent(in) allAte,
    real, dimension(:,:), intent(in) allAze,
    real, dimension(:,:), intent(in) allAto,
    real, dimension(:,:), intent(in) allAzo)
```

Write the magnetic vector potential Fourier harmonics to the output file group /vector potential.

The data is stacked in the radial direction over Lrad, since Lrad can be different in each volume, but HDF5 only supports rectangular arrays. So, one needs to split the sumLrad dimension into chunks given by the input Lrad array.

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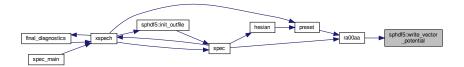
#### **Parameters**

sumLrad	total sum over Lrad in all nested volumes
allAte	$A_{\mathrm{even}}^{ heta}$ for all nested volumes
allAze	$A_{ m even}^{\zeta}$ for all nested volumes
allAto	$A_{\mathrm{odd}}^{ heta}$ for all nested volumes
allAzo	$A_{\mathrm{odd}}^{\zeta}$ for all nested volumes

References sphdf5::file id, and allglobal::mn.

Referenced by ra00aa().

Here is the caller graph for this function:



# 5.18.2.10 hdfint() subroutine sphdf5::hdfint

Write the final state of the equilibrium to the output file.

- In addition to the input variables, which are described in global(), the following quantities are written to ext. ← sp.h5:
- All quantities marked as real should be treated as double precision.

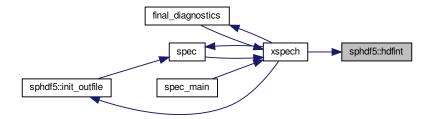
References inputlist::adiabatic, allglobal::beltramierror, inputlist::bnc, inputlist::bns, allglobal::bsupumn, allglobal::bsupumn, allglobal::bsupumn, allglobal::btomn, allglobal::btomn, allglobal::bzomn, allglobal::cpus, allglobal::drbc, allglobal::drbc, allglobal::drbc, allglobal::drbc, allglobal::ibnc, allglobal::ibnc, allglobal::ibnc, allglobal::in, allglobal::irbc, allglobal::irbc, allglobal::irbs, allglobal::ivnc, allglobal::ivns, inputlist::ivolume, allglobal::izbc, allglobal::izbc, inputlist::lcheck, allglobal::lmns, inputlist::lperturbed, inputlist::lrad, allglobal::mn, inputlist::mu, allglobal::ncpu, inputlist::nvol, fileunits::ounit, inputlist::pflux, inputlist::rbc, inputlist::rbs, inputlist::tflux, allglobal::tt, inputlist::vnc, inputlist::vns, volume(), allglobal::vvolume, inputlist::zbc, and inputlist::zbs.

Referenced by xspech().

Here is the call graph for this function:



Here is the caller graph for this function:



## 5.19 Coordinate axis

### **Functions/Subroutines**

• subroutine rzaxis (Mvol, mn, inRbc, inZbs, inRbs, inZbc, ivol, LcomputeDerivatives)

The coordinate axis is assigned via a poloidal average over an arbitrary surface.

## 5.19.1 Detailed Description

## 5.19.2 Function/Subroutine Documentation

The coordinate axis is assigned via a poloidal average over an arbitrary surface.

Specifies position of coordinate axis;  $\mathbf{x}_a(\zeta) \equiv \int \mathbf{x}_1(\theta, \zeta) dl / \int dl$ .

## coordinate axis

- The coordinate axis is *not* an independent degree-of-freedom of the geometry. It is constructed by extrapolating the geometry of a given interface, as determined by  $i \equiv \mathtt{ivol}$  which is given on input, down to a line
- If the coordinate axis depends only on the *geometry* of the interface and not the angle parameterization, then the block tri-diagonal structure of the the force-derivative matrix is preserved.

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· Define the arc-length-weighted averages,

$$R_0(\zeta) \equiv \frac{\int_0^{2\pi} R_i(\theta, \zeta) \, dl}{\int_0^{2\pi} dl}, \qquad Z_0(\zeta) \equiv \frac{\int_0^{2\pi} Z_i(\theta, \zeta) \, dl}{\int_0^{2\pi} dl}, \tag{217}$$

where  $dl \equiv \dot{l} d\theta = \sqrt{\partial_{\theta} R_i(\theta, \zeta)^2 + \partial_{\theta} Z_i(\theta, \zeta)^2} d\theta$ .

- (Note that if l does not depend on  $\theta$ , i.e. if  $\theta$  is the equal arc-length angle, then the expressions simplify. This constraint is not enforced.)
- The geometry of the coordinate axis thus constructed only depends on the geometry of the interface, i.e. the angular parameterization of the interface is irrelevant.

### coordinate axis: derivatives

 The derivatives of the coordinate axis with respect to the Fourier harmonics of the given interface are given by

$$\frac{\partial R_0}{\partial R_{i,j}^c} = \int \left(\cos \alpha_j \, \dot{l} - \Delta R_i R_{i,\theta} \, m_j \sin \alpha_j / \, \dot{l}\right) d\theta / L \tag{218}$$

$$\frac{\partial R_0}{\partial R_{i,j}^s} = \int \left( \sin \alpha_j \ \dot{l} + \Delta R_i R_{i,\theta} \ m_j \cos \alpha_j / \ \dot{l} \right) d\theta / L \tag{219}$$

$$\frac{\partial R_0}{\partial Z_{i,j}^c} = \int \left( -\Delta R_i Z_{i,\theta} \, m_j \sin \alpha_j / \, \dot{l} \right) d\theta / L \tag{220}$$

$$\frac{\partial R_{0}^{\sigma}}{\partial Z_{i,j}^{s}} = \int \left( +\Delta R_{i} Z_{i,\theta} \, m_{j} \cos \alpha_{j} / \, \dot{l} \right) d\theta / L \tag{221}$$

$$\frac{\partial Z_0}{\partial R_{i,j}^c} = \int \left( -\Delta Z_i R_{i,\theta} \, m_j \sin \alpha_j / \, \dot{l} \right) d\theta / L \tag{222}$$

$$\frac{\partial Z_0}{\partial R_{i,j}^s} = \int \left( +\Delta Z_i R_{i,\theta} \, m_j \cos \alpha_j / \, \dot{l} \right) d\theta / L \tag{223}$$

$$\frac{\partial Z_0}{\partial Z_{i,j}^c} = \int \left(\cos \alpha_j \ \dot{l} - \Delta Z_i Z_{i,\theta} \ m_j \sin \alpha_j / \ \dot{l}\right) d\theta / L \tag{224}$$

$$\frac{\partial Z_0}{\partial Z_{i,j}^s} = \int \left( \sin \alpha_j \ \dot{l} + \Delta Z_i Z_{i,\theta} \ m_j \cos \alpha_j / \ \dot{l} \right) d\theta / L \tag{225}$$

where 
$$L(\zeta) \equiv \int_0^{2\pi}\!\!dl.$$

## some numerical comments

- First, the differential poloidal length,  $\dot{l} \equiv \sqrt{R_{\theta}^2 + Z_{\theta}^2}$ , is computed in real space using an inverse FFT from the Fourier harmonics of R and Z.
- Second, the Fourier harmonics of dl are computed using an FFT. The integration over  $\theta$  to construct  $L \equiv \int dl$  is now trivial: just multiply the m=0 harmonics of dl by  $2\pi$ . The ajk (1:mn) variable is used, and this is assigned in readin().
- Next, the weighted R dl and Z dl are computed in real space, and the poloidal integral is similarly taken.
- Last, the Fourier harmonics are constructed using an FFT after dividing in real space.

### **Parameters**

in	Mvol	
in	mn	
	iRbc	
	iZbs	
	iRbs	
	iZbc	
in	ivol	
	LcomputeDerivatives	

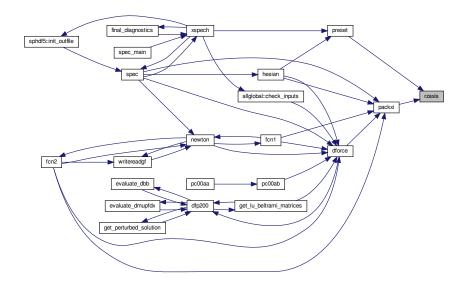
References allglobal::ajk, allglobal::cfmn, allglobal::comn, coords(), allglobal::cosi, allglobal::cpus, allglobal::dbdx, allglobal::dradz, allglobal::dradz, allglobal::dradz, allglobal::dzadz, allglobal::ijimag, allglobal::ipmag, allglobal::ipmag, allglobal::ipmag, allglobal::ipmag, allglobal::ipmag, allglobal::jimag, allglobal::jimag, allglobal::jimag, allglobal::jimag, allglobal::jimag, allglobal::jimag, allglobal::jimag, allglobal::jimag, allglobal::jimag, allglobal::myid, allglobal::myid, allglobal::myid, allglobal::myid, allglobal::mz, allglobal::nz, allglobal::nz, allglobal::nz, allglobal::nz, allglobal::mag, allglobal::simn, allglobal::simn, allglobal::simn, constants::one, fileunits::ounit, allglobal::yesstellsym, constants::zero, and allglobal::zij.

Referenced by packxi(), and preset().

Here is the call graph for this function:



Here is the caller graph for this function:



# 5.20 Rotational Transform

### **Functions/Subroutines**

subroutine tr00ab (Ivol, mn, NN, Nt, Nz, iflag, Idiota)
 Calculates rotational transform given an arbitrary tangential field.

## 5.20.1 Detailed Description

### 5.20.2 Function/Subroutine Documentation

```
5.20.2.1 tr00ab() subroutine tr00ab (
    integer, intent(in) lvol,
    integer, intent(in) mn,
    integer, intent(in) NN,
    integer, intent(in) Nt,
    integer, intent(in) Nz,
    integer, intent(in) iflag,
    real, dimension(0:1,-1:2), intent(inout) ldiota )
```

Calculates rotational transform given an arbitrary tangential field.

Calculates transform,  $\iota = \dot{\theta}(1 + \lambda_{\theta}) + \lambda_{\zeta}$ , given  $\mathbf{B}|_{\mathcal{I}}$ .

## constructing straight field line angle on interfaces

• The algorithm stems from introducing a straight field line angle  $\theta_s=\theta+\lambda(\theta,\zeta)$ , where

$$\lambda = \sum_{j} \lambda_{o,j} \sin(m_j \theta - n_j \zeta) + \sum_{j} \lambda_{e,j} \cos(m_j \theta - n_j \zeta)$$
 (226)

and insisting that

$$\frac{\mathbf{B} \cdot \nabla \theta_s}{\mathbf{B} \cdot \nabla \zeta} = \dot{\theta} (1 + \lambda_{\theta}) + \lambda_{\zeta} = \pm, \tag{227}$$

where + is a constant that is to be determined.

• Writing  $\dot{\theta}=-\partial_s A_\zeta/\partial_s A_\theta$ , we have

$$\partial_s A_\theta + \partial_s A_\zeta \lambda_\theta - \partial_s A_\theta \lambda_\zeta = -\partial_s A_\zeta \tag{228}$$

· Expanding this equation we obtain

$$(A'_{\theta,e,k}\cos\alpha_k + A'_{\theta,o,k}\sin\alpha_k) +$$

$$+ (A'_{\zeta,e,k}\cos\alpha_k + A'_{\zeta,o,k}\sin\alpha_k) (+m_j\lambda_{o,j}\cos\alpha_j - m_j\lambda_{e,j}\sin\alpha_j)$$

$$- (A'_{\theta,e,k}\cos\alpha_k + A'_{\theta,o,k}\sin\alpha_k) (-n_j\lambda_{o,j}\cos\alpha_j + n_j\lambda_{e,j}\sin\alpha_j)$$

$$= - (A'_{\zeta,e,k}\cos\alpha_k + A'_{\zeta,o,k}\sin\alpha_k), \qquad (229)$$

where summation over k=1, mn and j=2, mns is implied

· After applying double angle formulae,

$$(A'_{\theta,e,k}\cos\alpha_k + A'_{\theta,o,k}\sin\alpha_k) +$$

$$+ \lambda_{o,j} (+m_j A'_{\zeta,e,k} + n_j A'_{\theta,e,k}) [+\cos(\alpha_k + \alpha_j) + \cos(\alpha_k - \alpha_j)] / 2$$

$$+ \lambda_{e,j} (-m_j A'_{\zeta,e,k} - n_j A'_{\theta,e,k}) [+\sin(\alpha_k + \alpha_j) - \sin(\alpha_k - \alpha_j)] / 2$$

$$+ \lambda_{o,j} (+m_j A'_{\zeta,o,k} + n_j A'_{\theta,o,k}) [+\sin(\alpha_k + \alpha_j) + \sin(\alpha_k - \alpha_j)] / 2$$

$$+ \lambda_{e,j} (-m_j A'_{\zeta,o,k} - n_j A'_{\theta,o,k}) [-\cos(\alpha_k + \alpha_j) + \cos(\alpha_k - \alpha_j)] / 2$$

$$= - (A'_{\zeta,e,k}\cos\alpha_k + A'_{\zeta,o,k}\sin\alpha_k) ,$$
(230)

and equating coefficients, an equation of the form  $\mathbf{A} \cdot \mathbf{x} = \mathbf{b}$  is obtained, where

$$\mathbf{x} = \left(\underbrace{t}_{\mathbf{x}[1]}, \underbrace{\lambda_{o,2}, \lambda_{o,3}, \dots}_{\mathbf{x}[2:N]}, \underbrace{\lambda_{e,2}, \lambda_{e,3}, \dots}_{\mathbf{x}[N+1:2N-1]}\right)^{T}.$$
(231)

### alternative iterative method

• Consider the equation  $\dot{\theta}(1+\lambda_{\theta})+\lambda_{\zeta}=\pm$ , where  $\lambda=\sum_{j}\lambda_{j}\sin\alpha_{j}$ , given on a grid

$$\dot{\theta}_i + \dot{\theta}_i \sum_j m_j \cos \alpha_{i,j} \lambda_j - \sum_j n_j \cos \alpha_{i,j} \lambda_j = \pm, \tag{232}$$

where i labels the grid point.

· This is a matrix equation...

## **Parameters**

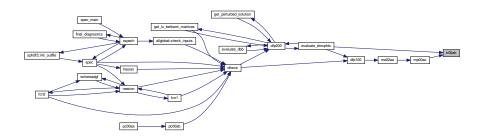
Ivol	
mn	
NN	
Nt	
Nz	
iflag	
Idiota	

References allglobal::cpus, allglobal::glambda, constants::goldenmean, constants::half, allglobal::im, inputlist::imethod, allglobal::ims, allglobal::ins, inputlist::iorder, inputlist::iotatol, inputlist::iprecon, inputlist::lrad, inputlist::lsparse, inputlist::lsvdiota, numerical::machprec, allglobal::mns, allglobal::mpi\_comm\_spec, inputlist::mpol, allglobal::myid, allglobal::ncpu, allglobal::notstellsym, inputlist::ntor, inputlist::nvol, constants::one, fileunits ::ounit, constants::pi2, numerical::small, numerical::sqrtmachprec, constants::third, constants::two, numerical ::vsmall, inputlist::wmacros, allglobal::yesstellsym, and constants::zero.

Referenced by evaluate\_dmupfdx(), and mp00ac().

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Here is the caller graph for this function:



#### 5.21 Plasma volume

### **Functions/Subroutines**

• subroutine volume (Ivol, vflag)

Computes volume of each region; and, if required, the derivatives of the volume with respect to the interface geometry.

# 5.21.1 Detailed Description

### 5.21.2 Function/Subroutine Documentation

Computes volume of each region; and, if required, the derivatives of the volume with respect to the interface geom-

Calculates volume of each region;  $V_i \equiv \int dv$ .

# volume integral

ullet The volume enclosed by the v-th interface is given by the integral

$$V = \int_{\mathcal{V}} dv = \frac{1}{3} \int_{\mathcal{V}} \nabla \cdot \mathbf{x} \, dv = \frac{1}{3} \int_{\mathcal{S}} \mathbf{x} \cdot d\mathbf{s} = \frac{1}{3} \int_{0}^{2\pi} d\theta \int_{0}^{2\pi/N} d\zeta \quad \mathbf{x} \cdot \mathbf{x}_{\theta} \times \mathbf{x}_{\zeta}|^{s}$$
(233)

where we have used  $\nabla \cdot \mathbf{x} = 3$ , and have assumed that the domain is periodic in the angles.

## representation of surfaces

· The coordinate functions are

$$R(\theta,\zeta) = \sum_{i} R_{e,i} \cos \alpha_i + \sum_{i} R_{o,i} \sin \alpha_i$$
 (234)

$$R(\theta,\zeta) = \sum_{i} R_{e,i} \cos \alpha_{i} + \sum_{i} R_{o,i} \sin \alpha_{i}$$

$$Z(\theta,\zeta) = \sum_{i} Z_{e,i} \cos \alpha_{i} + \sum_{i} Z_{o,i} \sin \alpha_{i},$$
(234)

where  $\alpha_i \equiv m_i \theta - n_i \zeta$ .

### geometry

- The geometry is controlled by the input parameter Igeometry as follows:
- Igeometry.eq.1: Cartesian:  $\sqrt{g}=R_s$

$$V = \int_0^{2\pi} d\theta \int_0^{2\pi/N} d\zeta R$$
$$= 2\pi \frac{2\pi}{N} R_{e,1}$$
(236)

• Igeometry.eq.2: cylindrical:  $\sqrt{g}=RR_s=\frac{1}{2}\partial_s(R^2)$ 

$$V = \frac{1}{2} \int_{0}^{2\pi} d\theta \int_{0}^{2\pi/N} d\zeta R^{2}$$

$$= \frac{1}{2} 2\pi \frac{2\pi}{N} \frac{1}{2} \sum_{i} \sum_{j} R_{e,i} R_{e,j} \left[ \cos(\alpha_{i} - \alpha_{j}) + \cos(\alpha_{i} + \alpha_{j}) \right]$$

$$+ \frac{1}{2} 2\pi \frac{2\pi}{N} \frac{1}{2} \sum_{i} \sum_{j} R_{o,i} R_{o,j} \left[ \cos(\alpha_{i} - \alpha_{j}) - \cos(\alpha_{i} + \alpha_{j}) \right]$$
(237)

• Igeometry.eq.3: toroidal:  $\mathbf{x} \cdot \mathbf{e}_{\theta} \times \mathbf{e}_{\zeta} = R(ZR_{\theta} - RZ_{\theta})$  This is computed by fast Fourier transform:

$$V = \frac{1}{3} \int_{0}^{2\pi} d\theta \int_{0}^{2\pi/N} d\zeta R(ZR_{\theta} - RZ_{\theta})$$

$$= \frac{1}{3} \sum_{i} \sum_{j} \sum_{k} R_{e,i} (Z_{e,j}R_{o,k} - R_{e,j}Z_{o,k}) (+m_{k}) \iint d\theta d\zeta \cos \alpha_{i} \cos \alpha_{j} \cos \alpha_{k}$$

$$+ \frac{1}{3} \sum_{i} \sum_{j} \sum_{k} R_{e,i} (Z_{o,j}R_{e,k} - R_{o,j}Z_{e,k}) (-m_{k}) \iint d\theta d\zeta \cos \alpha_{i} \sin \alpha_{j} \sin \alpha_{k}$$

$$+ \frac{1}{3} \sum_{i} \sum_{j} \sum_{k} R_{o,i} (Z_{e,j}R_{e,k} - R_{e,j}Z_{e,k}) (-m_{k}) \iint d\theta d\zeta \sin \alpha_{i} \cos \alpha_{j} \sin \alpha_{k}$$

$$+ \frac{1}{3} \sum_{i} \sum_{j} \sum_{k} R_{o,i} (Z_{o,j}R_{o,k} - R_{o,j}Z_{o,k}) (+m_{k}) \iint d\theta d\zeta \sin \alpha_{i} \sin \alpha_{j} \cos \alpha_{k}$$

$$(238)$$

- (Recall that the integral over an odd function is zero, so various terms in the above expansion have been ignored.)
- · The trigonometric terms are

$$4 \cos \alpha_i \cos \alpha_j \cos \alpha_k = + \cos(\alpha_i + \alpha_j + \alpha_k) + \cos(\alpha_i + \alpha_j - \alpha_k) + \cos(\alpha_i - \alpha_j + \alpha_k) + \cos(\alpha_i - \alpha_j - \alpha_k)$$

$$4 \cos \alpha_i \sin \alpha_j \sin \alpha_k = - \cos(\alpha_i + \alpha_j + \alpha_k) + \cos(\alpha_i + \alpha_j - \alpha_k) + \cos(\alpha_i - \alpha_j + \alpha_k) - \cos(\alpha_i - \alpha_j - \alpha_k)$$

$$4 \sin \alpha_i \cos \alpha_j \sin \alpha_k = - \cos(\alpha_i + \alpha_j + \alpha_k) + \cos(\alpha_i + \alpha_j - \alpha_k) - \cos(\alpha_i - \alpha_j + \alpha_k) + \cos(\alpha_i - \alpha_j - \alpha_k)$$

$$4 \sin \alpha_i \sin \alpha_j \cos \alpha_k = - \cos(\alpha_i + \alpha_j + \alpha_k) - \cos(\alpha_i + \alpha_j - \alpha_k) + \cos(\alpha_i - \alpha_j + \alpha_k) + \cos(\alpha_i - \alpha_j - \alpha_k)$$

· The required derivatives are

$$3\frac{\partial V}{\partial R_{e,i}} = (+Z_{e,j}R_{o,k}m_k - R_{e,j}Z_{o,k}m_k - R_{e,j}Z_{o,k}m_k) \qquad \iint d\theta d\zeta \cos \alpha_i \cos \alpha_j \cos \alpha_k$$

$$+ (-Z_{o,j}R_{e,k}m_k + R_{o,j}Z_{e,k}m_k + R_{o,j}Z_{e,k}m_k) \qquad \iint d\theta d\zeta \cos \alpha_i \sin \alpha_j \sin \alpha_k$$

$$+ (-R_{o,k}Z_{e,j}m_i) \qquad \qquad \iint d\theta d\zeta \sin \alpha_i \cos \alpha_j \sin \alpha_k$$

$$+ (-R_{e,k}Z_{o,j}m_i) \qquad \qquad \iint d\theta d\zeta \sin \alpha_i \sin \alpha_j \cos \alpha_k$$

$$(240)$$

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$$3\frac{\partial V}{\partial Z_{o,i}} = (-R_{e,k}R_{e,j}m_i) \quad \iint d\theta d\zeta \cos \alpha_i \cos \alpha_j \cos \alpha_k$$

$$+ (-R_{o,k}R_{o,j}m_i) \quad \iint d\theta d\zeta \cos \alpha_i \sin \alpha_j \sin \alpha_k$$

$$+ (-R_{e,j}R_{e,k}m_k) \quad \iint d\theta d\zeta \sin \alpha_i \cos \alpha_j \sin \alpha_k$$

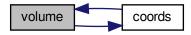
$$+ (+R_{o,j}R_{o,k}m_k) \quad \iint d\theta d\zeta \sin \alpha_i \sin \alpha_j \cos \alpha_k$$

$$(241)$$

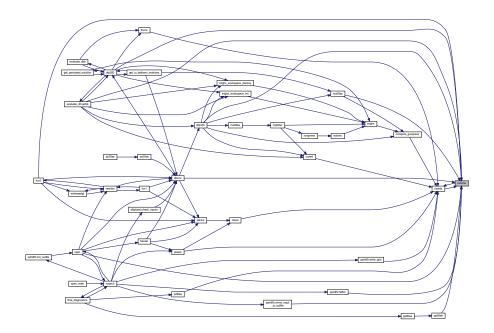
References coords(), allglobal::cosi, allglobal::cpus, allglobal::dbdx, allglobal::djkm, allglobal::djkp, allglobal::djkp, allglobal::dvolume, constants::four, constants::half, inputlist::igeometry, allglobal::im, allglobal::in, allglobal::irbc, allglobal::irbc, allglobal::mn, allglobal::mpi\_comm\_spec, allglobal::myid, allglobal::ntz, inputlist::nvol, constants::one, fileunits::ounit, constants::pi2, inputlist::pscale, constants::quart, allglobal::rij, allglobal::sini, numerical::small, constants::third, constants::two, numerical::vsmall, allglobal::vvolume, allglobal::vijesstellsym, constants::zero, and allglobal::zij.

Referenced by coords(), dforce(), dfp100(), dfp200(), evaluate\_dmupfdx(), fcn2(), sphdf5::hdfint(), ma00aa(), sphdf5::mirror\_input\_to\_outfile(), pp00ab(), and spec().

Here is the call graph for this function:



Here is the caller graph for this function:



# 5.22 Smooth boundary

### **Functions/Subroutines**

• subroutine wa00aa (iwa00aa)

Constructs smooth approximation to wall.

subroutine vacuumphi (Nconstraints, rho, fvec, iflag)

Compute vacuum magnetic scalar potential (?)

## 5.22.1 Detailed Description

### 5.22.2 Function/Subroutine Documentation

```
5.22.2.1 wa00aa() subroutine wa00aa ( integer iwa00aa )
```

Constructs smooth approximation to wall.

## solution of Laplace's equation in two-dimensions

- · The wall is given by a discrete set of points.
- · The points must go anti-clockwise.

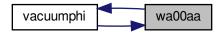
References laplaces::alpha, laplaces::cc, allglobal::cpus, laplaces::dorm, laplaces::exterior, fileunits::gunit, constants::half, laplaces::iangle, laplaces::ic, laplaces::icint, allglobal::im, allglobal::in, allglobal::irbc, allglobal::irbc, allglobal::irbs, allglobal::izbs, allglobal::lcoordinatesingularity, allglobal::mn, inputlist::mpol, allglobal::myid, allglobal::ncpu, laplaces::nintervals, laplaces::niterations, laplaces::np1, laplaces::np4, laplaces::nsegments, allglobal::nt, inputlist::ntor, allglobal::ntz, inputlist::nvol, allglobal::nz, inputlist::odetol, constants::one, laplaces::rmid, laplaces::phid, constants::pi2, allglobal::rij, laplaces::rmid, laplaces::stage1, constants::ten, vacuumphi(), numerical::vsmall, inputlist::wmacros, laplaces::xpoly, allglobal::yesstellsym, laplaces::ypoly, constants::zero, and allglobal::zij.

Referenced by vacuumphi().

Here is the call graph for this function:



Here is the caller graph for this function:



Compute vacuum magnetic scalar potential (?)

## **Parameters**

Nconstraints	
rho	
fvec	
iflag	

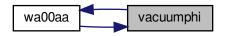
References laplaces::alpha, laplaces::cc, allglobal::cpus, laplaces::dorm, laplaces::exterior, constants::half, laplaces::iangle, laplaces::ic, laplaces::icint, allglobal::myid, allglobal::ncpu, laplaces::nintervals, laplaces::niterations, laplaces::np1, laplaces::np4, laplaces::nsegments, allglobal::ntz, constants::one, laplaces::originalalpha, fileunits::ounit, laplaces::phi, laplaces::phid, constants::pi2, allglobal::rij, laplaces::rmid, laplaces::stage1, wa00aa(), inputlist::wmacros, laplaces::xpoly, laplaces::ypoly, constants::zero, and allglobal::zij.

Referenced by wa00aa().

Here is the call graph for this function:



Here is the caller graph for this function:



## 5.23 Enhanced resolution for metric elements

Enhanced resolution is required for the metric elements,  $g_{ij}/\sqrt{g}$ , which is given by mne, ime, and ine. The Fourier resolution here is determined by 1 Mpol = 2 Mpol and 1 Ntor = 2 Ntor.

### **Variables**

- integer allglobal::mne
  - enhanced resolution for metric elements
- integer, dimension(:), allocatable allglobal::ime
   enhanced poloidal mode numbers for metric elements
- integer, dimension(:), allocatable allglobal::ine
   enhanced toroidal mode numbers for metric elements

# 5.23.1 Detailed Description

Enhanced resolution is required for the metric elements,  $g_{ij}/\sqrt{g}$ , which is given by mne, ime, and ine. The Fourier resolution here is determined by 1 Mpol = 2 Mpol and 1 Ntor = 2 Ntor.

# 5.24 Enhanced resolution for transformation to straight-field line angle

Enhanced resolution is required for the transformation to straight-field line angle on the interfaces, which is given by mns, ims and ins. The Fourier resolution here is determined by iMpol and iNtor.

## **Variables**

- · integer allglobal::mns
  - enhanced resolution for straight field line transformation
- integer, dimension(:), allocatable allglobal::ims
   enhanced poloidal mode numbers for straight field line transformation
- integer, dimension(:), allocatable allglobal::ins
  - enhanced toroidal mode numbers for straight field line transformation

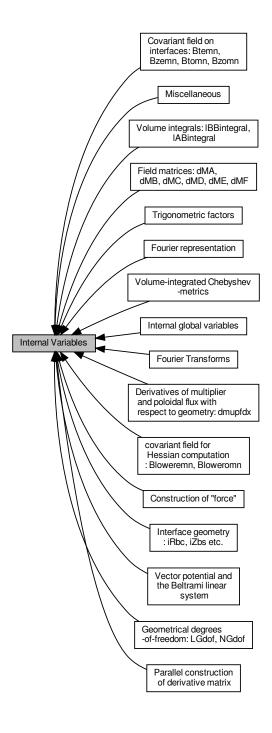
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## 5.24.1 Detailed Description

Enhanced resolution is required for the transformation to straight-field line angle on the interfaces, which is given by mns, ims and ins. The Fourier resolution here is determined by iMpol and iNtor.

## 5.25 Internal Variables

Collaboration diagram for Internal Variables:



## **Modules**

- · Fourier representation
- · Interface geometry: iRbc, iZbs etc.

The Fourier harmonics of the interfaces are contained in iRbc(1:mn, 0:Mvol) and iZbs(1:mn, 0:Mvol), where iRbc(1, j), iZbs(1, j) contains the Fourier harmonics,  $R_j$ ,  $Z_j$ , of the l-th interface.

· Fourier Transforms

The coordinate geometry and fields are mapped to/from Fourier space and real space using FFTW3. The resolution of the real space grid is given by Nt=Ndiscrete\*4\*Mpol and Nz=Ndiscrete\*4\*Ntor.

Volume-integrated Chebyshev-metrics

These are allocated in dforce(), defined in ma00aa(), and are used in matrix() to construct the matrices.

- · Vector potential and the Beltrami linear system
- Field matrices: dMA, dMB, dMC, dMD, dME, dMF
- · Construction of "force"

The force vector is comprised of Bomn and Iomn.

· Covariant field on interfaces: Btemn, Bzemn, Btomn, Bzomn

The covariant field.

- covariant field for Hessian computation: Bloweremn, Bloweromn
- · Geometrical degrees-of-freedom: LGdof, NGdof

The geometrical degrees-of-freedom.

- Parallel construction of derivative matrix
- · Derivatives of multiplier and poloidal flux with respect to geometry: dmupfdx
- · Trigonometric factors
- · Volume integrals: IBBintegral, IABintegral
- · Internal global variables

internal global variables; internal logical variables; default values are provided here; these may be changed according to input values

Miscellaneous

The following are miscellaneous flags required for the virtual casing field, external (vacuum) field integration, ...

# Variables

type(derivative) allglobal::dbdx

 $d\mathbf{B}/d\mathbf{X}$  (?)

### 5.25.1 Detailed Description

## 5.26 Fourier representation

Collaboration diagram for Fourier representation:



### **Variables**

· integer allglobal::mn

total number of Fourier harmonics for coordinates/fields; calculated from Mpol, Ntor in readin()

• integer, dimension(:), allocatable allglobal::im

poloidal mode numbers for Fourier representation

integer, dimension(:), allocatable allglobal::in

toroidal mode numbers for Fourier representation

real, dimension(:), allocatable allglobal::halfmm

I saw this already somewhere...

• real, dimension(:), allocatable allglobal::regumm

I saw this already somewhere...

· real allglobal::rscale

no idea

· real, dimension(:,:), allocatable allglobal::psifactor

no idea

real, dimension(:,:), allocatable allglobal::inifactor

no idea

 real, dimension(:), allocatable allglobal::bbweight weight on force-imbalance harmonics; used in dforce()

• real, dimension(:), allocatable allglobal::mmpp

spectral condensation factors

### 5.26.1 Detailed Description

## 5.27 Interface geometry: iRbc, iZbs etc.

The Fourier harmonics of the interfaces are contained in iRbc(1:mn, 0:Mvol) and iZbs(1:mn, 0:Mvol), where iRbc(1, j), iZbs(1, j) contains the Fourier harmonics,  $R_j$ ,  $Z_j$ , of the l-th interface.

Collaboration diagram for Interface geometry: iRbc, iZbs etc.:



## **Variables**

- real, dimension(:,:), allocatable allglobal::irbc
   cosine R harmonics of interface surface geometry; stellarator symmetric
- real, dimension(:,:), allocatable allglobal::izbs

sine Z harmonics of interface surface geometry; stellarator symmetric

real, dimension(:,:), allocatable allglobal::irbs

sine R harmonics of interface surface geometry; non-stellarator symmetric

```
    real, dimension(:,:), allocatable allglobal::izbc
    cosine Z harmonics of interface surface geometry; non-stellarator symmetric
```

• real, dimension(:,:), allocatable allglobal::drbc

cosine R harmonics of interface surface geometry; stellarator symmetric; linear deformation

real, dimension(:,:), allocatable allglobal::dzbs

sine Z harmonics of interface surface geometry; stellarator symmetric; linear deformation

real, dimension(:,:), allocatable allglobal::drbs

sine R harmonics of interface surface geometry; non-stellarator symmetric; linear deformation

real, dimension(:,:), allocatable allglobal::dzbc

cosine Z harmonics of interface surface geometry; non-stellarator symmetric; linear deformation

• real, dimension(:,:), allocatable allglobal::irij

interface surface geometry; real space

• real, dimension(:,:), allocatable allglobal::izij

interface surface geometry; real space

real, dimension(:,:), allocatable allglobal::drij

interface surface geometry; real space

• real, dimension(:,:), allocatable allglobal::dzij

interface surface geometry; real space

• real, dimension(:,:), allocatable allglobal::trij

interface surface geometry; real space

real, dimension(:,:), allocatable allglobal::tzij

interface surface geometry; real space

• real, dimension(:), allocatable allglobal::ivns

sine harmonics of vacuum normal magnetic field on interfaces; stellarator symmetric

real, dimension(:), allocatable allglobal::ibns

sine harmonics of plasma normal magnetic field on interfaces; stellarator symmetric

real, dimension(:), allocatable allglobal::ivnc

cosine harmonics of vacuum normal magnetic field on interfaces; non-stellarator symmetric

real, dimension(:), allocatable allglobal::ibnc

cosine harmonics of plasma normal magnetic field on interfaces; non-stellarator symmetric

• real, dimension(:), allocatable allglobal::lrbc

local workspace

• real, dimension(:), allocatable allglobal::lzbs

local workspace

real, dimension(:), allocatable allglobal::lrbs

local workspace

• real, dimension(:), allocatable allglobal::lzbc

local workspace

- integer allglobal::num\_modes
- integer, dimension(:), allocatable allglobal::mmrzrz
- integer, dimension(:), allocatable allglobal::nnrzrz
- real, dimension(:,:,:), allocatable allglobal::allrzrz

## 5.27.1 Detailed Description

The Fourier harmonics of the interfaces are contained in iRbc(1:mn, 0:Mvol) and iZbs(1:mn, 0:Mvol), where iRbc(1,j), iZbs(1,j) contains the Fourier harmonics,  $R_i$ ,  $Z_i$ , of the l-th interface.

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## 5.28 Fourier Transforms

The coordinate geometry and fields are mapped to/from Fourier space and real space using FFTW3. The resolution of the real space grid is given by Nt=Ndiscrete\*4\*Mpol and Nz=Ndiscrete\*4\*Ntor.

Collaboration diagram for Fourier Transforms:



#### **Variables**

· integer allglobal::nt

discrete resolution along  $\theta$  of grid in real space

integer allglobal::nz

discrete resolution along  $\zeta$  of grid in real space

· integer allglobal::ntz

discrete resolution; Ntz=Nt\*Nz shorthand

· integer allglobal::hnt

discrete resolution; Ntz=Nt\*Nz shorthand

integer allglobal::hnz

discrete resolution; Ntz=Nt\*Nz shorthand

· real allglobal::sontz

one / sqrt (one\*Ntz); shorthand

real, dimension(:,:,:), allocatable allglobal::rij

real-space grid; R

real, dimension(:,:,:), allocatable allglobal::zij

real-space grid; Z

real, dimension(:,:,:), allocatable allglobal::xij

what is this?

real, dimension(:,:,:), allocatable allglobal::yij

what is this?

real, dimension(:,:), allocatable allglobal::sg

real-space grid; jacobian and its derivatives

real, dimension(:,:,:,:), allocatable allglobal::guvij

real-space grid; metric elements

real, dimension(:,:,:), allocatable allglobal::gvuij

real-space grid; metric elements (?); 10 Dec 15;

• real, dimension(:,:,:), allocatable allglobal::guvijsave

what is this?

• integer, dimension(:,:), allocatable allglobal::ki

identification of Fourier modes

• integer, dimension(:,:,:), allocatable allglobal::kijs

identification of Fourier modes

- integer, dimension(:,:,:), allocatable allglobal::kija identification of Fourier modes
- integer, dimension(:), allocatable allglobal::iotakkii identification of Fourier modes
- integer, dimension(:,:), allocatable allglobal::iotaksub identification of Fourier modes
- integer, dimension(:,:), allocatable allglobal::iotakadd identification of Fourier modes
- integer, dimension(:,:), allocatable allglobal::iotaksgn identification of Fourier modes
- real, dimension(:), allocatable allglobal::efmn Fourier harmonics; dummy workspace.
- real, dimension(:), allocatable allglobal::ofmn Fourier harmonics; dummy workspace.
- real, dimension(:), allocatable allglobal::cfmn
   Fourier harmonics; dummy workspace.
- real, dimension(:), allocatable allglobal::sfmn
   Fourier harmonics; dummy workspace.
- real, dimension(:), allocatable allglobal::evmn Fourier harmonics; dummy workspace.
- real, dimension(:), allocatable allglobal::odmn
   Fourier harmonics; dummy workspace.
- real, dimension(:), allocatable allglobal::comn
   Fourier harmonics; dummy workspace.
- real, dimension(:), allocatable allglobal::simn
   Fourier harmonics; dummy workspace.
- real, dimension(:), allocatable allglobal::ijreal what is this?
- real, dimension(:), allocatable allglobal::ijimag
   what is this?
- real, dimension(:), allocatable allglobal::jireal what is this?
- real, dimension(:), allocatable allglobal::jiimag what is this?
- real, dimension(:), allocatable allglobal::jkreal what is this?
- real, dimension(:), allocatable allglobal::jkimag
   what is this ?
- real, dimension(:), allocatable allglobal::kjreal what is this?
- real, dimension(:), allocatable allglobal::kjimag
   what is this?
- $\bullet \quad \text{real, dimension}(:,:,:), \, \text{allocatable allglobal} :: bsupumn \\$ 
  - tangential field on interfaces;  $\theta$ -component; required for virtual casing construction of field; 11 Oct 12
- real, dimension(:,;,:), allocatable allglobal::bsupvmn
  - tangential field on interfaces;  $\zeta$  -component; required for virtual casing construction of field; 11 Oct 12
- real, dimension(:,:), allocatable allglobal::goomne described in preset()
- real, dimension(:,:), allocatable allglobal::goomno described in preset()
- real, dimension(:,:), allocatable allglobal::gssmne

described in preset()

- real, dimension(:,:), allocatable allglobal::gssmno described in preset()
- real, dimension(:,:), allocatable allglobal::gstmne described in preset()
- real, dimension(:,:), allocatable allglobal::gstmno described in preset()
- real, dimension(:,:), allocatable allglobal::gszmne described in preset()
- real, dimension(:,:), allocatable allglobal::gszmno described in preset()
- real, dimension(:,:), allocatable allglobal::gttmne described in preset()
- real, dimension(:,:), allocatable allglobal::gttmno described in preset()
- real, dimension(:,:), allocatable allglobal::gtzmne described in preset()
- real, dimension(:,:), allocatable allglobal::gtzmno described in preset()
- real, dimension(:,:), allocatable allglobal::gzzmne described in preset()
- real, dimension(:,:), allocatable allglobal::gzzmno described in preset()

## 5.28.1 Detailed Description

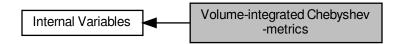
The coordinate geometry and fields are mapped to/from Fourier space and real space using FFTW3. The resolution of the real space grid is given by Nt=Ndiscrete\*4\*Mpol and Nz=Ndiscrete\*4\*Ntor.

Various workspace arrays are allocated. These include Rij(1:Ntz,0:3,0:3) and Zij(1:Ntz,0:3,0:3), which contain the coordinates in real space and their derivatives; sg(0:3,Ntz), which contains the Jacobian and its derivatives; and guv(0:6,0:3,1:Ntz), which contains the metric elements and their derivatives.

# 5.29 Volume-integrated Chebyshev-metrics

These are allocated in dforce(), defined in ma00aa(), and are used in matrix() to construct the matrices.

Collaboration diagram for Volume-integrated Chebyshev-metrics:



real, dimension(:,:,:,:), allocatable allglobal::dtoocc volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::dtoocs volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::dtoosc volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::dtooss volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::ttsscc volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::ttsscs volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::ttsssc volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::ttssss volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::tdstcc volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::tdstcs volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::tdstsc volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::tdstss volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::tdszcc volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::tdszcs volume-integrated Chebychev-metrics: see matrix() real, dimension(:,:,:,:), allocatable allglobal::tdszsc volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::tdszss volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::ddttcc volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::ddttcs volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::ddttsc volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::ddttss volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::ddtzcc volume-integrated Chebychev-metrics; see matrix() real, dimension(:.:::), allocatable allglobal::ddtzcs volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::ddtzsc volume-integrated Chebychev-metrics; see matrix() real, dimension(:,:,:,:), allocatable allglobal::ddtzss volume-integrated Chebychev-metrics; see matrix()

real, dimension(:,:,:,:), allocatable allglobal::ddzzcc

- volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:), allocatable allglobal::ddzzcs
   volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::ddzzsc volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:), allocatable allglobal::ddzzss
   volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:), allocatable allglobal::tsc what is this?
- real, dimension(:,:), allocatable allglobal::tss what is this?
- real, dimension(:,:), allocatable allglobal::dtc what is this?
- real, dimension(:,:), allocatable allglobal::dts
   what is this?
- real, dimension(:,:), allocatable allglobal::dzc what is this?
- real, dimension(:,:), allocatable allglobal::dzs what is this?
- real, dimension(:,:), allocatable allglobal::ttc what is this?
- real, dimension(:,:), allocatable allglobal::tzc what is this?
- real, dimension(:,:), allocatable allglobal::tts

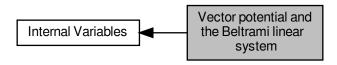
  what is this?
- real, dimension(:,:), allocatable allglobal::tzs what is this?
- real, dimension(:), allocatable allglobal::dtflux  $\delta \psi_{toroidal} \ \textit{in each annulus}$
- real, dimension(:), allocatable allglobal::dpflux  $\delta\psi_{poloidal}$  in each annulus
- real, dimension(:), allocatable allglobal::sweight minimum poloidal length constraint weight

## 5.29.1 Detailed Description

These are allocated in dforce(), defined in ma00aa(), and are used in matrix() to construct the matrices.

# 5.30 Vector potential and the Beltrami linear system

Collaboration diagram for Vector potential and the Beltrami linear system:



```
    integer, dimension(:), allocatable allglobal::nadof
degrees of freedom in Beltrami fields in each annulus
```

• integer, dimension(:), allocatable allglobal::nfielddof

degrees of freedom in Beltrami fields in each annulus, field only, no Lagrange multipliers

• type(subgrid), dimension(:,:,:), allocatable allglobal::ate

magnetic vector potential cosine Fourier harmonics; stellarator-symmetric

• type(subgrid), dimension(:,:,:), allocatable allglobal::aze

magnetic vector potential cosine Fourier harmonics; stellarator-symmetric

• type(subgrid), dimension(:,:,:), allocatable allglobal::ato

magnetic vector potential sine Fourier harmonics; non-stellarator-symmetric

type(subgrid), dimension(:,:,:), allocatable allglobal::azo

magnetic vector potential sine Fourier harmonics; non-stellarator-symmetric

• integer, dimension(:,:), allocatable allglobal::lma

Lagrange multipliers (?)

• integer, dimension(:,:), allocatable allglobal::Imb

Lagrange multipliers (?)

• integer, dimension(:,:), allocatable allglobal::lmc

Lagrange multipliers (?)

• integer, dimension(:,:), allocatable allglobal::Imd

Lagrange multipliers (?)

• integer, dimension(:,:), allocatable allglobal::lme

Lagrange multipliers (?)

integer, dimension(:,:), allocatable allglobal::lmf

Lagrange multipliers (?)

• integer, dimension(:,:), allocatable allglobal::Img

Lagrange multipliers (?)

integer, dimension(:,:), allocatable allglobal::lmh

Lagrange multipliers (?)

real, dimension(:,:), allocatable allglobal::lmavalue

what is this?

 real, dimension(:,:), allocatable allglobal::Imbvalue what is this?

real, dimension(:,:), allocatable allglobal::lmcvalue what is this?

 real, dimension(:,:), allocatable allglobal::Imdvalue what is this?

 real, dimension(:,:), allocatable allglobal::lmevalue what is this?

real, dimension(:,:), allocatable allglobal::Imfvalue
 what is this?

 real, dimension(:,:), allocatable allglobal::lmgvalue what is this?

 real, dimension(:,:), allocatable allglobal::Imhvalue what is this?

integer, dimension(:,:), allocatable allglobal::fso what is this?

integer, dimension(:,:), allocatable allglobal::fse what is this?

logical allglobal::lcoordinatesingularity

set by LREGION macro; true if inside the innermost volume

• logical allglobal::lplasmaregion

set by LREGION macro; true if inside the plasma region

· logical allglobal::lvacuumregion

set by LREGION macro; true if inside the vacuum region

· logical allglobal::lsavedguvij

flag used in matrix free

· logical allglobal::localconstraint

what is this?

## 5.30.1 Detailed Description

- In each volume, the total degrees of freedom in the Beltrami linear system is NAdof(1:Nvol). This depends on Mpol, Ntor and Lrad(vvol).
- · The covariant components of the vector potential are written as

$$A_{\theta} = \sum_{i} \sum_{l=0}^{L} A_{\theta,e,i,l} T_{l}(s) \cos \alpha_{i} + \sum_{i} \sum_{l=0}^{L} A_{\theta,o,i,l} T_{l}(s) \sin \alpha_{i}$$
 (242)

$$A_{\zeta} = \sum_{i} \sum_{l=0}^{L} A_{\zeta,e,i,l} T_{l}(s) \cos \alpha_{i} + \sum_{i} \sum_{l=0}^{L} A_{\zeta,o,i,l} T_{l}(s) \sin \alpha_{i},$$
 (243)

where  $T_l(s)$  are the Chebyshev polynomials and  $\alpha_i \equiv m_i \theta - n_i \zeta$ .

• The following internal arrays are declared in preset():

dAte (0, i) %s(I) 
$$\equiv A_{\theta,e,i,l}$$
 dAze (0, i) %s(I)  $\equiv A_{\zeta,e,i,l}$  dAto (0, i) %s(I)  $\equiv A_{\theta,o,i,l}$  dAzo (0, i) %s(I)  $\equiv A_{\zeta,o,i,l}$ 

# 5.31 Field matrices: dMA, dMB, dMC, dMD, dME, dMF

Collaboration diagram for Field matrices: dMA, dMB, dMC, dMD, dME, dMF:



- real, dimension(:,:), allocatable allglobal::dma
   energy and helicity matrices; quadratic forms
- real, dimension(:,:), allocatable allglobal::dmb
   energy and helicity matrices; quadratic forms
- real, dimension(:,:), allocatable allglobal::dmd energy and helicity matrices; quadratic forms
- real, dimension(:), allocatable allglobal::dmas sparse version of dMA, data
- real, dimension(:), allocatable allglobal::dmds
   sparse version of dMD, data
- integer, dimension(:), allocatable allglobal::idmas sparse version of dMA and dMD, indices
- integer, dimension(:), allocatable allglobal::jdmas sparse version of dMA and dMD, indices
- integer, dimension(:), allocatable allglobal::ndmasmax
  - number of elements for sparse matrices
- integer, dimension(:), allocatable allglobal::ndmas number of elements for sparse matrices
- real, dimension(:), allocatable allglobal::dmg what is this?
- real, dimension(:), allocatable allglobal::adotx the matrix-vector product
- real, dimension(:), allocatable allglobal::ddotx
  - the matrix-vector product
- real, dimension(:,:), allocatable allglobal::solution
  - this is allocated in dforce; used in mp00ac and ma02aa; and is passed to packab
- real, dimension(:,:,:), allocatable allglobal::gmreslastsolution
  - used to store the last solution for restarting GMRES
- real, dimension(:), allocatable allglobal::mbpsi
  - matrix vector products
- · logical allglobal::liluprecond
  - whether to use ILU preconditioner for GMRES
- real, dimension(:,:), allocatable allglobal::beltramiinverse
   Beltrami inverse matrix.
- real, dimension(:,:,:), allocatable allglobal::diotadxup
  - measured rotational transform on inner/outer interfaces for each volume; d(transform)/dx; (see dforce)
- real, dimension(:,:,:), allocatable allglobal::ditgpdxtp
  - measured toroidal and poloidal current on inner/outer interfaces for each volume; d(ltor,Gpol)/dx; (see dforce)
- real, dimension(:,:,:,:), allocatable allglobal::glambda
  - save initial guesses for iterative calculation of rotational-transform
- integer allglobal::lmns
  - what is this?

# 5.31.1 Detailed Description

• The energy,  $W \equiv \int dv \, \mathbf{B} \cdot \mathbf{B}$ , and helicity,  $K \equiv \int dv \, \mathbf{A} \cdot \mathbf{B}$ , functionals may be written

$$W = \frac{1}{2} a_i A_{i,j} a_j + a_i B_{i,j} \psi_j + \frac{1}{2} \psi_i C_{i,j} \psi_j$$

$$K = \frac{1}{2} a_i D_{i,j} a_j + a_i E_{i,j} \psi_j + \frac{1}{2} \psi_i F_{i,j} \psi_j$$
(244)

$$K = \frac{1}{2} a_i D_{i,j} a_j + a_i E_{i,j} \psi_j + \frac{1}{2} \psi_i F_{i,j} \psi_j$$
 (245)

where  $\mathbf{a} \equiv \{A_{\theta,e,i,l}, A_{\zeta,e,i,l}, A_{\theta,o,i,l}, A_{\zeta,o,i,l}, f_{e,i}, f_{o,i}\}$  contains the independent degrees of freedom and  $\psi \equiv \{\Delta\psi_t, \Delta\psi_p\}.$ 

These are allocated and deallocated in dforce(), assigned in matrix(), and used in mp00ac() and (?) df00aa().

# 5.32 Construction of "force"

The force vector is comprised of Bomn and Iomn.

Collaboration diagram for Construction of "force":



# **Variables**

- real, dimension(:,:,:), allocatable allglobal::bemn force vector; stellarator-symmetric (?)
- real, dimension(:,:), allocatable allglobal::iomn force vector; stellarator-symmetric (?)
- real, dimension(:,:,:), allocatable allglobal::somn force vector; non-stellarator-symmetric (?)
- real, dimension(:,:,:), allocatable allglobal::pomn force vector; non-stellarator-symmetric (?)
- real, dimension(:,:,:), allocatable allglobal::bomn force vector; stellarator-symmetric (?)
- real, dimension(:,:), allocatable allglobal::iemn force vector; stellarator-symmetric (?)
- real, dimension(:,:,:), allocatable allglobal::semn force vector; non-stellarator-symmetric (?)
- real, dimension(:,:,:), allocatable allglobal::pemn force vector; non-stellarator-symmetric (?)
- real, dimension(:), allocatable allglobal::bbe force vector (?); stellarator-symmetric (?)
- real, dimension(:), allocatable allglobal::iio force vector (?); stellarator-symmetric (?)
- real, dimension(:), allocatable allglobal::bbo force vector (?); non-stellarator-symmetric (?)
- real, dimension(:), allocatable allglobal::iie force vector (?); non-stellarator-symmetric (?)

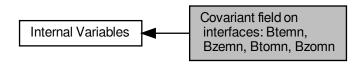
# 5.32.1 Detailed Description

The force vector is comprised of Bomn and Iomn.

# 5.33 Covariant field on interfaces: Btemn, Bzemn, Btomn, Bzomn

The covariant field.

Collaboration diagram for Covariant field on interfaces: Btemn, Bzemn, Btomn, Bzomn:



#### **Variables**

- real, dimension(:,:,:), allocatable allglobal::btemn
   covariant θ cosine component of the tangential field on interfaces; stellarator-symmetric
- real, dimension(:,:,:), allocatable allglobal::bzemn
   covariant ζ cosine component of the tangential field on interfaces; stellarator-symmetric
- real, dimension(:,;,:), allocatable allglobal::btomn
   covariant θ sine component of the tangential field on interfaces; non-stellarator-symmetric
- real, dimension(:,:,:), allocatable allglobal::bzomn
   covariant ζ sine component of the tangential field on interfaces; non-stellarator-symmetric

# 5.33.1 Detailed Description

The covariant field.

# 5.34 covariant field for Hessian computation: Bloweremn, Bloweromn

Collaboration diagram for covariant field for Hessian computation: Bloweremn, Bloweremn:



- real, dimension(:,:), allocatable allglobal::bloweremn covariant field for Hessian computation
- real, dimension(:,:), allocatable allglobal::bloweromn covariant field for Hessian computation

# 5.34.1 Detailed Description

# 5.35 Geometrical degrees-of-freedom: LGdof, NGdof

The geometrical degrees-of-freedom.

Collaboration diagram for Geometrical degrees-of-freedom: LGdof, NGdof:



# **Variables**

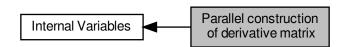
- integer allglobal::lgdof geometrical degrees of freedom associated with each interface
- integer allglobal::ngdof
   total geometrical degrees of freedom

## 5.35.1 Detailed Description

The geometrical degrees-of-freedom.

# 5.36 Parallel construction of derivative matrix

Collaboration diagram for Parallel construction of derivative matrix:



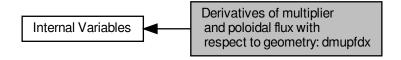
- real, dimension(:,:,:), allocatable allglobal::dbbdrz
   derivative of magnetic field w.r.t. geometry (?)
- real, dimension(:,:), allocatable allglobal::diidrz derivative of spectral constraints w.r.t. geometry (?)
- real, dimension(:,:,:,:), allocatable allglobal::dffdrz derivatives of B<sup>^2</sup> 2 at the interfaces wrt geometry
- real, dimension(:,:,:,:), allocatable allglobal::dbbdmp derivatives of B^2 at the interfaces wrt mu and dpflux

## 5.36.1 Detailed Description

- The derivatives of force-balance,  $[[p + B^2/2]]$ , and the spectral constraints (see sw03aa()), with respect to the interface geometry is constructed in parallel by dforce().
- force-balance across the l-th interface depends on the fields in the adjacent interfaces.

# 5.37 Derivatives of multiplier and poloidal flux with respect to geometry: dmupfdx

Collaboration diagram for Derivatives of multiplier and poloidal flux with respect to geometry: dmupfdx:



## **Variables**

- real, dimension(:,:,:,:), allocatable allglobal::dmupfdx
   derivatives of mu and dpflux wrt geometry at constant interface transform
- · logical allglobal::lhessianallocated

flag to indicate that force gradient matrix is allocated (?)

- real, dimension(:,:), allocatable allglobal::hessian force gradient matrix (?)
- real, dimension(:,:), allocatable allglobal::dessian derivative of force gradient matrix (?)

# 5.37.1 Detailed Description

- The information in dmupfdx describes how the helicity multiplier,  $\mu$ , and the enclosed poloidal flux,  $\Delta \psi_p$ , must vary as the geometry is varied in order to satisfy the interface transform constraint.
- The internal variable dmupfdx (1:Mvol, 1:2, 1:LGdof, 0:1) is allocated/deallocated in newton(), and hesian() if selected.
- The magnetic field depends on the Fourier harmonics of both the inner and outer interface geometry (represented here as  $x_j$ ), the helicity multiplier, and the enclosed poloidal flux, i.e.  $\mathbf{B}_{\pm} = \mathbf{B}_{\pm}(x_j, \mu, \Delta \psi_p)$ , so that

$$\delta \mathbf{B}_{\pm} = \frac{\partial \mathbf{B}_{\pm}}{\partial x_{j}} \delta x_{j} + \frac{\partial \mathbf{B}_{\pm}}{\partial \mu} \delta \mu + \frac{\partial \mathbf{B}_{\pm}}{\partial \Delta \psi_{p}} \delta \Delta \psi_{p}. \tag{246}$$

• This information is used to adjust the calculation of how force-balance, i.e.  $B^2$  at the interfaces, varies with geometry at fixed interface rotational transform. Given

$$B_{+}^{2} = B_{+}^{2}(x_{j}, \mu, \Delta \psi_{p}), \tag{247}$$

we may derive

$$\frac{\partial B_{\pm}^{2}}{\partial x_{j}} = \frac{\partial B_{\pm}^{2}}{\partial x_{j}} + \frac{\partial B_{\pm}^{2}}{\partial \mu} \frac{\partial \mu}{\partial x_{j}} + \frac{\partial B_{\pm}^{2}}{\partial \Delta \psi_{p}} \frac{\partial \Delta \psi_{p}}{\partial x_{j}}$$
(248)

• The constraint to be enforced is that  $\mu$  and  $\Delta\psi_p$  must generally vary as the geometry is varied if the value of the rotational-transform constraint on the inner/outer interface is to be preserved, i.e.

$$\begin{pmatrix}
\frac{\partial \boldsymbol{t}_{-}}{\partial \mathbf{B}_{-}} \cdot \frac{\partial \mathbf{B}_{-}}{\partial \mu} & , & \frac{\partial \boldsymbol{t}_{-}}{\partial \mathbf{B}_{-}} \cdot \frac{\partial \mathbf{B}_{-}}{\partial \Delta \psi_{p}} \\
\frac{\partial \boldsymbol{t}_{+}}{\partial \mathbf{B}_{+}} \cdot \frac{\partial \mathbf{B}_{+}}{\partial \mu} & , & \frac{\partial \boldsymbol{t}_{+}}{\partial \mathbf{B}_{+}} \cdot \frac{\partial \mathbf{B}_{+}}{\partial \Delta \psi_{p}}
\end{pmatrix}
\begin{pmatrix}
\frac{\partial \mu}{\partial x_{j}} \\
\frac{\partial \Delta \psi_{p}}{\partial x_{j}}
\end{pmatrix} = - \begin{pmatrix}
\frac{\partial \boldsymbol{t}_{-}}{\partial \mathbf{B}_{-}} \cdot \frac{\partial \mathbf{B}_{-}}{\partial x_{j}} \\
\frac{\partial \boldsymbol{t}_{+}}{\partial \mathbf{B}_{+}} \cdot \frac{\partial \mathbf{B}_{+}}{\partial x_{j}}
\end{pmatrix}.$$
(249)

- This  $2 \times 2$  linear equation is solved in dforce() and the derivatives of the rotational-transform are given in diotadxup, see preset.f90.
- A finite-difference estimate is computed if Lcheck==4.

# 5.38 Trigonometric factors

Collaboration diagram for Trigonometric factors:



- real, dimension(:,:), allocatable allglobal::cosi some precomputed cosines
- real, dimension(:,:), allocatable allglobal::sini some precomputed sines
- real, dimension(:), allocatable allglobal::gteta something related to  $\sqrt{g}$  and  $\theta$ ?
- real, dimension(:), allocatable allglobal::gzeta something related to  $\sqrt{g}$  and  $\zeta$ ?
- real, dimension(:), allocatable allglobal::ajk
   definition of coordinate axis
- real, dimension(:,:,:,:), allocatable allglobal::dradr derivatives of coordinate axis
- real, dimension(:,:,:,:), allocatable allglobal::dradz
   derivatives of coordinate axis
- real, dimension(:,:,:,:), allocatable allglobal::dzadr derivatives of coordinate axis
- real, dimension(:,:,:,:), allocatable allglobal::dzadz derivatives of coordinate axis
- real, dimension(:,:,:), allocatable allglobal::drodr derivatives of coordinate axis
- real, dimension(:,:,:), allocatable allglobal::drodz derivatives of coordinate axis
- real, dimension(:,:,:), allocatable allglobal::dzodr derivatives of coordinate axis
- real, dimension(:,:,:), allocatable allglobal::dzodz derivatives of coordinate axis
- integer, dimension(:,:), allocatable allglobal::djkp for calculating cylindrical volume
- integer, dimension(:,:), allocatable allglobal::djkm for calculating cylindrical volume

# 5.38.1 Detailed Description

- To facilitate construction of the metric integrals, various trigonometric identities are exploited.
- The following are used for volume integrals (see volume()):

$$a_{i,j,k} = 4 m_k \oint d\theta d\zeta \cos(\alpha_i) \cos(\alpha_j) \cos(\alpha_k) / (2\pi)^2,$$
 (250)

$$b_{i,j,k} = 4 m_j \oint d\theta d\zeta \cos(\alpha_i) \sin(\alpha_j) \sin(\alpha_k) / (2\pi)^2,$$
 (251)

# 5.39 Volume integrals: IBBintegral, IABintegral

Collaboration diagram for Volume integrals: IBBintegral, IABintegral:



### **Variables**

- real, dimension(:), allocatable allglobal::lbbintegral
   B.B integral.
- real, dimension(:), allocatable allglobal::labintegral
   A.B integral.
- real, dimension(:), allocatable allglobal::vvolume volume integral of  $\sqrt{g}$ ; computed in volume
- · real allglobal::dvolume

derivative of volume w.r.t. interface geometry

## 5.39.1 Detailed Description

• The energy functional,  $F \equiv \sum_l F_l$ , where

$$F_{l} \equiv \left( \int_{\mathcal{V}_{l}} \frac{p_{l}}{\gamma - 1} + \frac{B_{l}^{2}}{2} dv \right) = \frac{P_{l}}{\gamma - 1} V_{l}^{1 - \gamma} + \int_{\mathcal{V}_{l}} \frac{B_{l}^{2}}{2} dv, \tag{252}$$

where the second expression is derived using  $p_l V_l^{\gamma} = P_l$ , where  $P_l$  is the adiabatic-constant. In Eqn. (252), it is implicit that  ${\bf B}$  satisfies (i) the toroidal and poloidal flux constraints; (ii) the interface constraint,  ${\bf B} \cdot \nabla s = 0$ ; and (iii) the helicity constraint (or the transform constraint).

• The derivatives of  $F_l$  with respect to the inner and outer adjacent interface geometry are stored in  $dFF(1 \leftarrow :Nvol,0:1,0:mn+mn-1)$ , where

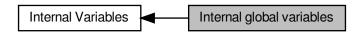
$$\begin{split} F_l &\equiv \text{dFF} \, (\text{1,0,0}) \\ \partial F_l / \partial R_{l-1,j} &\equiv \text{dFF} \, (\text{11,0,j}) \\ \partial F_l / \partial Z_{l-1,j} &\equiv \text{dFF} \, (\text{11,0,mn j}) \\ \partial F_l / \partial R_{l,j} &\equiv \text{dFF} \, (\text{11,1,j}) \\ \partial F_l / \partial Z_{l,j} &\equiv \text{dFF} \, (\text{11,1,mn j}) \end{split}$$

• The volume integrals  $\int dv$ ,  $\int B^2 dv$  and  $\int \mathbf{A} \cdot \mathbf{B} dv$  in each volume are computed and saved in volume (0  $\leftarrow$  :2,1:Nvol).

# 5.40 Internal global variables

internal global variables; internal logical variables; default values are provided here; these may be changed according to input values

Collaboration diagram for Internal global variables:



#### **Variables**

· integer allglobal::ivol

labels volume; some subroutines (called by NAG) are fixed argument list but require the volume label

· real allglobal::gbzeta

toroidal (contravariant) field; calculated in bfield; required to convert  $\dot{\theta}$  to  $B^{\theta}$ ,  $\dot{s}$  to  $B^{s}$ 

• integer, dimension(:), allocatable allglobal::iquad

internal copy of Nquad

real, dimension(:,:), allocatable allglobal::gaussianweight

weights for Gaussian quadrature

• real, dimension(:,:), allocatable allglobal::gaussianabscissae

abscissae for Gaussian quadrature

· logical allglobal::lblinear

controls selection of Beltrami field solver; depends on LBeltrami

logical allglobal::lbnewton

controls selection of Beltrami field solver; depends on LBeltrami

· logical allglobal::lbsequad

controls selection of Beltrami field solver; depends on LBeltrami

real, dimension(1:3) allglobal::orzp

used in mg00aa() to determine  $(s,\theta,\zeta)$  given  $(R,Z,\varphi)$ 

# 5.40.1 Detailed Description

internal global variables; internal logical variables; default values are provided here; these may be changed according to input values

5.41 Miscellaneous 119

# 5.41 Miscellaneous

The following are miscellaneous flags required for the virtual casing field, external (vacuum) field integration, ...

Collaboration diagram for Miscellaneous:



#### **Variables**

• integer allglobal::globaljk

labels position

real, dimension(:,:), allocatable allglobal::dxyz

computational boundary; position

real, dimension(:,:), allocatable allglobal::nxyz

computational boundary; normal

real, dimension(:,:), allocatable allglobal::jxyz

plasma boundary; surface current

real, dimension(1:2) allglobal::tetazeta

what is this?

real allglobal::virtualcasingfactor = -one / (four\*pi)

this agrees with diagno

· integer allglobal::iberror

for computing error in magnetic field

integer allglobal::nfreeboundaryiterations

number of free-boundary iterations already performed

• integer, parameter allglobal::node = 2

best to make this global for consistency between calling and called routines

• logical allglobal::first\_free\_bound = .false.

flag to indicate that this is the first free-boundary iteration

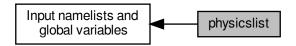
# 5.41.1 Detailed Description

The following are miscellaneous flags required for the virtual casing field, external (vacuum) field integration, ...

# 5.42 physicslist

The namelist physicslist controls the geometry, profiles, and numerical resolution.

Collaboration diagram for physicslist:



## **Variables**

```
• integer inputlist::igeometry = 3

selects Cartesian, cylindrical or toroidal geometry;
```

• integer inputlist::istellsym = 1

stellarator symmetry is enforced if Istellsym==1

• integer inputlist::Ifreebound = 0

compute vacuum field surrounding plasma

• real inputlist::phiedge = 1.0

total enclosed toroidal magnetic flux;

• real inputlist::curtor = 0.0

total enclosed (toroidal) plasma current;

• real inputlist::curpol = 0.0

total enclosed (poloidal) linking current;

• real inputlist::gamma = 0.0

adiabatic index; cannot set  $|\gamma|=1$ 

• integer inputlist::nfp = 1

field periodicity

• integer inputlist::nvol = 1

number of volumes

• integer inputlist::mpol = 0

number of poloidal Fourier harmonics

• integer inputlist::ntor = 0

number of toroidal Fourier harmonics

• integer, dimension(1:mnvol+1) inputlist::lrad = 4

Chebyshev resolution in each volume.

• integer inputlist::lconstraint = -1

selects constraints; primarily used in ma02aa() and mp00ac().

• real, dimension(1:mnvol+1) inputlist::tflux = 0.0

toroidal flux,  $\psi_t$ , enclosed by each interface

real, dimension(1:mnvol+1) inputlist::pflux = 0.0

poloidal flux,  $\psi_p$ , enclosed by each interface

real, dimension(1:mnvol) inputlist::helicity = 0.0

helicity, K, in each volume,  $V_i$ 

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```
real inputlist::pscale = 0.0
      pressure scale factor

    real, dimension(1:mnvol+1) inputlist::pressure = 0.0

      pressure in each volume
• integer inputlist::ladiabatic = 0
      logical flag

    real, dimension(1:mnvol+1) inputlist::adiabatic = 0.0

      adiabatic constants in each volume

    real, dimension(1:mnvol+1) inputlist::mu = 0.0

      helicity-multiplier, \mu, in each volume

    real, dimension(1:mnvol+1) inputlist::ivolume = 0.0

       Toroidal current constraint normalized by \mu_0 ( I_{volume} = \mu_0 \cdot [A]), in each volume. This is a cumulative quantity:
       I_{\mathcal{V},i} = \int_0^{\psi_{t,i}} \mathbf{J} \cdot \mathbf{dS}. Physically, it represents the sum of all non-pressure driven currents.

    real, dimension(1:mnvol) inputlist::isurf = 0.0

       Toroidal current normalized by \mu_0 at each interface (cumulative). This is the sum of all pressure driven currents.

    integer, dimension(0:mnvol) inputlist::pl = 0

       "inside" interface rotational-transform is \iota=(p_l+\gamma p_r)/(q_l+\gamma q_r), where \gamma is the golden mean, \gamma=(1+\sqrt{5})/2.

    integer, dimension(0:mnvol) inputlist::ql = 0

       "inside" interface rotational-transform is \iota=(p_l+\gamma p_r)/(q_l+\gamma q_r), where \gamma is the golden mean, \gamma=(1+\sqrt{5})/2.
• integer, dimension(0:mnvol) inputlist::pr = 0
       "inside" interface rotational-transform is \iota=(p_l+\gamma p_r)/(q_l+\gamma q_r), where \gamma is the golden mean, \gamma=(1+\sqrt{5})/2.
• integer, dimension(0:mnvol) inputlist::qr = 0
       "inside" interface rotational-transform is \iota=(p_l+\gamma p_r)/(q_l+\gamma q_r), where \gamma is the golden mean, \gamma=(1+\sqrt{5})/2.

    real, dimension(0:mnvol) inputlist::iota = 0.0

      rotational-transform, ε, on inner side of each interface
• integer, dimension(0:mnvol) inputlist::lp = 0
       "outer" interface rotational-transform is \,\iota=(p_l+\gamma p_r)/(q_l+\gamma q_r), where \gamma is the golden mean, \gamma=(1+\sqrt{5})/2.

    integer, dimension(0:mnvol) inputlist::lq = 0

       "outer" interface rotational-transform is \,\iota=(p_l+\gamma p_r)/(q_l+\gamma q_r), where \gamma is the golden mean, \gamma=(1+\sqrt{5})/2.
• integer, dimension(0:mnvol) inputlist::rp = 0
       "outer" interface rotational-transform is \,\iota=(p_l+\gamma p_r)/(q_l+\gamma q_r), where \gamma is the golden mean, \gamma=(1+\sqrt{5})/2.
integer, dimension(0:mnvol) inputlist::rq = 0
       "outer" interface rotational-transform is \,\iota=(p_l+\gamma p_r)/(q_l+\gamma q_r), where \gamma is the golden mean, \gamma=(1+\sqrt{5})/2.
• real, dimension(0:mnvol) inputlist::oita = 0.0
      rotational-transform, ε, on outer side of each interface

    real inputlist::mupftol = 1.0e-14

      accuracy to which \mu and \Delta\psi_p are required
• integer inputlist::mupfits = 8
      an upper limit on the transform/helicity constraint iterations;
real inputlist::rpol = 1.0
      poloidal extent of slab (effective radius)
real inputlist::rtor = 1.0
      toroidal extent of slab (effective radius)
• integer inputlist::lreflect = 0
      =1 reflect the upper and lower bound in slab, =0 do not reflect

    real, dimension(0:mntor) inputlist::rac = 0.0

      stellarator symmetric coordinate axis;

    real, dimension(0:mntor) inputlist::zas = 0.0

      stellarator symmetric coordinate axis;
  real, dimension(0:mntor) inputlist::ras = 0.0
      non-stellarator symmetric coordinate axis;
```

- real, dimension( 0:mntor) inputlist::zac = 0.0
   non-stellarator symmetric coordinate axis;
- real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::rbc = 0.0 stellarator symmetric boundary components;
- real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::zbs = 0.0 stellarator symmetric boundary components;
- real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::rbs = 0.0
   non-stellarator symmetric boundary components;
- real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::zbc = 0.0 non-stellarator symmetric boundary components;
- real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::rwc = 0.0 stellarator symmetric boundary components of wall;
- real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::zws = 0.0 stellarator symmetric boundary components of wall;
- real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::rws = 0.0
   non-stellarator symmetric boundary components of wall;
- real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::zwc = 0.0
   non-stellarator symmetric boundary components of wall;
- real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::vns = 0.0 stellarator symmetric normal field at boundary; vacuum component;
- real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::bns = 0.0 stellarator symmetric normal field at boundary; plasma component;
- real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::vnc = 0.0
   non-stellarator symmetric normal field at boundary; vacuum component;
- real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::bnc = 0.0
   non-stellarator symmetric normal field at boundary; plasma component;

## 5.42.1 Detailed Description

The namelist physicslist controls the geometry, profiles, and numerical resolution.

# 5.42.2 Variable Documentation

## **5.42.2.1 igeometry** integer inputlist::igeometry = 3

selects Cartesian, cylindrical or toroidal geometry;

- Igeometry=1: Cartesian; geometry determined by R;
- Igeometry=2 : cylindrical; geometry determined by R;
- Igeometry=3 : toroidal; geometry determined by R and Z;

Referenced by bnorml(), allglobal::broadcast\_inputs(), allglobal::check\_inputs(), coords(), dfpred(), dfpred(), dfpred(), dfpred(), dfpred(), fcnred(), fcnr

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**5.42.2.2 nfp** integer inputlist::nfp = 1

field periodicity

• all Fourier representations are of the form  $\cos(m\theta - nN\zeta)$ ,  $\sin(m\theta - nN\zeta)$ , where  $N \equiv \text{Nfp}$ 

• constraint: Nfp >= 1

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), jo00aa(), sphdf5::mirror\_input\_to\_outfile(), preset(), ra00aa(), spec(), and allglobal::wrtend().

**5.42.2.3 nvol** integer inputlist::nvol = 1

number of volumes

- each volume  $\mathcal{V}_l$  is bounded by the  $\mathcal{I}_{l-1}$  and  $\mathcal{I}_l$  interfaces
- note that in cylindrical or toroidal geometry,  $\mathcal{I}_0$  is the degenerate coordinate axis
- constraint: Nvol<=MNvol

Referenced by brcast(), allglobal::broadcast\_inputs(), allglobal::check\_inputs(), df00ab(), dforce(), dfp100(), dfp200(), dvcfield(), evaluate\_dbb(), evaluate\_dmupfdx(), final\_diagnostics(), sphdf5::hdfint(), hesian(), jo00aa(), lforce(), sphdf5::mirror\_input\_to\_outfile(), packxi(), pc00ab(), pp00aa(), pp00ab(), preset(), spec(), stzxyz(), tr00ab(), volume(), wa00aa(), sphdf5::write\_grid(), writereadgf(), and allglobal::wrtend().

**5.42.2.4 mpol** integer inputlist::mpol = 0

number of poloidal Fourier harmonics

· all Fourier representations of doubly-periodic functions are of the form

$$f(\theta,\zeta) = \sum_{n=0}^{\mathrm{Ntor}} f_{0,n} \cos(-n \operatorname{Nfp} \zeta) + \sum_{m=1}^{\mathrm{Mpol}} \sum_{n=-\mathrm{Ntor}}^{\mathrm{Ntor}} f_{m,n} \cos(m\theta - n \operatorname{Nfp} \zeta), \qquad \text{(253)}$$

Internally these "double" summations are written as a "single" summation, e.g.  $f(\theta, \zeta) = \sum_j f_j \cos(m_j \theta - n_j \zeta)$ .

Referenced by allocate\_geometry\_matrices(), bfield(), bfield\_tangent(), allglobal::broadcast\_inputs(), allglobal ::check\_inputs(), dfp200(), intghs(), intghs\_workspace\_init(), jo00aa(), ma00aa(), matrix(), sphdf5::mirror\_input - to\_outfile(), mtrxhs(), preset(), ra00aa(), spsint(), spsmat(), tr00ab(), wa00aa(), writereadgf(), and allglobal ::wrtend().

**5.42.2.5 ntor** integer inputlist::ntor = 0

number of toroidal Fourier harmonics

· all Fourier representations of doubly-periodic functions are of the form

$$f(\theta,\zeta) = \sum_{n=0}^{\text{Ntor}} f_{0,n} \cos(-n \operatorname{Nfp} \zeta) + \sum_{m=1}^{\text{Mpol}} \sum_{n=-\text{Ntor}}^{\text{Ntor}} f_{m,n} \cos(m\theta - n \operatorname{Nfp} \zeta), \quad (254)$$

Internally these "double" summations are written as a "single" summation, e.g.  $f(\theta, \zeta) = \sum_j f_j \cos(m_j \theta - n_j \zeta)$ .

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), coords(), dforce(), dfp200(), evaluate\_dbb(), sphdf5::mirror\_input\_to\_outfile(), mp00ac(), packxi(), preset(), ra00aa(), rzaxis(), stzxyz(), tr00ab(), wa00aa(), writereadgf(), and allglobal::wrtend().

**5.42.2.6 Irad** integer, dimension(1:mnvol+1) inputlist::lrad = 4

Chebyshev resolution in each volume.

• constraint : Lrad(1:Mvol) >= 2

Referenced by allocate\_geometry\_matrices(), bfield(), bfield\_tangent(), bnorml(), brcast(), allglobal::broadcast \_\_inputs(), allglobal::check\_inputs(), curent(), dforce(), dfp100(), dfp200(), dvcfield(), evaluate\_dbb(), evaluate \_\_dmupfdx(), get\_lu\_beltrami\_matrices(), get\_perturbed\_solution(), sphdf5::hdfint(), intghs\_workspace\_init(), jo00aa(), lforce(), ma02aa(), matvec(), sphdf5::mirror\_input\_to\_outfile(), mp00ac(), packab(), pp00aa(), ra00aa(), spec(), tr00ab(), sphdf5::write\_grid(), and allglobal::wrtend().

### **5.42.2.7 | constraint** integer inputlist::lconstraint = -1

selects constraints; primarily used in ma02aa() and mp00ac().

- if Lconstraint==-1, then in the plasma regions  $\Delta \psi_t$ ,  $\mu$  and  $\Delta \psi_p$  are *not* varied and in the vacuum region (only for free-boundary)  $\Delta \psi_t$  and  $\Delta \psi_p$  are *not* varied, and  $\mu=0$ .
- if Lconstraint==0, then in the plasma regions  $\Delta\psi_t$ ,  $\mu$  and  $\Delta\psi_p$  are not varied and in the vacuum region (only for free-boundary)  $\Delta\psi_t$  and  $\Delta\psi_p$  are varied to match the prescribed plasma current, current, and the "linking" current, curpol, and  $\mu=0$
- if Lconstraint==1, then in the plasma regions  $\mu$  and  $\Delta\psi_p$  are adjusted in order to satisfy the inner and outer interface transform constraints (except in the simple torus, where the enclosed poloidal flux is irrelevant, and only  $\mu$  is varied to satisfy the outer interface transform constraint); and in the vacuum region  $\Delta\psi_t$  and  $\Delta\psi_p$  are varied to match the transform constraint on the boundary and to obtain the prescribed linking current, curpol, and  $\mu=0$ .
- Todo if Lconstraint==2, under reconstruction.
- if Lconstraint.eq.3, then the  $\mu$  and  $\psi_p$  variables are adjusted in order to satisfy the volume and surface toroidal current computed with lbpol() (excepted in the inner most volume, where the volume current is irrelevant). Not implemented yet in free boundary.

Referenced by brcast(), allglobal::broadcast\_inputs(), allglobal::check\_inputs(), dforce(), dfp100(), dfp200(), evaluate\_dbb(), evaluate\_dmupfdx(), get\_lu\_beltrami\_matrices(), get\_perturbed\_solution(), ma02aa(), sphdf5columntrices(), pp00aa(), preset(), spec(), and allglobal::wrtend().

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```
5.42.2.8 tflux real, dimension(1:mnvol+1) inputlist::tflux = 0.0
```

toroidal flux,  $\psi_t$ , enclosed by each interface

- For each of the plasma volumes, this is a constraint: tflux is not varied
- For the vacuum region (only if Lfreebound==1), tflux may be allowed to vary to match constraints
- Note that tflux will be normalized so that tflux (Nvol) = 1.0, so that tflux is arbitrary up to a scale factor

See also

phiedge

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), dfp200(), sphdf5::hdfint(), sphdf5::mirror\_
input\_to\_outfile(), preset(), spec(), and allglobal::wrtend().

```
5.42.2.9 helicity real, dimension(1:mnvol) inputlist::helicity = 0.0
```

helicity,  $\mathcal{K}$ , in each volume,  $\mathcal{V}_i$ 

• on exit, helicity is set to the computed values of  $\mathcal{K} \equiv \int \mathbf{A} \cdot \mathbf{B} \; dv$ 

Referenced by brcast(), allglobal::broadcast\_inputs(), allglobal::check\_inputs(), df00ab(), sphdf5::hdfint(), hesian(), ma02aa(), sphdf5::mirror\_input\_to\_outfile(), mp00ac(), preset(), spec(), and allglobal::wrtend().

```
5.42.2.10 pscale real inputlist::pscale = 0.0
```

pressure scale factor

the initial pressure profile is given by pscale \* pressure

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), dfp200(), evaluate\_dbb(), lforce(), sphdf5 ::mirror\_input\_to\_outfile(), spec(), volume(), and allglobal::wrtend().

```
5.42.2.11 pressure real, dimension(1:mnvol+1) inputlist::pressure = 0.0
```

pressure in each volume

- The pressure is *not* held constant, but  $p_l V_l^{\gamma} = P_l$  is held constant, where  $P_l$  is determined by the initial pressures and the initial volumes,  $V_l$ .
- Note that if gamma==0.0, then  $p_l \equiv P_l$ .
- On output, the pressure is given by  $p_l = P_l/V_l^{\gamma}$ , where  $V_l$  is the final volume.
- pressure is only used in calculation of interface force-balance.

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), spec(), and allglobal::wrtend().

## **5.42.2.12 ladiabatic** integer inputlist::ladiabatic = 0

logical flag

- If Ladiabatic==0, the adiabatic constants are determined by the initial pressure and volume.
- If Ladiabatic==1, the adiabatic constants are determined by the given input adiabatic.

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), spec(), and allglobal::wrtend().

#### **5.42.2.13 adiabatic** real, dimension(1:mnvol+1) inputlist::adiabatic = 0.0

adiabatic constants in each volume

- The pressure is *not* held constant, but  $p_l V_l^{\gamma} = P_l \equiv \texttt{adiabatic}$  is constant.
- Note that if gamma==0.0, then pressure==adiabatic.
- pressure is only used in calculation of interface force-balance.

Referenced by allglobal::broadcast\_inputs(), dfp200(), evaluate\_dbb(), sphdf5::hdfint(), lforce(), sphdf5::mirror\_ input\_to\_outfile(), spec(), and allglobal::wrtend().

### **5.42.2.14 pl** integer, dimension(0:mnvol) inputlist::pl = 0

"inside" interface rotational-transform is  $\iota = (p_l + \gamma p_r)/(q_l + \gamma q_r)$ , where  $\gamma$  is the golden mean,  $\gamma = (1 + \sqrt{5})/2$ .

If both  $q_l=0$  and  $q_r=0$ , then the (inside) interface rotational-transform is defined by  ${\tt iota}$  .

Referenced by allglobal::broadcast\_inputs(), sphdf5::mirror\_input\_to\_outfile(), preset(), and allglobal::wrtend().

## **5.42.2.15 ql** integer, dimension(0:mnvol) inputlist::ql = 0

"inside" interface rotational-transform is  $\ell=(p_l+\gamma p_r)/(q_l+\gamma q_r)$ , where  $\gamma$  is the golden mean,  $\gamma=(1+\sqrt{5})/2$ .

If both  $q_l=0$  and  $q_r=0$ , then the (inside) interface rotational-transform is defined by  ${\tt iota}$  .

Referenced by allglobal::broadcast\_inputs(), sphdf5::mirror\_input\_to\_outfile(), preset(), and allglobal::wrtend().

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**5.42.2.16 pr** integer, dimension(0:mnvol) inputlist::pr = 0

"inside" interface rotational-transform is  $\iota=(p_l+\gamma p_r)/(q_l+\gamma q_r)$ , where  $\gamma$  is the golden mean,  $\gamma=(1+\sqrt{5})/2$ .

If both  $q_l=0$  and  $q_r=0$ , then the (inside) interface rotational-transform is defined by  ${\tt iota}$  .

Referenced by allglobal::broadcast\_inputs(), sphdf5::mirror\_input\_to\_outfile(), preset(), and allglobal::wrtend().

**5.42.2.17 qr** integer, dimension(0:mnvol) inputlist::qr = 0

"inside" interface rotational-transform is  $\ \iota=(p_l+\gamma p_r)/(q_l+\gamma q_r)$ , where  $\gamma$  is the golden mean,  $\gamma=(1+\sqrt{5})/2$ .

If both  $q_l=0$  and  $q_r=0$ , then the (inside) interface rotational-transform is defined by  ${\tt iota}$  .

Referenced by allglobal::broadcast inputs(), sphdf5::mirror input to outfile(), preset(), and allglobal::wrtend().

**5.42.2.18** iota real, dimension(0:mnvol) inputlist::iota = 0.0

rotational-transform, t, on inner side of each interface

only relevant if illogical input for ql and qr are provided

Referenced by allglobal::broadcast\_inputs(), sphdf5::mirror\_input\_to\_outfile(), mp00ac(), pp00aa(), preset(), and allglobal::wrtend().

**5.42.2.19 Ip** integer, dimension(0:mnvol) inputlist::lp = 0

"outer" interface rotational-transform is  $\epsilon = (p_l + \gamma p_r)/(q_l + \gamma q_r)$ , where  $\gamma$  is the golden mean,  $\gamma = (1 + \sqrt{5})/2$ .

If both  $q_l=0$  and  $q_r=0$ , then the (outer) interface rotational-transform is defined by  ${\tt oita}$  .

Referenced by allglobal::broadcast inputs(), sphdf5::mirror input to outfile(), preset(), and allglobal::wrtend().

**5.42.2.20** Iq integer, dimension(0:mnvol) inputlist::lq = 0

"outer" interface rotational-transform is  $\iota=(p_l+\gamma p_r)/(q_l+\gamma q_r)$ , where  $\gamma$  is the golden mean,  $\gamma=(1+\sqrt{5})/2$ .

If both  $q_l=0$  and  $q_r=0$ , then the (outer) interface rotational-transform is defined by  ${\tt oita}$  .

Referenced by allglobal::broadcast inputs(), sphdf5::mirror input to outfile(), preset(), and allglobal::wrtend().

```
5.42.2.21 rp integer, dimension(0:mnvol) inputlist::rp = 0
```

"outer" interface rotational-transform is  $t = (p_l + \gamma p_r)/(q_l + \gamma q_r)$ , where  $\gamma$  is the golden mean,  $\gamma = (1 + \sqrt{5})/2$ .

If both  $q_l=0$  and  $q_r=0$ , then the (outer) interface rotational-transform is defined by oita.

Referenced by allglobal::broadcast\_inputs(), sphdf5::mirror\_input\_to\_outfile(), preset(), and allglobal::wrtend().

```
5.42.2.22 rq integer, dimension(0:mnvol) inputlist::rq = 0
```

"outer" interface rotational-transform is  $\epsilon=(p_l+\gamma p_r)/(q_l+\gamma q_r)$ , where  $\gamma$  is the golden mean,  $\gamma=(1+\sqrt{5})/2$ .

If both  $q_l=0$  and  $q_r=0$ , then the (outer) interface rotational-transform is defined by oita.

Referenced by allglobal::broadcast\_inputs(), sphdf5::mirror\_input\_to\_outfile(), preset(), and allglobal::wrtend().

```
5.42.2.23 oita real, dimension(0:mnvol) inputlist::oita = 0.0
```

rotational-transform, t, on outer side of each interface

- only relevant if illogical input for  ${\tt ql}$  and  ${\tt qr}$  are provided

Referenced by allglobal::broadcast\_inputs(), sphdf5::mirror\_input\_to\_outfile(), mp00ac(), pp00aa(), preset(), and allglobal::wrtend().

```
5.42.2.24 mupftol real inputlist::mupftol = 1.0e-14
```

accuracy to which  $\mu$  and  $\Delta\psi_p$  are required

• only relevant if constraints on transform, enclosed currents etc. are to be satisfied iteratively, see Lconstraint

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), dforce(), evaluate\_dmupfdx(), ma02aa(), sphdf5::mirror\_input\_to\_outfile(), and allglobal::wrtend().

```
5.42.2.25 mupfits integer inputlist::mupfits = 8
```

an upper limit on the transform/helicity constraint iterations;

- only relevant if constraints on transform, enclosed currents etc. are to be satisfied iteratively, see Lconstraint
- constraint: mupfits > 0

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), ma02aa(), sphdf5::mirror\_input\_to\_outfile(), and allglobal::wrtend().

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```
5.42.2.26 rpol real inputlist::rpol = 1.0
```

poloidal extent of slab (effective radius)

- only relevant if Igeometry==1
- poloidal size is  $L=2\pi*{\tt rpol}$

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), coords(), sphdf5::mirror\_input\_to\_outfile(), sphdf5::write\_grid(), and allglobal::wrtend().

```
5.42.2.27 rtor real inputlist::rtor = 1.0
```

toroidal extent of slab (effective radius)

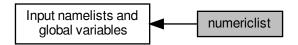
- only relevant if Igeometry==1
- toroidal size is  $L=2\pi*{\tt rtor}$

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), coords(), sphdf5::mirror\_input\_to\_outfile(), sphdf5::write\_grid(), and allglobal::wrtend().

# 5.43 numericlist

The namelist numericlist controls internal resolution parameters that the user rarely needs to consider.

Collaboration diagram for numericlist:



• integer inputlist::linitialize = 0

Used to initialize geometry using a regularization / extrapolation method.

• integer inputlist::lautoinitbn = 1

Used to initialize  $B_{ns}$  using an initial fixed-boundary calculation.

• integer inputlist::lzerovac = 0

Used to adjust vacuum field to cancel plasma field on computational boundary.

• integer inputlist::ndiscrete = 2

resolution of the real space grid on which fast Fourier transforms are performed is given by Ndiscrete\*Mpol\*4

• integer inputlist::nquad = -1

Resolution of the Gaussian quadrature.

• integer inputlist::impol = -4

Fourier resolution of straight-fieldline angle on interfaces.

• integer inputlist::intor = -4

Fourier resolution of straight-fieldline angle on interfaces;.

• integer inputlist::lsparse = 0

controls method used to solve for rotational-transform on interfaces

• integer inputlist::lsvdiota = 0

controls method used to solve for rotational-transform on interfaces; only relevant if Lsparse = 0

• integer inputlist::imethod = 3

controls iterative solution to sparse matrix arising in real-space transformation to the straight-fieldline angle; only relevant if Lsparse.eq.2;

• integer inputlist::iorder = 2

controls real-space grid resolution for constructing the straight-fieldline angle; only relevant if Lsparse>0

• integer inputlist::iprecon = 0

controls iterative solution to sparse matrix arising in real-space transformation to the straight-fieldline angle; only relevant if Lsparse.eq.2;

• real inputlist::iotatol = -1.0

tolerance required for iterative construction of straight-fieldline angle; only relevant if Lsparse.ge.2

• integer inputlist::lextrap = 0

geometry of innermost interface is defined by extrapolation

• integer inputlist::mregular = -1

maximum regularization factor

• integer inputlist::lrzaxis = 1

controls the guess of geometry axis in the innermost volume or initialization of interfaces

• integer inputlist::ntoraxis = 3

the number of n harmonics used in the Jacobian m=1 harmonic elimination method; only relevant if  $Lrzaxis. \leftarrow ge.1$ .

# 5.43.1 Detailed Description

The namelist numericlist controls internal resolution parameters that the user rarely needs to consider.

#### 5.43.2 Variable Documentation

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#### **5.43.2.1 linitialize** integer inputlist::linitialize = 0

Used to initialize geometry using a regularization / extrapolation method.

• if Linitialize = -I, where I is a positive integer, the geometry of the  $i=1,N_V-I$  surfaces constructed by an extrapolation

- if Linitialize = 0, the geometry of the interior surfaces is provided after the namelists in the input file
- if Linitialize = 1, the interior surfaces will be intialized as  $R_{l,m,n} = R_{N,m,n} \psi_{t,l}^{m/2}$ , where  $R_{N,m,n}$  is the plasma boundary and  $\psi_{t,l}$  is the given toroidal flux enclosed by the l-th interface, normalized to the total enclosed toroidal flux; a similar extrapolation is used for  $Z_{l,m,n}$
- Note that the Fourier harmonics of the boundary is always given by the Rbc and Zbs given in physicslist.
- if Linitialize = 2, the interior surfaces and the plasma boundary will be intialized as  $R_{l,m,n} = R_{W,m,n}\psi_{t,l}^{m/2}$ , where  $R_{W,m,n}$  is the computational boundary and  $\psi_{t,l}$  is the given toroidal flux enclosed by the l-th interface, normalized to the total enclosed toroidal flux; a similar extrapolation is used for  $Z_{l,m,n}$
- Note that, for free-boundary calculations, the Fourier harmonics of the computational boundary are *always* given by the Rwc and Zws given in physicslist.
- if Linitialize = 1, 2, it is not required to provide the geometry of the interfaces after the namelists

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), preset(), and allglobal::wrtend().

## **5.43.2.2 lautoinithn** integer inputlist::lautoinithn = 1

Used to initialize  $B_{ns}$  using an initial fixed-boundary calculation.

- only relevant if Lfreebound = 1
- user-supplied Bns will only be considered if LautoinitBn = 0

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), spec(), and allglobal::wrtend().

## **5.43.2.3 | Izerovac** integer inputlist::lzerovac = 0

Used to adjust vacuum field to cancel plasma field on computational boundary.

• only relevant if Lfreebound = 1

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), spec(), and allglobal::wrtend().

#### **5.43.2.4 ndiscrete** integer inputlist::ndiscrete = 2

resolution of the real space grid on which fast Fourier transforms are performed is given by Ndiscrete\*Mpol\*4

• constraint Ndiscrete>0

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), preset(), and allglobal::wrtend().

```
5.43.2.5 nquad integer inputlist::nquad = -1
```

Resolution of the Gaussian quadrature.

- The resolution of the Gaussian quadrature,  $\int \!\! f(s) ds = \sum_k \omega_k f(s_k)$ , in each volume is given by Iquad  $_v$ ,
- Iquad v is set in preset()

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), preset(), and allglobal::wrtend().

```
5.43.2.6 impol integer inputlist::impol = -4
```

Fourier resolution of straight-fieldline angle on interfaces.

- the rotational-transform on the interfaces is determined by a transformation to the straight-fieldline angle, with poloidal resolution given by iMpol
- if iMpol <= 0, then iMpol = Mpol iMpol

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), preset(), and allglobal::wrtend().

```
5.43.2.7 intor integer inputlist::intor = -4
```

Fourier resolution of straight-fieldline angle on interfaces;.

- the rotational-transform on the interfaces is determined by a transformation to the straight-fieldline angle, with toroidal resolution given by iNtor
- if iNtor<=0 then iNtor = Ntor iNtor
- if Ntor==0, then the toroidal resolution of the angle transformation is set 1Ntor = 0

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), preset(), and allglobal::wrtend().

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```
5.43.2.8 Isparse integer inputlist::lsparse = 0
```

controls method used to solve for rotational-transform on interfaces

• if Lsparse = 0, the transformation to the straight-fieldline angle is computed in Fourier space using a dense matrix solver, F04AAF

- if Lsparse = 1, the transformation to the straight-fieldline angle is computed in real space using a dense matrix solver, F04ATF
- if Lsparse = 2, the transformation to the straight-fieldline angle is computed in real space using a sparse matrix solver, F11DEF
- if Lsparse = 3, the different methods for constructing the straight-fieldline angle are compared

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), tr00ab(), and allglobal::wrtend().

```
5.43.2.9 Isvdiota integer inputlist::lsvdiota = 0
```

controls method used to solve for rotational-transform on interfaces; only relevant if Lsparse = 0

- if Lsvdiota = 0, use standard linear solver to construct straight fieldline angle transformation
- if Lsvdiota = 1, use SVD method to compute rotational-transform

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), tr00ab(), and allglobal::wrtend().

```
5.43.2.10 imethod integer inputlist::imethod = 3
```

controls iterative solution to sparse matrix arising in real-space transformation to the straight-fieldline angle; only relevant if Lsparse.eq.2;

See also

tr00ab() for details

- if imethod = 1, the method is RGMRES
- if imethod = 2, the method is CGS
- if imethod = 3, the method is BICGSTAB

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), tr00ab(), and allglobal::wrtend().

```
5.43.2.11 iorder integer inputlist::iorder = 2
```

controls real-space grid resolution for constructing the straight-fieldline angle; only relevant if Lsparse>0

determines order of finite-difference approximation to the derivatives

- if iorder = 2,
- if iorder = 4,
- if iorder = 6,

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), tr00ab(), and allglobal::wrtend().

```
5.43.2.12 iprecon integer inputlist::iprecon = 0
```

controls iterative solution to sparse matrix arising in real-space transformation to the straight-fieldline angle; only relevant if Lsparse.eq.2;

See also

tr00ab() for details

- if iprecon = 0, the preconditioner is 'N'
- if iprecon = 1, the preconditioner is 'J'
- if iprecon = 2, the preconditioner is 'S'

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), tr00ab(), and allglobal::wrtend().

```
5.43.2.13 mregular integer inputlist::mregular = -1
```

maximum regularization factor

• if Mregular.ge.2, then regumm  $_i$  = Mregular /2 where m  $_i$  > Mregular

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), preset(), and allglobal::wrtend().

```
5.43.2.14 Irzaxis integer inputlist::lrzaxis = 1
```

controls the guess of geometry axis in the innermost volume or initialization of interfaces

- if iprecon = 1, the centroid is used
- if iprecon = 2, the Jacobian m = 1 harmonic elimination method is used

 $Referenced\ by\ allglobal::broadcast\_inputs(),\ allglobal::check\_inputs(),\ sphdf5::mirror\_input\_to\_outfile(),\ rzaxis(),\ and\ allglobal::wrtend().$ 

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## 5.44 locallist

The namelist locallist controls the construction of the Beltrami fields in each volume.

Collaboration diagram for locallist:



#### **Variables**

• integer inputlist::lbeltrami = 4

Control flag for solution of Beltrami equation.

• integer inputlist::linitgues = 1

controls how initial guess for Beltrami field is constructed

• integer inputlist::lposdef = 0

redundant;

real inputlist::maxrndgues = 1.0

the maximum random number of the Beltrami field if Linitgues = 3

• integer inputlist::lmatsolver = 3

1 for LU factorization, 2 for GMRES, 3 for GMRES matrix-free

integer inputlist::nitergmres = 200

number of max iteration for GMRES

• real inputlist::epsgmres = 1e-14

the precision of GMRES

• integer inputlist::lgmresprec = 1

type of preconditioner for GMRES, 1 for ILU sparse matrix

• real inputlist::epsilu = 1e-12

the precision of incomplete LU factorization for preconditioning

## 5.44.1 Detailed Description

The namelist locallist controls the construction of the Beltrami fields in each volume.

The transformation to straight-fieldline coordinates is singular when the rotational-transform of the interfaces is rational; however, the rotational-transform is still well defined.

### 5.44.2 Variable Documentation

## **5.44.2.1 | Ibeltrami** integer inputlist::lbeltrami = 4

Control flag for solution of Beltrami equation.

- if LBeltrami = 1,3,5 or 7, (SQP) then the Beltrami field in each volume is constructed by minimizing the magnetic energy with the constraint of fixed helicity; this is achieved by using sequential quadratic programming as provided by E04UFF. This approach has the benefit (in theory) of robustly constructing minimum energy solutions when multiple, i.e. bifurcated, solutions exist.
- if LBeltrami = 2,3,6 or 7, (Newton) then the Beltrami fields are constructed by employing a standard Newton method for locating an extremum of  $F \equiv \int B^2 dv \mu (\int \mathbf{A} \cdot \mathbf{B} dv \mathcal{K})$ , where  $\mu$  is treated as an independent degree of freedom similar to the parameters describing the vector potential and  $\mathcal{K}$  is the required value of the helicity; this is the standard Lagrange multipler approach for locating the constrained minimum; this method cannot distinguish saddle-type extrema from minima, and which solution that will be obtained depends on the initial guess;
- if LBeltrami = 4,5,6 or 7, (linear) it is assumed that the Beltrami fields are parameterized by  $\mu$ ; in this case, it is only required to solve  $\nabla \times \mathbf{B} = \mu \mathbf{B}$  which reduces to a system of linear equations;  $\mu$  may or may not be adjusted iteratively, depending on Lconstraint, to satisfy either rotational-transform or helicity constraints;
- for flexibility and comparison, each of the above methods can be employed; for example:
  - if LBeltrami = 1, only the SQP method will be employed;
  - if LBeltrami = 2, only the Newton method will be employed;
  - if LBeltrami = 4, only the linear method will be employed;
  - if LBeltrami = 3, the SQP and the Newton method are used;
  - if LBeltrami = 5, the SQP and the linear method are used;
  - if LBeltrami = 6, the Newton and the linear method are used;
  - if LBeltrami = 7, all three methods will be employed;

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), preset(), and allglobal::wrtend().

### **5.44.2.2 linitgues** integer inputlist::linitgues = 1

controls how initial guess for Beltrami field is constructed

- only relevant for routines that require an initial guess for the Beltrami fields, such as the SQP and Newton methods, or the sparse linear solver;
- if Linitgues = 0, the initial guess for the Beltrami field is trivial
- if Linitgues = 1, the initial guess for the Beltrami field is an integrable approximation
- if Linitgues = 2, the initial guess for the Beltrami field is read from file
- if Linitques = 3, the initial guess for the Beltrami field will be randomized with the maximum maxrndques

 $Referenced\ by\ allglobal::broadcast\_inputs(),\ allglobal::check\_inputs(),\ sphdf5::mirror\_input\_to\_outfile(),\ preset(),\ and\ allglobal::wrtend().$ 

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# 5.45 globallist

The namelist globallist controls the search for global force-balance.

Collaboration diagram for globallist:

```
Input namelists and global variables globallist
```

## **Variables**

```
• integer inputlist::lfindzero = 0
```

use Newton methods to find zero of force-balance, which is computed by dforce()

real inputlist::escale = 0.0

controls the weight factor, BBweight, in the force-imbalance harmonics

• real inputlist::opsilon = 1.0

weighting of force-imbalance

real inputlist::pcondense = 2.0

spectral condensation parameter

• real inputlist::epsilon = 0.0

weighting of spectral-width constraint

real inputlist::wpoloidal = 1.0

"star-like" poloidal angle constraint radial exponential factor used in preset() to construct sweight

• real inputlist::upsilon = 1.0

weighting of "star-like" poloidal angle constraint used in preset() to construct sweight

• real inputlist::forcetol = 1.0e-10

required tolerance in force-balance error; only used as an initial check

• real inputlist::c05xmax = 1.0e-06

required tolerance in position,  $\mathbf{x} \equiv \{R_{i,v}, Z_{i,v}\}$ 

• real inputlist::c05xtol = 1.0e-12

required tolerance in position,  $\mathbf{x} \equiv \{R_{i,v}, Z_{i,v}\}$ 

• real inputlist::c05factor = 1.0e-02

used to control initial step size in C05NDF and C05PDF

• logical inputlist::lreadgf = .true.

read  $\nabla_{\mathbf{x}}\mathbf{F}$  from file <code>ext.GF</code>

• integer inputlist::mfreeits = 0

maximum allowed free-boundary iterations

real inputlist::bnstol = 1.0e-06

redundant;

real inputlist::bnsblend = 0.666

redundant;

• real inputlist::gbntol = 1.0e-06

required tolerance in free-boundary iterations

• real inputlist::gbnbld = 0.666

normal blend

• real inputlist::vcasingeps = 1.e-12

regularization of Biot-Savart; see bnorml(), casing()

• real inputlist::vcasingtol = 1.e-08

accuracy on virtual casing integral; see bnorml(), casing()

• integer inputlist::vcasingits = 8

minimum number of calls to adaptive virtual casing routine; see casing()

• integer inputlist::vcasingper = 1

periods of integragion in adaptive virtual casing routine; see casing()

• integer inputlist::mcasingcal = 8

minimum number of calls to adaptive virtual casing routine; see casing(); redundant;

### 5.45.1 Detailed Description

The namelist globallist controls the search for global force-balance.

Comments:

The "force" vector, F, which is constructed in dforce(), is a combination of pressure-imbalance Fourier harmonics.

$$F_{i,v} \equiv [[p+B^2/2]]_{i,v} \times \exp\left[-\operatorname{escale}(m_i^2 + n_i^2)\right] \times \operatorname{opsilon}, \tag{255}$$

and spectral-condensation constraints,  $I_{i,v}$ , and the "star-like" angle constraints,  $S_{i,v}$ , (see Iforce() for details)

$$F_{i,v} \equiv \operatorname{epsilon} \times I_{i,v} + \operatorname{upsilon} \times \left( \psi_v^{\omega} S_{i,v,1} - \psi_{v+1}^{\omega} S_{i,v+1,0} \right), \tag{256}$$

where  $\psi_v \equiv \text{normalized toroidal flux}$ , tflux, and  $\omega \equiv \text{wpoloidal}$ .

### 5.45.2 Variable Documentation

## **5.45.2.1 Ifindzero** integer inputlist::lfindzero = 0

use Newton methods to find zero of force-balance, which is computed by dforce()

- if Lfindzero = 0, then dforce() is called once to compute the Beltrami fields consistent with the given geometry and constraints
- if Lfindzero = 1, then call C05NDF (uses function values only), which iteratively calls dforce()
- if Lfindzero = 2, then call COSPDF (uses derivative information), which iteratively calls dforce()

Referenced by brcast(), allglobal::broadcast\_inputs(), allglobal::check\_inputs(), dfp200(), hesian(), sphdf5::mirror — \_input\_to\_outfile(), packxi(), preset(), spec(), and allglobal::wrtend().

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```
5.45.2.2 escale real inputlist::escale = 0.0
```

controls the weight factor, BBweight, in the force-imbalance harmonics

- BBweight (i)  $\equiv$  opsilon  $\times \exp\left[-\text{escale} \times (m_i^2 + n_i^2)\right]$
- defined in preset(); used in dforce()
- also see Eqn. (255)

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), preset(), and allglobal::wrtend().

```
5.45.2.3 opsilon real inputlist::opsilon = 1.0
```

weighting of force-imbalance

• used in dforce(); also see Eqn. (255)

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), preset(), and allglobal::wrtend().

## **5.45.2.4 pcondense** real inputlist::pcondense = 2.0

spectral condensation parameter

- used in preset() to define mmpp (i)  $\equiv m_i^p$ , where  $p \equiv {\tt pcondense}$
- the angle freedom is exploited to minimize  $\operatorname{epsilon} \sum_i m_i^p (R_i^2 + Z_i^2)$  with respect to tangential variations in the interface geometry
- also see Eqn. (256)

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), preset(), and allglobal::wrtend().

```
5.45.2.5 epsilon real inputlist::epsilon = 0.0
```

weighting of spectral-width constraint

• used in dforce(); also see Eqn. (256)

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), dforce(), dfp200(), evaluate\_dbb(), sphdf5 ::mirror\_input\_to\_outfile(), pc00ab(), and allglobal::wrtend().

### **5.45.2.6 forcetol** real inputlist::forcetol = 1.0e-10

required tolerance in force-balance error; only used as an initial check

- if the initially supplied interfaces are consistent with force-balance to within forcetol then the geometry of the interfaces is not altered
- if not, then the geometry of the interfaces is changed in order to bring the configuration into force balance so that the geometry of interfaces is within c05xtol, defined below, of the true solution
- to force execution of either C05NDF or C05PDF, regardless of the initial force imbalance, set forcetol < o

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), pc00aa(), pc00ab(), preset(), and allglobal::wrtend().

### **5.45.2.7 c05xtol** real inputlist::c05xtol = 1.0e-12

required tolerance in position,  $\mathbf{x} \equiv \{R_{i,v}, Z_{i,v}\}$ 

- used by both C05NDF and C05PDF; see the NAG documents for further details on how the error is defined
- constraint c05xtol > 0.0

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), and allglobal::wrtend().

### **5.45.2.8 c05factor** real inputlist::c05factor = 1.0e-02

used to control initial step size in C05NDF and C05PDF

- constraint c05factor > 0.0
- only relevant if Lfindzero > 0

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), and allglobal::wrtend().

## **5.45.2.9 | lreadgf** | logical inputlist::lreadgf = .true.

read  $\nabla_{\mathbf{x}} \mathbf{F}$  from file ext . GF

- only used if Lfindzero = 2
- only used in newton()

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), and allglobal::wrtend().

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**5.45.2.10** mfreeits integer inputlist::mfreeits = 0

maximum allowed free-boundary iterations

- only used if Lfreebound = 1
- only used in xspech()

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), spec(), and allglobal::wrtend().

**5.45.2.11 gbntol** real inputlist::gbntol = 1.0e-06

required tolerance in free-boundary iterations

- only used if Lfreebound = 1
- only used in xspech()

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), spec(), and allglobal::wrtend().

**5.45.2.12 gbnbld** real inputlist::gbnbld = 0.666

normal blend

• The "new" magnetic field at the computational boundary produced by the plasma currents is updated using a Picard scheme:

$$(\mathbf{B} \cdot \mathbf{n})^{j+1} = gBnbld \times (\mathbf{B} \cdot \mathbf{n})^j + (1 - gBnbld) \times (\mathbf{B} \cdot \mathbf{n})^*, \tag{257}$$

where j labels free-boundary iterations, and  $(\mathbf{B} \cdot \mathbf{n})^*$  is computed by virtual casing.

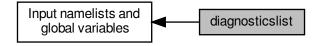
- only used if Lfreebound = 1
- only used in xspech()

Referenced by allglobal::broadcast\_inputs(), allglobal::check\_inputs(), sphdf5::mirror\_input\_to\_outfile(), spec(), and allglobal::wrtend().

## 5.46 diagnosticslist

The namelist diagnosticslist controls post-processor diagnostics, such as Poincaré plot resolution, etc.

Collaboration diagram for diagnosticslist:



### **Variables**

```
real inputlist::odetol = 1.0e-07
      o.d.e. integration tolerance for all field line tracing routines
• real inputlist::absreq = 1.0e-08
      redundant
• real inputlist::relreq = 1.0e-08
      redundant

    real inputlist::absacc = 1.0e-04

      redundant
• real inputlist::epsr = 1.0e-08
      redundant
• integer inputlist::nppts = 0
      number of toroidal transits used (per trajectory) in following field lines for constructing Poincaré plots; if nPpts<1,
      no Poincaré plot is constructed;
• real inputlist::ppts = 0.0
      stands for Poincare plot theta start. Chose at which angle (normalized over \pi) the Poincare field-line tracing start.
• integer, dimension(1:mnvol+1) inputlist::nptrj = -1
      number of trajectories in each annulus to be followed in constructing Poincaré plot

    logical inputlist::lhevalues = .false.

      to compute eigenvalues of 
abla \mathbf{F}

    logical inputlist::lhevectors = .false.

      to compute eigenvectors (and also eigenvalues) of \nabla \mathbf{F}
• logical inputlist::lhmatrix = .false.
      to compute and write to file the elements of \nabla \mathbf{F}
• integer inputlist::lperturbed = 0
      to compute linear, perturbed equilibrium
• integer inputlist::dpp = -1
      perturbed harmonic

    integer inputlist::dqq = -1

      perturbed harmonic
• integer inputlist::lerrortype = 0
      the type of error output for Lcheck=1
• integer inputlist::ngrid = -1
      the number of points to output in the grid, -1 for Lrad(vvol)

    real inputlist::drz = 1E-5

      difference in geometry for finite difference estimate (debug only)
• integer inputlist::lcheck = 0
      implement various checks
• logical inputlist::ltiming = .false.
      to check timing
• real inputlist::fudge = 1.0e-00
      redundant
• real inputlist::scaling = 1.0e-00
      redundant
```

### 5.46.1 Detailed Description

The namelist diagnosticslist controls post-processor diagnostics, such as Poincaré plot resolution, etc.

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### 5.46.2 Variable Documentation

```
5.46.2.1 nptrj integer, dimension(1:mnvol+1) inputlist::nptrj = -1
```

number of trajectories in each annulus to be followed in constructing Poincaré plot

• if nPtrj(1) < 0, then nPtrj(1) = Ni(I), where Ni(I) is the grid resolution used to construct the Beltrami field in volume l

Referenced by allglobal::broadcast\_inputs(), final\_diagnostics(), sphdf5::mirror\_input\_to\_outfile(), pp00aa(), spec(), and allglobal::wrtend().

### **5.46.2.2 | Icheck** integer inputlist::lcheck = 0

implement various checks

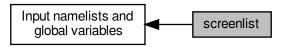
- if Lcheck = 0, no additional check on the calculation is performed
- if Lcheck = 1, the error in the current, i.e.  $\nabla \times \mathbf{B} \mu \mathbf{B}$  is computed as a post-diagnostic
- if Lcheck = 2, the analytic derivatives of the interface transform w.r.t. the helicity multiplier,  $\mu$ , and the enclosed poloidal flux,  $\Delta \psi_p$ , are compared to a finite-difference estimate
  - only if Lconstraint==1
  - only for dspec executable, i.e. must compile with DFLAGS = "-D DEBUG"
- if Lcheck = 3, the analytic derivatives of the volume w.r.t. interface Fourier harmonic is compared to a finite-difference estimate
  - must set Lfindzero = 2
  - set forcetol sufficiently small and set LreadGF = F, so that the matrix of second derivatives is calculated
  - only for dspec executable, i.e. must compile with DFLAGS = "-D DEBUG"
- if Lcheck = 4, the analytic calculation of the derivatives of the magnetic field,  $B^2$ , at the interfaces is compared to a finite-difference estimate
  - $\mathsf{must}\,\mathsf{set}\,\mathsf{Lfindzero} = 2$
  - set forcetol sufficiently small
  - set LreadGF=F
  - only for dspec executable, i.e. must compile with DFLAGS = "-D DEBUG"
- if Lcheck = 5, the analytic calculation of the matrix of the derivatives of the force imbalance is compared to a finite-difference estimate
- if Lcheck = 6, the virtual casing calculation is compared to xdiagno (Lazerson 2013 [6])
  - the input file for xdiagno is written by bnorml()
  - this provides the Cartesian coordinates on the computational boundary where the virtual casing routine casing() computes the magnetic field, with the values of the magnetic field being written to the screen for comparison
  - must set Freebound=1, Lfindzero>0, mfreeits!=0
  - xdiagno must be executed manually

Referenced by bnorml(), allglobal::broadcast\_inputs(), allglobal::check\_inputs(), dforce(), dfp200(), evaluate\_dbb(), evaluate\_dmupfdx(), final\_diagnostics(), sphdf5::hdfint(), hesian(), lforce(), ma02aa(), sphdf5::mirror\_input\_to\_ $\leftarrow$  outfile(), preset(), rzaxis(), spec(), and allglobal::wrtend().

### 5.47 screenlist

The namelist screenlist controls screen output. Every subroutine, e.g. xy00aa.h, has its own write flag, wxy00aa.h

Collaboration diagram for screenlist:



### **Variables**

- logical inputlist::wmanual = .false.
- logical inputlist::wrzaxis = .false.
- logical inputlist::wpackxi = .false.
- logical inputlist::wvolume = .false.
- logical inputlist::wcoords = .false.
- logical inputlist::wbasefn = .false.
- logical **inputlist::wmemory** = .false.
- logical inputlist::wmetrix = .false.
- logical inputlist::wma00aa = .false.
- logical inputlist::wmatrix = .false.
- logical inputlist::wspsmat = .false.
- logical inputlist::wspsint = .false.
- logical inputlist::wmp00ac = .false.
- logical inputlist::wma02aa = .false.
- logical inputlist::wpackab = .false.
- logical inputlist::wtr00ab = .false.
   logical inputlist::wcurent = .false.
- logical inputlist::wdf00ab = .false.
- logical inputlist::wlforce = .false.
- logical inputlist::wintghs = .false.
- logical inputlist::wmtrxhs = .false.
- logical inputlist::wlbpol = .false.
- logical inputlist::wbrcast = .false.
- logical inputlist::wdfp100 = .false.
- logical inputlist::wdfp200 = .false.
- logical inputlist::wdforce = .false.
- logical inputlist::wnewton = .false.
- logical inputlist::wcasing = .false.
- logical inputlist::wbnorml = .false.
- logical inputlist::wjo00aa = .false.
- logical inputlist::wpp00aa = .false.
- logical inputlist::wpp00ab = .false.
- logical inputlist::wbfield = .false.
- logical inputlist::wstzxyz = .false.

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- logical inputlist::whesian = .false.
- logical inputlist::wra00aa = .false.
- logical inputlist::wnumrec = .false.
- logical inputlist::wdcuhre = .false.
- logical inputlist::wminpack = .false.
- logical inputlist::wiqpack = .false.
- logical inputlist::wrksuite = .false.
- logical inputlist::wi1mach = .false.
- logical inputlist::wd1mach = .false.
- logical inputlist::wilut = .false.
- logical inputlist::witers = .false.
- logical inputlist::wsphdf5 = .false.
- logical inputlist::wpreset = .false.
- logical inputlist::wglobal = .false.
- logical inputlist::wxspech = .false.
- logical inputlist::wbuild\_vector\_potential = .false.
- logical inputlist::wreadin = .false.

write screen output of readin()

• logical inputlist::wwrtend = .false.

write screen output of wrtend()

• logical inputlist::wmacros = .false.

write screen output from expanded macros

### 5.47.1 Detailed Description

The namelist screenlist controls screen output. Every subroutine, e.g. xy00aa.h, has its own write flag, Wxy00aa.h

## 5.47.2 Variable Documentation

**5.47.2.1 wbuild\_vector\_potential** logical inputlist::wbuild\_vector\_potential = .false.

Todo: what is this?

# 6 Module Documentation

## 6.1 aligiobal Module Reference

global variable storage used as "workspace" throughout the code

### **Functions/Subroutines**

- subroutine build\_vector\_potential (Ivol, iocons, aderiv, tderiv)
- · subroutine set mpi comm (comm)
- subroutine read\_inputlists\_from\_file ()
- subroutine check\_inputs ()
- subroutine broadcast inputs
- · subroutine wrtend

The restart file is written.

• subroutine ismyvolume (vvol)

Check if volume vvol is associated to the corresponding MPI node.

subroutine whichcpuid (vvol, cpu\_id)

Returns which MPI node is associated to a given volume.

## **Variables**

· integer myid

MPI rank of current CPU.

integer ncpu

number of MPI tasks

· integer ismyvolumevalue

flag to indicate if a CPU is operating on its assigned volume

· real cpus

initial time

• integer mpi\_comm\_spec

SPEC MPI communicator.

- logical skip\_write = .false.
- · real pi2nfp
- · real pi2pi2nfp
- · real pi2pi2nfphalf
- real pi2pi2nfpquart
- character(len=1000) ext
- · real forceerr

total force-imbalance

· real energy

MHD energy.

- real, dimension(:), allocatable ipdt
- · real, dimension(:,:), allocatable ipdtdpf

Toroidal pressure-driven current.

- integer mvol
- logical yesstellsym

internal shorthand copies of Istellsym, which is an integer input;

· logical notstellsym

internal shorthand copies of Istellsym, which is an integer input;

- logical yesmatrixfree
- · logical notmatrixfree

to use matrix-free method or not

real, dimension(:,:), allocatable cheby

local workspace for evaluation of Chebychev polynomials

real, dimension(:,:,:), allocatable zernike

local workspace for evaluation of Zernike polynomials

```
real, dimension(:,:,:), allocatable tt
      derivatives of Chebyshev polynomials at the inner and outer interfaces;
 real, dimension(:,:,:,:), allocatable rtt
      derivatives of Zernike polynomials at the inner and outer interfaces;
  real, dimension(:,:), allocatable rtm
      r^m term of Zernike polynomials at the origin

    real, dimension(:), allocatable zernikedof

      Zernike degree of freedom for each m.

    integer mne

      enhanced resolution for metric elements
• integer, dimension(:), allocatable ime
      enhanced poloidal mode numbers for metric elements

    integer, dimension(:), allocatable ine

      enhanced toroidal mode numbers for metric elements
· integer mns
      enhanced resolution for straight field line transformation
• integer, dimension(:), allocatable ims
      enhanced poloidal mode numbers for straight field line transformation
• integer, dimension(:), allocatable ins
      enhanced toroidal mode numbers for straight field line transformation

    integer Impol

      what is this?
 integer Intor
      what is this?

    integer smpol

      what is this?
  integer sntor
      what is this?
 real xoffset = 1.0
      used to normalize NAG routines (which ones exacly where?)
· logical, dimension(:), allocatable imagneticok
      used to indicate if Beltrami fields have been correctly constructed;
· logical iconstraintok
      Used to break iteration loops of slaves in the global constraint minimization.
• real, dimension(:,:), allocatable beltramierror
      to store the integral of |curlB-mu*B| computed by jo00aa;
· integer mn
      total number of Fourier harmonics for coordinates/fields; calculated from Mpol, Ntor in readin()

    integer, dimension(:), allocatable im

      poloidal mode numbers for Fourier representation
· integer, dimension(:), allocatable in
      toroidal mode numbers for Fourier representation
• real, dimension(:), allocatable halfmm
      I saw this already somewhere...
• real, dimension(:), allocatable regumm
      I saw this already somewhere...

    real rscale

      no idea

    real, dimension(:,:), allocatable psifactor
```

real, dimension(:,:), allocatable inifactor

integer num\_modes

integer, dimension(:), allocatable mmrzrz

```
no idea
· real, dimension(:), allocatable bbweight
      weight on force-imbalance harmonics; used in dforce()
· real, dimension(:), allocatable mmpp
      spectral condensation factors
• real, dimension(:,:), allocatable irbc
      cosine R harmonics of interface surface geometry; stellarator symmetric

    real, dimension(:,:), allocatable izbs

      sine Z harmonics of interface surface geometry; stellarator symmetric

    real, dimension(:,:), allocatable irbs

      sine R harmonics of interface surface geometry; non-stellarator symmetric

    real, dimension(:,:), allocatable izbc

      cosine Z harmonics of interface surface geometry; non-stellarator symmetric

    real, dimension(:,:), allocatable drbc

      cosine R harmonics of interface surface geometry; stellarator symmetric; linear deformation

    real, dimension(:,:), allocatable dzbs

      sine Z harmonics of interface surface geometry; stellarator symmetric; linear deformation

    real, dimension(:,:), allocatable drbs

      sine R harmonics of interface surface geometry; non-stellarator symmetric; linear deformation

    real, dimension(:,:), allocatable dzbc

      cosine Z harmonics of interface surface geometry; non-stellarator symmetric; linear deformation

    real, dimension(:,:), allocatable irij

      interface surface geometry; real space

    real, dimension(:,:), allocatable izij

      interface surface geometry; real space

    real, dimension(:,:), allocatable drij

      interface surface geometry; real space

    real, dimension(:,:), allocatable dzij

      interface surface geometry; real space
• real, dimension(:,:), allocatable trij
      interface surface geometry; real space

    real, dimension(:,:), allocatable tzij

      interface surface geometry; real space
· real, dimension(:), allocatable ivns
      sine harmonics of vacuum normal magnetic field on interfaces; stellarator symmetric
• real, dimension(:), allocatable ibns
      sine harmonics of plasma normal magnetic field on interfaces; stellarator symmetric
· real, dimension(:), allocatable ivnc
      cosine harmonics of vacuum normal magnetic field on interfaces; non-stellarator symmetric

    real, dimension(:), allocatable ibnc

      cosine harmonics of plasma normal magnetic field on interfaces; non-stellarator symmetric

    real, dimension(:), allocatable lrbc

      local workspace

    real, dimension(:), allocatable lzbs

      local workspace

    real, dimension(:), allocatable Irbs

      local workspace
• real, dimension(:), allocatable lzbc
      local workspace
```

 integer, dimension(:), allocatable nnrzrz • real, dimension(:,:,:), allocatable allrzrz · integer nt discrete resolution along  $\theta$  of grid in real space integer nz discrete resolution along  $\zeta$  of grid in real space integer ntz discrete resolution; Ntz=Nt\*Nz shorthand integer hnt discrete resolution; Ntz=Nt\*Nz shorthand integer hnz discrete resolution; Ntz=Nt\*Nz shorthand real sontz one / sqrt (one\*Ntz); shorthand real, dimension(:,:,:), allocatable rij real-space grid; R • real, dimension(:,:,:), allocatable zij real-space grid; Z real, dimension(:,:,:), allocatable xij what is this? real, dimension(:,:,:), allocatable yij what is this? real, dimension(:,:), allocatable sg real-space grid; jacobian and its derivatives real, dimension(:,:,:,:), allocatable guvij real-space grid; metric elements real, dimension(:,:,:), allocatable gvuij real-space grid; metric elements (?); 10 Dec 15; • real, dimension(:,:,:,:), allocatable guvijsave what is this? • integer, dimension(:,:), allocatable ki identification of Fourier modes • integer, dimension(:,:,:), allocatable kijs identification of Fourier modes integer, dimension(:,:,:), allocatable kija identification of Fourier modes integer, dimension(:), allocatable iotakkii identification of Fourier modes integer, dimension(:,:), allocatable iotaksub identification of Fourier modes • integer, dimension(:,:), allocatable iotakadd identification of Fourier modes integer, dimension(:,:), allocatable iotaksgn identification of Fourier modes • real, dimension(:), allocatable efmn Fourier harmonics; dummy workspace. · real, dimension(:), allocatable ofmn Fourier harmonics; dummy workspace.

real, dimension(:), allocatable cfmn

real, dimension(:), allocatable sfmn

Fourier harmonics; dummy workspace.

Fourier harmonics; dummy workspace.

```
• real, dimension(:), allocatable evmn
      Fourier harmonics; dummy workspace.
• real, dimension(:), allocatable odmn
      Fourier harmonics; dummy workspace.
· real, dimension(:), allocatable comn
      Fourier harmonics; dummy workspace.

    real, dimension(:), allocatable simn

      Fourier harmonics; dummy workspace.
• real, dimension(:), allocatable ijreal
      what is this?
· real, dimension(:), allocatable ijimag
      what is this?
• real, dimension(:), allocatable jireal
      what is this?
· real, dimension(:), allocatable jiimag
      what is this?
• real, dimension(:), allocatable jkreal
      what is this?

    real, dimension(:), allocatable jkimag

      what is this?
• real, dimension(:), allocatable kireal
      what is this?
· real, dimension(:), allocatable kjimag
      what is this?
• real, dimension(:,:,:), allocatable bsupumn
      tangential field on interfaces; \theta-component; required for virtual casing construction of field; 11 Oct 12

    real, dimension(:,:,:), allocatable bsupvmn

      tangential field on interfaces; \zeta -component; required for virtual casing construction of field; 11 Oct 12

    real, dimension(:,:), allocatable goomne

     described in preset()
• real, dimension(:,:), allocatable goomno
     described in preset()

    real, dimension(:,:), allocatable gssmne

     described in preset()

    real, dimension(:,:), allocatable gssmno

      described in preset()
• real, dimension(:,:), allocatable gstmne
      described in preset()
• real, dimension(:,:), allocatable gstmno
     described in preset()
• real, dimension(:,:), allocatable gszmne
     described in preset()
• real, dimension(:,:), allocatable gszmno
      described in preset()

    real, dimension(:,:), allocatable gttmne

     described in preset()
• real, dimension(:,:), allocatable gttmno
      described in preset()
• real, dimension(:,:), allocatable gtzmne
      described in preset()
```

```
    real, dimension(:,:), allocatable gtzmno

      described in preset()

    real, dimension(:,:), allocatable gzzmne

      described in preset()
• real, dimension(:,:), allocatable gzzmno
      described in preset()

    real, dimension(:,:,:,:), allocatable dtoocc

      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable dtoocs

      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable dtoosc

      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable dtooss

      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable ttsscc

      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable ttsscs

      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable ttsssc

      volume-integrated Chebychev-metrics; see matrix()
• real, dimension(:,:,:,:), allocatable ttssss
      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable tdstcc

      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable tdstcs

      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable tdstsc

      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable tdstss

      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable tdszcc

      volume-integrated Chebychev-metrics; see matrix()
• real, dimension(:,:,:,:), allocatable tdszcs
      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable tdszsc

      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable tdszss

      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable ddttcc

      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable ddttcs

      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable ddttsc

      volume-integrated Chebychev-metrics; see matrix()
• real, dimension(:,:,:,:), allocatable ddttss
      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable ddtzcc

      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable ddtzcs

      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable ddtzsc
```

```
volume-integrated Chebychev-metrics; see matrix()
• real, dimension(:,:,:,:), allocatable ddtzss
      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable ddzzcc

      volume-integrated Chebychev-metrics; see matrix()
• real, dimension(:,:,:,:), allocatable ddzzcs
      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable ddzzsc

      volume-integrated Chebychev-metrics; see matrix()

    real, dimension(:,:,:,:), allocatable ddzzss

      volume-integrated Chebychev-metrics; see matrix()
• real, dimension(:,:), allocatable tsc
      what is this?
• real, dimension(:,:), allocatable tss
      what is this?

    real, dimension(:,:), allocatable dtc

      what is this?
• real, dimension(:,:), allocatable dts
      what is this?

    real, dimension(:,:), allocatable dzc

      what is this?
• real, dimension(:,:), allocatable dzs
      what is this?
• real, dimension(:,:), allocatable ttc
      what is this?
• real, dimension(:,:), allocatable tzc
      what is this?
• real, dimension(:,:), allocatable tts
      what is this?

    real, dimension(:,:), allocatable tzs

      what is this?

    real, dimension(:), allocatable dtflux

      \delta \psi_{toroidal} in each annulus
· real, dimension(:), allocatable dpflux
      \delta\psi_{poloidal} in each annulus

    real, dimension(:), allocatable sweight

      minimum poloidal length constraint weight
· integer, dimension(:), allocatable nadof
      degrees of freedom in Beltrami fields in each annulus
· integer, dimension(:), allocatable nfielddof
      degrees of freedom in Beltrami fields in each annulus, field only, no Lagrange multipliers

    type(subgrid), dimension(:,:,:), allocatable ate

      magnetic vector potential cosine Fourier harmonics; stellarator-symmetric

    type(subgrid), dimension(:,:,:), allocatable aze

      magnetic vector potential cosine Fourier harmonics; stellarator-symmetric

    type(subgrid), dimension(:,:,:), allocatable ato

      magnetic vector potential sine Fourier harmonics; non-stellarator-symmetric
• type(subgrid), dimension(:,:,:), allocatable azo
      magnetic vector potential sine Fourier harmonics; non-stellarator-symmetric

    integer, dimension(:,:), allocatable Ima

      Lagrange multipliers (?)
```

```
    integer, dimension(:,:), allocatable lmb

      Lagrange multipliers (?)

    integer, dimension(:,:), allocatable lmc

      Lagrange multipliers (?)

    integer, dimension(:,:), allocatable Imd

      Lagrange multipliers (?)
• integer, dimension(:,:), allocatable Ime
      Lagrange multipliers (?)

    integer, dimension(:,:), allocatable Imf

      Lagrange multipliers (?)
• integer, dimension(:,:), allocatable Img
      Lagrange multipliers (?)

    integer, dimension(:,:), allocatable lmh

      Lagrange multipliers (?)
• real, dimension(:,:), allocatable Imavalue
      what is this?
• real, dimension(:,:), allocatable Imbvalue
      what is this?
• real, dimension(:,:), allocatable Imcvalue
      what is this?
• real, dimension(:,:), allocatable Imdvalue
      what is this?
• real, dimension(:,:), allocatable Imevalue
      what is this?
• real, dimension(:,:), allocatable Imfvalue
      what is this?
• real, dimension(:,:), allocatable Imgvalue
      what is this?
• real, dimension(:,:), allocatable Imhvalue
      what is this?
• integer, dimension(:,:), allocatable fso
      what is this?
• integer, dimension(:,:), allocatable fse
      what is this?

    logical lcoordinatesingularity

      set by LREGION macro; true if inside the innermost volume

    logical lplasmaregion

      set by LREGION macro; true if inside the plasma region

    logical lvacuumregion

      set by LREGION macro; true if inside the vacuum region

    logical Isavedguvij

      flag used in matrix free

    logical localconstraint

      what is this?
• real, dimension(:,:), allocatable dma
      energy and helicity matrices; quadratic forms

    real, dimension(:,:), allocatable dmb

      energy and helicity matrices; quadratic forms

    real, dimension(:,:), allocatable dmd

      energy and helicity matrices; quadratic forms

    real, dimension(:), allocatable dmas
```

```
sparse version of dMA, data
• real, dimension(:), allocatable dmds
      sparse version of dMD, data

    integer, dimension(:), allocatable idmas

      sparse version of dMA and dMD, indices
• integer, dimension(:), allocatable jdmas
      sparse version of dMA and dMD, indices

    integer, dimension(:), allocatable ndmasmax

      number of elements for sparse matrices
• integer, dimension(:), allocatable ndmas
      number of elements for sparse matrices
· real, dimension(:), allocatable dmg
      what is this?
• real, dimension(:), allocatable adotx
      the matrix-vector product

    real, dimension(:), allocatable ddotx

      the matrix-vector product
• real, dimension(:,:), allocatable solution
      this is allocated in dforce; used in mp00ac and ma02aa; and is passed to packab
• real, dimension(:,:,:), allocatable gmreslastsolution
      used to store the last solution for restarting GMRES

    real, dimension(:), allocatable mbpsi

      matrix vector products

    logical liluprecond

      whether to use ILU preconditioner for GMRES
• real, dimension(:,:), allocatable beltramiinverse
      Beltrami inverse matrix.

    real, dimension(:,:,:), allocatable diotadxup

      measured rotational transform on inner/outer interfaces for each volume; d(transform)/dx; (see dforce)

    real, dimension(:,:,:), allocatable ditgpdxtp

      measured toroidal and poloidal current on inner/outer interfaces for each volume; d(ltor, Gpol)/dx; (see dforce)
• real, dimension(:,:,:,:), allocatable glambda
      save initial guesses for iterative calculation of rotational-transform

    integer Imns

      what is this?

    real, dimension(:,:,:), allocatable bemn

      force vector; stellarator-symmetric (?)
• real, dimension(:,:), allocatable iomn
      force vector; stellarator-symmetric (?)

    real, dimension(:,:,:), allocatable somn

      force vector; non-stellarator-symmetric (?)

    real, dimension(:,:,:), allocatable pomn

      force vector; non-stellarator-symmetric (?)

    real, dimension(:,:,:), allocatable bomn

      force vector; stellarator-symmetric (?)

    real, dimension(:,:), allocatable iemn

      force vector; stellarator-symmetric (?)
• real, dimension(:,:,:), allocatable semn
      force vector; non-stellarator-symmetric (?)

    real, dimension(:,:,:), allocatable pemn

      force vector; non-stellarator-symmetric (?)
```

```
    real, dimension(:), allocatable bbe

      force vector (?); stellarator-symmetric (?)
· real, dimension(:), allocatable iio
      force vector (?); stellarator-symmetric (?)

    real, dimension(:), allocatable bbo

      force vector (?); non-stellarator-symmetric (?)
· real, dimension(:), allocatable iie
      force vector (?); non-stellarator-symmetric (?)

    real, dimension(:,:,:), allocatable btemn

      covariant \theta cosine component of the tangential field on interfaces; stellarator-symmetric

    real, dimension(:,:,:), allocatable bzemn

      covariant \zeta cosine component of the tangential field on interfaces; stellarator-symmetric

    real, dimension(:,:,:), allocatable btomn

      covariant \theta sine component of the tangential field on interfaces; non-stellarator-symmetric

    real, dimension(:,:,:), allocatable bzomn

      covariant ζ sine component of the tangential field on interfaces; non-stellarator-symmetric
• real, dimension(:,:), allocatable bloweremn
      covariant field for Hessian computation

    real, dimension(:,:), allocatable bloweromn

      covariant field for Hessian computation
· integer lgdof
      geometrical degrees of freedom associated with each interface

    integer ngdof

      total geometrical degrees of freedom

    real, dimension(:,:,:), allocatable dbbdrz

      derivative of magnetic field w.r.t. geometry (?)

    real, dimension(:,:), allocatable diidrz

      derivative of spectral constraints w.r.t. geometry (?)

    real, dimension(:,:,:,:), allocatable dffdrz

      derivatives of B^{\wedge}2 at the interfaces wrt geometry
• real, dimension(:,:,:,:), allocatable dbbdmp
      derivatives of B^2 at the interfaces wrt mu and dpflux
• real, dimension(:,:,:,:), allocatable dmupfdx
      derivatives of mu and dpflux wrt geometry at constant interface transform
· logical Ihessianallocated
      flag to indicate that force gradient matrix is allocated (?)

    real, dimension(:,:), allocatable hessian

      force gradient matrix (?)

    real, dimension(:,:), allocatable dessian

      derivative of force gradient matrix (?)

    real, dimension(:,:), allocatable cosi

      some precomputed cosines

    real, dimension(:,:), allocatable sini

      some precomputed sines
• real, dimension(:), allocatable gteta
      something related to \sqrt{g} and \theta ?

    real, dimension(:), allocatable gzeta

      something related to \sqrt{g} and \zeta?

    real, dimension(:), allocatable aik

      definition of coordinate axis
```

real, dimension(:,:,:,:), allocatable dradr

```
derivatives of coordinate axis

    real, dimension(:,:,:,:), allocatable dradz

      derivatives of coordinate axis

    real, dimension(:,:,:,:), allocatable dzadr

      derivatives of coordinate axis

    real, dimension(:,:,:,:), allocatable dzadz

      derivatives of coordinate axis

    real, dimension(:,:,:), allocatable drodr

      derivatives of coordinate axis
• real, dimension(:,:,:), allocatable drodz
      derivatives of coordinate axis
• real, dimension(:,:,:), allocatable dzodr
      derivatives of coordinate axis
• real, dimension(:,:,:), allocatable dzodz
      derivatives of coordinate axis

    integer, dimension(:,:), allocatable djkp

      for calculating cylindrical volume

    integer, dimension(:,:), allocatable djkm

      for calculating cylindrical volume

    real, dimension(:), allocatable lbbintegral

      B.B integral.
• real, dimension(:), allocatable labintegral
      A.B integral.

    real, dimension(:), allocatable vvolume

      volume integral of \sqrt{g}; computed in volume
· real dvolume
      derivative of volume w.r.t. interface geometry

    integer ivol

      labels volume; some subroutines (called by NAG) are fixed argument list but require the volume label
· real gbzeta
      toroidal (contravariant) field; calculated in bfield; required to convert \dot{\theta} to B^{\theta}, \dot{s} to B^{s}
• integer, dimension(:), allocatable iquad
      internal copy of Nquad
• real, dimension(:,:), allocatable gaussianweight
      weights for Gaussian quadrature

    real, dimension(:,:), allocatable gaussianabscissae

      abscissae for Gaussian quadrature
· logical Iblinear
      controls selection of Beltrami field solver; depends on LBeltrami

    logical lbnewton

      controls selection of Beltrami field solver; depends on LBeltrami

    logical lbsequad

      controls selection of Beltrami field solver; depends on LBeltrami

    real, dimension(1:3) orzp

      used in mg00aa() to determine (s, \theta, \zeta) given (R, Z, \varphi)
• type(derivative) dbdx
      d\mathbf{B}/d\mathbf{X} (?)
· integer globaljk
      labels position

    real, dimension(:,:), allocatable dxyz
```

computational boundary; position

real, dimension(:,:), allocatable nxyz

computational boundary; normal

real, dimension(:,:), allocatable jxyz

plasma boundary; surface current

• real, dimension(1:2) tetazeta

what is this?

real virtualcasingfactor = -one / (four\*pi)

this agrees with diagno

· integer iberror

for computing error in magnetic field

· integer nfreeboundaryiterations

number of free-boundary iterations already performed

integer, parameter node = 2

best to make this global for consistency between calling and called routines

logical first free bound = .false.

flag to indicate that this is the first free-boundary iteration

### 6.1.1 Detailed Description

global variable storage used as "workspace" throughout the code

### 6.1.2 Function/Subroutine Documentation

### **6.1.2.1 check\_inputs()** subroutine allglobal::check\_inputs

## reading of physicslist

- The internal variable, Mvol=Nvol+Lfreebound, gives the number of computational domains.
- The input value for the fluxes enclosed within each interface, tflux (1:Mvol) and tflux (1:Mvol), are immediately normalized:

```
tflux(1:Mvol) \rightarrow tflux(1:Mvol)/tflux(Nvol).
pflux(1:Mvol) \rightarrow pflux(1:Mvol)/tflux(Nvol).
```

The input  $\Phi_{edge} \equiv \text{phiedge}$  will provide the total toroidal flux; see preset().

• The input value for the toroidal current constraint (Isurf (1:Mvol)) and Ivolume (1:Mvol)) are also immediately normalized, using curtor .  $Ivolume \rightarrow Ivolume \cdot \frac{curtor}{\sum_i Isurf_i + Ivolume_i} Isurf \rightarrow Isurf \cdot \frac{curtor}{\sum_i Isurf_i + Ivolume_i}$ 

### **Current profiles normalization**

In case of a free boundary calculation (Lfreebound=1) and using a current constraint (Lconstraint=3), the current profiles are renormalized in order to match the linking current curtor. More specifically,

$$Isurf_{i} \rightarrow Isurf_{i} \cdot \frac{curtor}{\sum_{i=1}^{Mvol-1} Isurf_{i} + Ivol_{i}} Ivol_{i} \rightarrow Ivol_{i} \cdot \frac{curtor}{\sum_{i=1}^{Mvol-1} Isurf_{i} + Ivol_{i}}$$
(258)

Finally, the volume current in the vacuum region is set to 0.

reading of numericlist

reading of locallist

reading of globallist

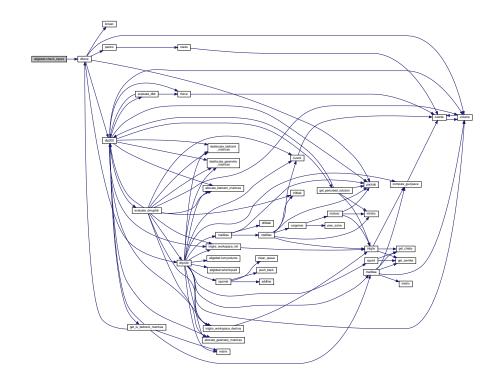
reading of diagnosticslist

### reading of screenlist

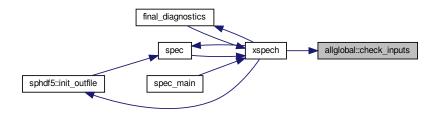
References inputlist::c05factor, inputlist::c05xmax, inputlist::c05xtol, cpus, inputlist::curpol, inputlist: ::curtor, dforce(), inputlist::dpp, inputlist::dqq, inputlist::drz, inputlist::epsgmres, inputlist::epsilon, inputlist::epsilon, inputlist::escale, inputlist::forcetol, inputlist::gamma, inputlist::gbnbld, inputlist::gbntol, inputlist::helicity, inputlist. ::igeometry, inputlist::imethod, inputlist::impol, in, inputlist::intor, inputlist::iorder, inputlist::iotatol, inputlist::iprecon, inputlist::istellsym, inputlist::isurf, inputlist::ivolume, inputlist::ladiabatic, inputlist::lautoinitbn, inputlist::lbeltrami, inputlist::lcheck, inputlist::lcneck, inputlist::lcneck, inputlist::lgmresprec, inputlist::lfreebound, inputlist::lgmresprec, inputlist::lhevalues, inputlist::lhevectors, inputlist::lhmatrix, inputlist::linitgues, inputlist::linitialize, inputlist::lmatsolver, inputlist::lperturbed, inputlist::lrad, inputlist::lreadgf, inputlist::lreflect, inputlist::lrzaxis, inputlist::lsparse, inputlist ::Isvdiota, inputlist::Itiming, inputlist::Izerovac, numerical::machprec, inputlist::mfreeits, inputlist::mmpol, inputlist. ::mntor, inputlist::mnvol, inputlist::mpol, inputlist::mregular, inputlist::mu, inputlist::mupfits, inputlist::mupftol, inputlist::ndiscrete, inputlist::nfp, inputlist::nitergmres, inputlist::nppts, inputlist::nquad, inputlist::ntor, inputlist ::ntoraxis, inputlist::nvol, inputlist::odetol, constants::one, inputlist::opsilon, fileunits::ounit, inputlist::pcondense, inputlist::pflux, inputlist::phiedge, inputlist::pressure, inputlist::pscale, inputlist::rbs, inputlist::rpol, inputlist::rtor, inputlist::rws, numerical::small, inputlist::tflux, inputlist::upsilon, inputlist::vcasingeps, inputlist::vcasingits, inputlist: ::vcasingper, inputlist::vcasingtol, inputlist::vnc, numerical::vsmall, inputlist::wpoloidal, inputlist::wreadin, inputlist ::zbc, constants::zero, and inputlist::zwc.

Referenced by xspech().

Here is the call graph for this function:



Here is the caller graph for this function:



## **6.1.2.2 broadcast\_inputs()** subroutine allglobal::broadcast\_inputs

broadcast physicslist

broadcast numericlist

broadcast globallist

broadcast locallist

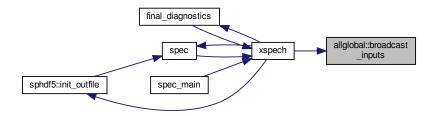
broadcast diagnosticslist

## broadcast screenlist

References inputlist::adiabatic, inputlist::c05factor, inputlist::c05xmax, inputlist::c05xtol, cpus, inputlist::curpol, inputlist::curtor, inputlist::dpp, inputlist::dqq, inputlist::drz, inputlist::epsgmres, inputlist::epsilon, inputlist::epsilon, inputlist::escale, inputlist::forcetol, inputlist::gamma, inputlist::gbnbld, inputlist::gbntol, inputlist::helicity, inputlist. ::igeometry, inputlist::imethod, inputlist::impol, inputlist::intor, inputlist::iorder, inputlist::iota, inputlist::iotatol, inputlist::iprecon, inputlist::istellsym, inputlist::isurf, inputlist::ivolume, inputlist::ladiabatic, inputlist::lautoinitbn, inputlist::lbeltrami, inputlist::lcheck, inputlist::lcnstraint, inputlist::lerrortype, inputlist::lextrap, inputlist::lfindzero, inputlist::Ifreebound, inputlist::Igmresprec, inputlist::Ihevalues, inputlist::Ihevectors, inputlist::Ihmatrix, inputlist ::linitgues, inputlist::linitialize, inputlist::lmatsolver, inputlist::lp, inputlist::lperturbed, inputlist::lq, inputlist::lrad, inputlist::lreadgf, inputlist::lreflect, inputlist::lrzaxis, inputlist::lsparse, inputlist::lsvdiota, inputlist::ltiming, inputlist ::lzerovac, inputlist::maxrndgues, inputlist::mfreeits, inputlist::mnvol, inputlist::mpol, inputlist::mregular, inputlist::mu, inputlist::mupfits, inputlist::mupftol, inputlist::ndiscrete, inputlist::nfp, inputlist::narid, inputlist::niteramres, inputlist; ::nppts, inputlist::nptrj, inputlist::nquad, inputlist::ntor, inputlist::ntoraxis, inputlist::nvol, inputlist::odetol, inputlist::oita, inputlist::opsilon, fileunits::ounit, inputlist::pcondense, inputlist::pflux, inputlist::phiedge, inputlist::pl, inputlist::pts, inputlist::pr, inputlist::pressure, inputlist::pscale, inputlist::ql, inputlist::qr, inputlist::rp, inputlist::rpol, inputlist: ::rq, inputlist::rtor, inputlist::tflux, inputlist::upsilon, inputlist::vcasingeps, inputlist::vcasingits, inputlist::vcasingepr, inputlist::vcasingtol, inputlist::wmacros, inputlist::wpoloidal, inputlist::wreadin, and inputlist::wwrtend.

Referenced by xspech().

Here is the caller graph for this function:



```
6.1.2.3 ismyvolume() subroutine allglobal::ismyvolume ( integer, intent(in) vvol )
```

Check if volume vvol is associated to the corresponding MPI node.

The global variable IsMyVolumeValue is updated to 0 or 1, depending on vvol. A value of -1 is set if an error occured.

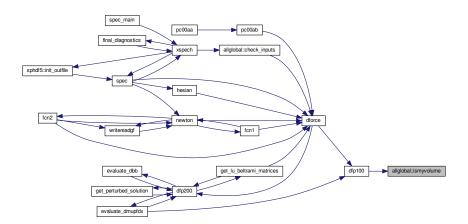
### **Parameters**

vvol	volume to check
------	-----------------

References ismyvolumevalue, myid, and ncpu.

Referenced by dfp100().

Here is the caller graph for this function:



## 6.2 constants Module Reference

some constants used throughout the code

### **Variables**

```
• real, parameter zero = 0.0
• real, parameter one = 1.0
• real, parameter two = 2.0
• real, parameter three = 3.0
• real, parameter four = 4.0
• real, parameter five = 5.0
• real, parameter six = 6.0
• real, parameter seven = 7.0
• real, parameter eight = 8.0
• real, parameter nine = 9.0
• real, parameter ten = 10.0
• real, parameter eleven = 11.0
• real, parameter twelve = 12.0
• real, parameter hundred = 100.0
• real, parameter thousand = 1000.0
     1000
• real, parameter half = one / two
     1/2

 real, parameter third = one / three

• real, parameter quart = one / four

    real, parameter fifth = one / five

• real, parameter sixth = one / six

    real, parameter pi2 = 6.28318530717958623

• real, parameter pi = pi2 / two
• real, parameter mu0 = 2.0E-07 * pi2
• real, parameter goldenmean = 1.618033988749895
     golden mean = (1+\sqrt{5})/2;
• real, parameter version = 3.10
     version of SPEC
```

## 6.2.1 Detailed Description

some constants used throughout the code

# 6.3 cputiming Module Reference

timing variables

### **Variables**

- real **tmanual** = 0.0
- real manualt = 0.0
- real trzaxis = 0.0
- real **rzaxist** = 0.0
- real **tpackxi** = 0.0
- real packxit = 0.0
- real **tvolume** = 0.0
- real volumet = 0.0
- real tcoords = 0.0
- real **coordst** = 0.0
- real tbasefn = 0.0
- real **basefnt** = 0.0
- real tmemory = 0.0
- real **memoryt** = 0.0
- real tmetrix = 0.0
- real **metrixt** = 0.0
- real tma00aa = 0.0
- real ma00aat = 0.0
- real tmatrix = 0.0
- real matrixt = 0.0
- real **tspsmat** = 0.0
- real **spsmatt** = 0.0
- real **tspsint** = 0.0
- real **spsintt** = 0.0
- real **tmp00ac** = 0.0
- real **mp00act** = 0.0
- real **tma02aa** = 0.0
- real **ma02aat** = 0.0
- real tpackab = 0.0
- real packabt = 0.0
- real ttr00ab = 0.0
- real tr00abt = 0.0
- real tcurent = 0.0
- real curentt = 0.0
- real **tdf00ab** = 0.0
- real **df00abt** = 0.0
- real tlforce = 0.0
- real **Iforcet** = 0.0
- real tintghs = 0.0
- real intghst = 0.0
- real **tmtrxhs** = 0.0
- real **mtrxhst** = 0.0

- real **tlbpol** = 0.0
- real **lbpolt** = 0.0
- real tbrcast = 0.0
- real brcastt = 0.0
- real tdfp100 = 0.0
- real dfp100t = 0.0
- real tdfp200 = 0.0
- real dfp200t = 0.0
- real tdforce = 0.0
- real dforcet = 0.0
- real tnewton = 0.0
- real newtont = 0.0
- real tcasing = 0.0
- real casingt = 0.0
- real **tbnorml** = 0.0
- real **bnormlt** = 0.0
- real **tjo00aa** = 0.0
- real jo00aat = 0.0
- real tpp00aa = 0.0
- real pp00aat = 0.0
- real tpp00ab = 0.0
- real **pp00abt** = 0.0
- real **tbfield** = 0.0
- real **bfieldt** = 0.0
- real tstzxyz = 0.0
- real stzxyzt = 0.0
- real thesian = 0.0
- real **hesiant** = 0.0
- real **tra00aa** = 0.0
- real **ra00aat** = 0.0
- real tnumrec = 0.0
- real numrect = 0.0
- real tdcuhre = 0.0
- real dcuhret = 0.0
- real tminpack = 0.0
- real minpackt = 0.0
- real tiqpack = 0.0
- real iqpackt = 0.0
- real trksuite = 0.0 • real rksuitet = 0.0
- real ti1mach = 0.0
- real i1macht = 0.0
- real td1mach = 0.0
- real d1macht = 0.0
- real tilut = 0.0
- real ilutt = 0.0
- real **titers** = 0.0
- real iterst = 0.0 real tsphdf5 = 0.0
- real sphdf5t = 0.0
- real tpreset = 0.0
- real presett = 0.0
- real tglobal = 0.0
- real globalt = 0.0
- real **txspech** = 0.0

- real **xspecht** = 0.0
- real tinputlist = 0.0
- real inputlistt = 0.0
- real treadin = 0.0
- real twrtend = 0.0

# 6.3.1 Detailed Description

timing variables

# 6.4 fftw\_interface Module Reference

Interface to FFTW library.

### **Variables**

```
    type(c_ptr) planf
```

FFTW-related (?)

type(c\_ptr) planb

FFTW-related (?)

• complex(c\_double\_complex), dimension(:,:,:), allocatable cplxin

FFTW-related (?)

complex(c\_double\_complex), dimension(:,:,:), allocatable cplxout
 FFTW-related (?)

# 6.4.1 Detailed Description

Interface to FFTW library.

# 6.5 fileunits Module Reference

central definition of file units to avoid conflicts

# Functions/Subroutines

• subroutine mute (action)

### **Variables**

```
• integer iunit = 10
```

input; used in global/readin:ext.sp, global/wrtend:ext.sp.end

• integer ounit = 6

screen output;

• integer gunit = 13

wall geometry; used in wa00aa

• integer aunit = 11

vector potential; used in ra00aa:.ext.AtAzmn;

• integer dunit = 12

derivative matrix; used in newton:.ext.GF;

integer hunit = 14

eigenvalues of Hessian; under re-construction;

• integer munit = 14

matrix elements of Hessian;

integer lunit = 20

local unit; used in lunit+myid: pp00aa:.ext.poincare,.ext.transform;

• integer vunit = 15

for examination of adaptive quadrature; used in casing:.ext.vcint;

## 6.5.1 Detailed Description

central definition of file units to avoid conflicts

# 6.6 laplaces Module Reference

...todo...

### **Variables**

logical stage1

what is this?

· logical exterior

what is this?

· logical dorm

what is this?

· integer nintervals

what is this?

integer nsegments

what is this?

· integer ic

what is this?

integer np4

what is this?

integer np1

what is this?

• integer, dimension(:), allocatable icint

```
what is this?
· real originalalpha
      what is this?
· real, dimension(:), allocatable xpoly
      what is this?

    real, dimension(:), allocatable ypoly

      what is this?
· real, dimension(:), allocatable phi
      what is this?
· real, dimension(:), allocatable phid
      what is this?
• real, dimension(:,:), allocatable cc
      what is this?
· integer ilength
      what is this?
· real totallength
      what is this?

    integer niterations

      counter; eventually redundant; 24 Oct 12;

    integer iangle

      angle; eventually redundant; 24 Oct 12;

    real rmid

      used to define local polar coordinate; eventually redundant; 24 Oct 12;

    real zmid

      used to define local polar coordinate; eventually redundant; 24 Oct 12;

    real alpha
```

## 6.6.1 Detailed Description

...todo...

## 6.7 newtontime Module Reference

eventually redundant; 24 Oct 12;

timing of Newton iterations

## **Variables**

integer nfcalls

number of calls to get function values (?)

· integer ndcalls

number of calls to get derivative values (?)

real lastcpu

last CPU that called this (?)

# 6.7.1 Detailed Description

timing of Newton iterations

### 6.8 numerical Module Reference

platform-dependant numerical resolution

#### **Variables**

• real, parameter machprec = 1.11e-16

machine precision: 0.5\*epsilon(one) for 64 bit double precision

• real, parameter vsmall = 100\*machprec

very small number

real, parameter small = 10000\*machprec

small number

real, parameter sqrtmachprec = sqrt(machprec)

square root of machine precision

real, parameter logtolerance = 1.0e-32

this is used to avoid taking alog10(zero); see e.g. dforce;

### 6.8.1 Detailed Description

platform-dependant numerical resolution

# 6.9 sphdf5 Module Reference

writing the HDF5 output file

## **Functions/Subroutines**

· subroutine init outfile

Initialize the interface to the HDF5 library and open the output file.

• subroutine mirror\_input\_to\_outfile

Mirror input variables into output file.

· subroutine init convergence output

Prepare convergence evolution output.

• subroutine write\_convergence\_output (nDcalls, ForceErr)

Write convergence output (evolution of interface geometry, force, etc).

· subroutine write grid

Write the magnetic field on a grid.

• subroutine init\_flt\_output (numTrajTotal)

Initialize field line tracing output group and create array datasets.

• subroutine write\_poincare (offset, data, success)

Write a hyperslab of Poincare data corresponding to the output of one parallel worker.

subroutine write\_transform (offset, length, lvol, diotadxup, fiota)

Write the rotational transform output from field line following.

· subroutine finalize\_flt\_output

Finalize Poincare output.

subroutine write\_vector\_potential (sumLrad, allAte, allAze, allAto, allAzo)

Write the magnetic vector potential Fourier harmonics to the output file group /vector\_potential.

· subroutine hdfint

Write the final state of the equilibrium to the output file.

· subroutine finish outfile

Close all open HDF5 objects (we know of) and list any remaining still-open objects.

### **Variables**

• logical, parameter hdfdebug = .false.

global flag to enable verbal diarrhea commenting HDF5 operations

```
    integer, parameter internalhdf5msg = 0

      1: print internal HDF5 error messages; 0: only error messages from sphdf5
· integer hdfier
      error flag for HDF5 library
· integer rank
      rank of data to write using macros
  integer(hid_t) file_id
      default file ID used in macros

    integer(hid_t) space_id

      default dataspace ID used in macros
integer(hid_t) dset_id
      default dataset ID used in macros
• integer(hsize_t), dimension(1:1) onedims
      dimension specifier for one-dimensional data used in macros
• integer(hsize_t), dimension(1:2) twodims
      dimension specifier for two-dimensional data used in macros
• integer(hsize_t), dimension(1:3) threedims
      dimension specifier for three-dimensional data used in macros

    logical grp_exists

      flags used to signal if a group already exists

    logical var_exists

      flags used to signal if a variable already exists
· integer(hid t) iteration dset id
      Dataset identifier for "iteration".

    integer(hid_t) dataspace

      dataspace for extension by 1 iteration object

    integer(hid t) memspace

      memspace for extension by 1 iteration object

    integer(hsize_t), dimension(1) old_data_dims

      current dimensions of "iterations" dataset

    integer(hsize_t), dimension(1) data_dims

      new dimensions for "iterations" dataset

    integer(hsize_t), dimension(1) max_dims

      maximum dimensions for "iterations" dataset
integer(hid_t) plist_id
      Property list identifier used to activate dataset transfer property.
• integer(hid_t) dt_ndcalls_id
      Memory datatype identifier (for "nDcalls" dataset in "/grid")
integer(hid_t) dt_energy_id
      Memory datatype identifier (for "Energy" dataset in "/grid")
· integer(hid t) dt forceerr id
      Memory datatype identifier (for "ForceErr" dataset in "/grid")
integer(hid_t) dt_irbc_id
      Memory datatype identifier (for "iRbc" dataset in "/grid")

    integer(hid t) dt izbs id

      Memory datatype identifier (for "iZbs" dataset in "/grid")

    integer(hid_t) dt_irbs_id
```

Memory datatype identifier (for "iRbs" dataset in "/grid")

integer(hid\_t) dt\_izbc\_id

Memory datatype identifier (for "iZbc" dataset in "/grid")

integer, parameter rankp =3

rank of Poincare data

integer, parameter rankt =2

rank of rotational transform data

integer(hid\_t) grppoincare

group for Poincare data

integer(hid\_t) dset\_id\_t

Dataset identifier for  $\theta$  coordinate of field line following.

integer(hid\_t) dset\_id\_s

Dataset identifier for s coordinate of field line following.

integer(hid\_t) dset\_id\_r

Dataset identifier for R coordinate of field line following.

integer(hid\_t) dset\_id\_z

Dataset identifier for Z coordinate of field line following.

integer(hid\_t) dset\_id\_success

Dataset identifier for success flag of trajectories to follow.

integer(hid t) filespace t

Dataspace identifier in file for  $\theta$  coordinate of field line following.

integer(hid\_t) filespace\_s

Dataspace identifier in file for s coordinate of field line following.

integer(hid\_t) filespace\_r

Dataspace identifier in file for R coordinate of field line following.

integer(hid\_t) filespace\_z

Dataspace identifier in file for Z coordinate of field line following.

integer(hid\_t) filespace\_success

Dataspace identifier in file for success flag of trajectories to follow.

integer(hid t) memspace t

Dataspace identifier in memory for  $\theta$  coordinate of field line following.

• integer(hid t) memspace s

Dataspace identifier in memory for s coordinate of field line following.

integer(hid\_t) memspace\_r

Dataspace identifier in memory for  ${\cal R}$  coordinate of field line following.

• integer(hid\_t) memspace\_z

Dataspace identifier in memory for  ${\cal Z}$  coordinate of field line following.

integer(hid\_t) memspace\_success

Dataspace identifier in memory for success flag of trajectories to follow.

integer(hid\_t) grptransform

group for rotational transform data

• integer(hid\_t) dset\_id\_diotadxup

Dataset identifier for diotadxup (derivative of rotational transform ?)

integer(hid\_t) dset\_id\_fiota

Dataset identifier for fiota ( rotational transform ?)

• integer(hid\_t) filespace\_diotadxup

Dataspace identifier in file for diotadxup.

• integer(hid\_t) filespace\_fiota

Dataspace identifier in file for fiota.

integer(hid\_t) memspace\_diotadxup

Dataspace identifier in memory for diotadxup.

• integer(hid\_t) memspace\_fiota

Dataspace identifier in memory for fiota.

• character(len=15), parameter aname = "description"

Attribute name for descriptive info.

integer(hid\_t) attr\_id

Attribute identifier.

• integer(hid\_t) aspace\_id

Attribute Dataspace identifier.

integer(hid\_t) atype\_id

Attribute Datatype identifier.

• integer, parameter arank = 1

Attribure rank.

• integer(hsize\_t), dimension(arank) adims = (/1/)

Attribute dimension.

• integer(size\_t) attrlen

Length of the attribute string.

• character(len=:), allocatable attr\_data

Attribute data.

## 6.9.1 Detailed Description

writing the HDF5 output file

## 6.10 typedefns Module Reference

type definitions for custom datatypes

# **Data Types**

· type subgrid

used for quantities which have different resolutions in different volumes, e.g. the vector potential More...

- type matrixlu
- type derivative

 $\mathrm{d}\mathbf{B}/\mathrm{d}\mathbf{X}$  (?) More...

### 6.10.1 Detailed Description

type definitions for custom datatypes

# 6.10.2 Data Type Documentation

**6.10.2.1 type typedefns::subgrid** used for quantities which have different resolutions in different volumes, e.g. the vector potential

### **Class Members**

real, dimension(:), allocatable		coefficients
integer, dimension(:), allocatable		indices

### **Class Members**

real, dimension(:,:), allocatable	mat	
integer, dimension(:), allocatable	ipivot	

## 6.10.2.2 type typedefns::matrixlu

## 6.10.2.3 type typedefns::derivative $d\mathbf{B}/d\mathbf{X}$ (?)

### **Class Members**

logical	I	what is this?
integer	vol	Used in coords(); required for global constraint force gradient evaluation.
integer	innout	what is this?
integer	ii	what is this?
integer	irz	what is this?
integer	issym	what is this?

# 7 Data Type Documentation

# 7.1 intghs\_module::intghs\_workspace Type Reference

This calculates the integral of something related to matrix-vector-multiplication.

# **Public Attributes**

- real, dimension(:,:), allocatable efmn

  This is efmn.
- real, dimension(:,:), allocatable ofmn
   This is ofmn.
- real, dimension(:,:), allocatable cfmn
- real, dimension(:,:), allocatable sfmn
- real, dimension(:,:), allocatable evmn
- real, dimension(:,:), allocatable odmn
- real, dimension(:,:), allocatable ijreal
- real, dimension(:,:), allocatable jireal
- real, dimension(:,:), allocatable jkreal
- real, dimension(:,:), allocatable kireal
- real, dimension(:,:,:), allocatable bloweremn
- real, dimension(:,:,:), allocatable **bloweromn**
- real, dimension(:,:,:), allocatable gbupper
- real, dimension(:,:,:), allocatable blower
- real, dimension(:,:,:,:), allocatable basis

### 7.1.1 Detailed Description

This calculates the integral of something related to matrix-vector-multiplication.

**Todo** Zhisong might need to update the documentation of this type.

### 7.1.2 Member Data Documentation

**7.1.2.1 efmn** real, dimension(:,:), allocatable intghs\_module::intghs\_workspace::efmn This is efmn.

**7.1.2.2 ofmn** real, dimension(:,:), allocatable intghs\_module::intghs\_workspace::ofmn

This is ofmn.

- $\textbf{7.1.2.3 cfmn} \quad \texttt{real, dimension(:,:), allocatable intghs\_module::intghs\_workspace::cfmn}$
- $\textbf{7.1.2.4} \quad \textbf{sfmn} \quad \texttt{real, dimension(:,:), allocatable intghs\_module::intghs\_workspace::sfmn}$
- $\textbf{7.1.2.5} \quad \textbf{evmn} \quad \texttt{real, dimension(:,:), allocatable intghs\_module::intghs\_workspace::evmn}$
- $\textbf{7.1.2.6} \quad \textbf{odmn} \quad \texttt{real, dimension(:,:), allocatable intghs\_module::intghs\_workspace::odmn}$
- $\textbf{7.1.2.7} \quad \textbf{ijreal} \quad \texttt{real, dimension(:,:), allocatable intghs\_module::intghs\_workspace::ijreal}$
- $\textbf{7.1.2.8} \quad \textbf{jireal} \quad \texttt{real, dimension(:,:), allocatable intghs\_module::intghs\_workspace::jireal}$

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```
\textbf{7.1.2.9} \quad \textbf{jkreal} \quad \texttt{real, dimension(:,:), allocatable intghs\_module::intghs\_workspace::jkreal}
```

- 7.1.2.10 **kjreal** real, dimension(:,:), allocatable intghs\_module::intghs\_workspace::kjreal
- **7.1.2.11 bloweremn** real, dimension(:,:,:), allocatable intghs\_module::intghs\_workspace  $\leftarrow$  ::bloweremn
- **7.1.2.12 bloweromn** real, dimension(:,:,:), allocatable intghs\_module::intghs\_workspace 
  ::bloweromn
- 7.1.2.13 **gbupper** real, dimension(:,:,:), allocatable intghs\_module::intghs\_workspace::gbupper
- 7.1.2.14 blower real, dimension(:,:,:), allocatable intghs\_module::intghs\_workspace::blower
- **7.1.2.15 basis** real, dimension(:,:,:), allocatable intghs\_module::intghs\_workspace::basis

  The documentation for this type was generated from the following file:
  - src/intghs.f90

# 8 File Documentation

## 8.1 src/basefn.f90 File Reference

Polynomials evaluation.

### **Functions/Subroutines**

- subroutine get\_cheby (lss, lrad, cheby)
  - Get the Chebyshev polynomials with zeroth, first derivatives.
- subroutine get\_cheby\_d2 (lss, lrad, cheby)
  - Get the Chebyshev polynomials with zeroth, first and second derivatives The Chebyshev polynomial has been recombined and rescaled. See get\_cheby for more detail.
- subroutine get\_zernike (r, Irad, mpol, zernike)
  - Get the Zernike polynomials  $\hat{R}_l^m$  with zeroth, first derivatives.
- subroutine get\_zernike\_d2 (r, Irad, mpol, zernike)
  - Get the Zernike polynomials  $\hat{R}_l^m$  with zeroth, first, second derivatives.
- subroutine <a href="mailto:get\_zernike\_rm">get\_zernike\_rm</a> (r, lrad, mpol, zernike)
  - Get the Zernike polynomials  $\hat{R}_l^m/r^m$  .

# 8.1.1 Detailed Description

Polynomials evaluation.

### 8.1.2 Function/Subroutine Documentation

Get the Chebyshev polynomials with zeroth, first derivatives.

The Chebyshev polynomial has been recombined and rescaled. By doing so, the Chebyshev polynomial satisfy the zero Dirichlet boundary condition on the inner surface of the annulus with reduced ill-conditioning problem.

Let  $T_l$  be the Chebyshev polynomial of the first kind with degree l. This subroutine computes

$$\bar{T}_0 = 1,$$

and

$$\bar{T}_l = \frac{T_l - (-1)^l}{l+1}.$$

 $T_l$  are computed iteratively.

$$T_0(s) = 1,$$
 
$$T_1(s) = s,$$
 
$$T_{l+1}(s) = 2sT_l(s) - T_{l-1}(s).$$

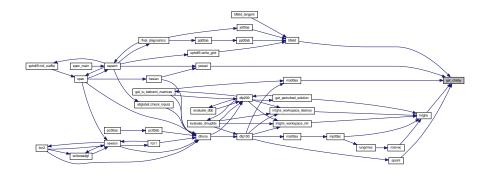
# Parameters

in	Iss	coordinate input lss
in	Irad	radial resolution
out	cheby	the value, first derivative of Chebyshev polynomial

References constants::one, constants::two, and constants::zero.

Referenced by bfield(), intghs(), ma00aa(), preset(), and spsint().

Here is the caller graph for this function:



Get the Chebyshev polynomials with zeroth, first and second derivatives The Chebyshev polynomial has been recombined and rescaled. See get\_cheby for more detail.

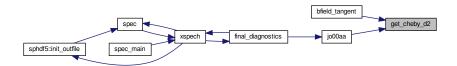
### **Parameters**

ſ	in	Iss	coordinate input lss
ſ	in	Irad	radial resolution
	out	cheby	the value, first and second derivative of Chebyshev polynomial

References constants::one, constants::two, and constants::zero.

Referenced by bfield\_tangent(), and jo00aa().

Here is the caller graph for this function:



```
integer, intent(in) mpol,
real, dimension(0:lrad,0:mpol,0:1), intent(inout) zernike)
```

Get the Zernike polynomials  $\hat{R}_l^m$  with zeroth, first derivatives.

The original Zernike polynomial is defined by The Zernike polynomials take the form

$$\begin{split} Z_l^{-m}(s,\theta) &= R_l^m(s) \sin m\theta, \\ Z_l^m(s,\theta) &= R_l^m(s) \cos m\theta, \end{split}$$

where  $R_l^m(s)$  is a l-th order polynomial given by

$$R_l^m(s) = \sum_{k=0}^{\frac{l-m}{2}} \frac{(-1)^k (l-k)!}{k! \left[\frac{1}{2} (l+m) - k\right]! \left[\frac{1}{2} (l-m) - k\right]!} s^{l-2k},$$

and is only non-zero for  $l \geq m$  and even l-m.

In this subroutine,  $R_l^m(s)$  is computed using the iterative relationship

$$R_l^m(s) = \frac{2(l-1)(2l(l-2)s^2 - m^2 - l(l-2))R_{l-2}^m(s) - l(l+m-2)(l-m-2)R_{l-4}^m(s)}{(l+m)(l-m)(l-2)}$$

For m=0 and m=1, a basis recombination method is used by defining new radial basis functions as

$$\begin{split} \hat{R}_0^0 &= 1, \hat{R}_l^0 &= \frac{1}{l+1} R_l^0 - \frac{(-1)^{l/2}}{l+1}, \\ \hat{R}_1^1 &= s, \hat{R}_l^1 &= \frac{1}{l+1} R_l^1 - \frac{(-1)^{(l-1)/2}}{2} s. \end{split}$$

so that the basis scales as  $s^{m+2}$  except for  $\hat{R}_0^0$  and  $\hat{R}_1^1$ , which are excluded from the representation of  $A_{\theta,m,n}$ . For  $m \geq 2$ , the radial basis functions are only rescaled as

$$\hat{R}_l^m = \frac{1}{l+1} R_l^m.$$

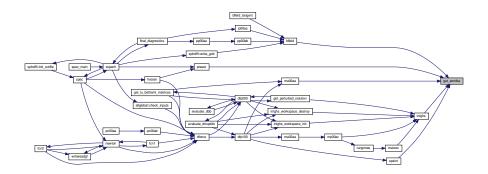
# **Parameters**

in	r	coordinate input, note that this is normalized to $\left[0,1\right]$	
in	Irad	radial resolution	
in	mpol	poloidal resolution	
out	zernike	the value, first derivative of Zernike polynomial	

References constants::one, constants::two, and constants::zero.

Referenced by bfield(), intghs(), ma00aa(), preset(), and spsint().

Here is the caller graph for this function:



Get the Zernike polynomials  $\hat{R}_l^m$  with zeroth, first, second derivatives.

See get\_zernike for more detail.

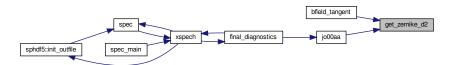
### **Parameters**

in	r	coordinate input, note that this is normalized to $\left[0,1\right]$
in	Irad	radial resolution
in	mpol	poloidal resolution
out	zernike	the value, first/second derivative of Zernike polynomial

References constants::one, constants::two, and constants::zero.

Referenced by bfield\_tangent(), and jo00aa().

Here is the caller graph for this function:



### 8.1.2.5 get\_zernike\_rm() subroutine get\_zernike\_rm (

```
real, intent(in) r,
integer, intent(in) lrad,
integer, intent(in) mpol,
real, dimension(0:lrad,0:mpol), intent(inout) zernike)
```

Get the Zernike polynomials  $\hat{R}_l^m/r^m$ .

See get\_zernike for more detail.

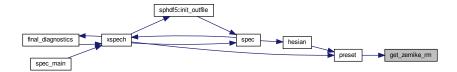
#### **Parameters**

in	r	coordinate input, note that this is normalized to $\left[0,1\right]$
in	Irad	radial resolution
in	mpol	poloidal resolution
out	zernike	the value

References constants::one, constants::two, and constants::zero.

Referenced by preset().

Here is the caller graph for this function:



# 8.2 src/bfield.f90 File Reference

Returns  $\dot{s} \equiv B^s/B^\zeta$  and  $\dot{\theta} \equiv B^\theta/B^\zeta$ .

## Functions/Subroutines

- subroutine bfield (zeta, st, Bst)
  - Compute the magnetic field.
- subroutine bfield\_tangent (zeta, st, Bst) compute the tangential magnetic field

## 8.2.1 Detailed Description

Returns  $\dot{s} \equiv B^s/B^\zeta$  and  $\dot{\theta} \equiv B^\theta/B^\zeta$ .

## 8.2.2 Function/Subroutine Documentation

# 

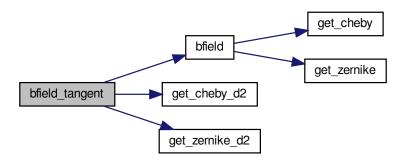
compute the tangential magnetic field

#### **Parameters**

in	zeta	toroidal angle
in	st	radial(s) and poloidal(theta) positions
out	Bst	tangential magnetic field

References allglobal::ate, allglobal::ate, allglobal::aze, allglobal::aze, bfield(), allglobal::cpus, allglobal::gbzeta, get\_cheby\_d2(), get\_zernike\_d2(), constants::half, allglobal::halfmm, allglobal::im, allglobal::in, allglobal::ivol, allglobal::lcoordinatesingularity, inputlist::lrad, allglobal::mn, allglobal::mpi\_comm\_spec, inputlist::mpol, allglobal::myid, allglobal::ncpu, allglobal::node, allglobal::notstellsym, constants::one, fileunits::ounit, allglobal::regumm, numerical::small, constants::two, numerical::vsmall, inputlist::wmacros, and constants::zero.

Here is the call graph for this function:



# 8.3 src/bnorml.f90 File Reference

Computes  $\mathbf{B}_{Plasma} \cdot \mathbf{e}_{\theta} \times \mathbf{e}_{\zeta}$  on the computational boundary,  $\partial \mathcal{D}$ .

#### **Functions/Subroutines**

• subroutine bnorml (mn, Ntz, efmn, ofmn)  $\textit{Computes $B_{Plasma} \cdot e_{\theta} \times e_{\zeta}$ on the computational boundary, $\partial \mathcal{D}$.}$ 

## 8.3.1 Detailed Description

Computes  $\mathbf{B}_{Plasma} \cdot \mathbf{e}_{\theta} \times \mathbf{e}_{\zeta}$  on the computational boundary,  $\partial \mathcal{D}$ .

# 8.4 src/brcast.f90 File Reference

Broadcasts Beltrami fields, profiles, . . .

### **Functions/Subroutines**

• subroutine brcast (Ivol)

Broadcasts Beltrami fields, profiles, . . .

### 8.4.1 Detailed Description

Broadcasts Beltrami fields, profiles, . . .

# 8.5 src/casing.f90 File Reference

Constructs the field created by the plasma currents, at an arbitrary, external location using virtual casing.

### **Functions/Subroutines**

- subroutine casing (teta, zeta, gBn, icasing)
  - Constructs the field created by the plasma currents, at an arbitrary, external location using virtual casing.
- subroutine dvcfield (Ndim, tz, Nfun, vcintegrand)

Differential virtual casing integrand.

# 8.5.1 Detailed Description

Constructs the field created by the plasma currents, at an arbitrary, external location using virtual casing.

## 8.6 src/coords.f90 File Reference

Calculates coordinates,  $\mathbf{x}(s, \theta, \zeta) \equiv R \mathbf{e}_R + Z \mathbf{e}_Z$ , and metrics, using FFTs.

### **Functions/Subroutines**

• subroutine coords (Ivol, Iss, Lcurvature, Ntz, mn) Calculates coordinates,  $\mathbf{x}(s,\theta,\zeta) \equiv R\,\mathbf{e}_R + Z\,\mathbf{e}_Z$ , and metrics, using FFTs.

# 8.6.1 Detailed Description

Calculates coordinates,  $\mathbf{x}(s, \theta, \zeta) \equiv R \mathbf{e}_R + Z \mathbf{e}_Z$ , and metrics, using FFTs.

# 8.7 src/curent.f90 File Reference

Computes the plasma current,  $I \equiv \int B_{\theta} d\theta$ , and the "linking" current,  $G \equiv \int B_{\zeta} d\zeta$ .

#### **Functions/Subroutines**

• subroutine curent (Ivol, mn, Nt, Nz, iflag, IdItGp)

Computes the plasma current,  $I \equiv \int B_{\theta} d\theta$ , and the "linking" current,  $G \equiv \int B_{\zeta} d\zeta$ .

# 8.7.1 Detailed Description

Computes the plasma current,  $I \equiv \int B_{\theta} d\theta$ , and the "linking" current,  $G \equiv \int B_{\zeta} d\zeta$ .

# 8.8 src/df00ab.f90 File Reference

Evaluates volume integrals, and their derivatives w.r.t. interface geometry, using "packed" format.

#### **Functions/Subroutines**

subroutine df00ab (pNN, xi, Fxi, DFxi, Ldfjac, iflag)
 Evaluates volume integrals, and their derivatives w.r.t. interface geometry, using "packed" format.

## 8.8.1 Detailed Description

Evaluates volume integrals, and their derivatives w.r.t. interface geometry, using "packed" format.

# 8.9 src/dforce.f90 File Reference

Calculates  $\mathbf{F}(\mathbf{x})$ , where  $\mathbf{x} \equiv \{\text{geometry}\} \equiv \{R_{i,v}, Z_{i,v}\}$  and  $\mathbf{F} \equiv [[p+B^2/2]] + \{\text{spectral constraints}\}$ , and  $\nabla \mathbf{F}$ .

# **Functions/Subroutines**

- subroutine dforce (NGdof, position, force, LComputeDerivatives, LComputeAxis)
   Calculates F(x), where x ≡ {geometry} ≡ {R<sub>i,v</sub>, Z<sub>i,v</sub>} and F ≡ [[p + B²/2]] + {spectral constraints}, and ∇F.
   subroutine fndiff\_dforce (NGdof)
- oubloatine mam\_alores (reader

# 8.9.1 Detailed Description

Calculates  $\mathbf{F}(\mathbf{x})$ , where  $\mathbf{x} \equiv \{\text{geometry}\} \equiv \{R_{i,v}, Z_{i,v}\}$  and  $\mathbf{F} \equiv [[p+B^2/2]] + \{\text{spectral constraints}\}$ , and  $\nabla \mathbf{F}$ .

# 8.10 src/dfp100.f90 File Reference

Split the work between MPI nodes and evaluate the global constraint.

#### **Functions/Subroutines**

subroutine dfp100 (Ndofgl, x, Fvec, LComputeDerivatives)
 Split the work between MPI nodes and evaluate the global constraint.

## 8.10.1 Detailed Description

Split the work between MPI nodes and evaluate the global constraint.

### 8.10.2 Function/Subroutine Documentation

Split the work between MPI nodes and evaluate the global constraint.

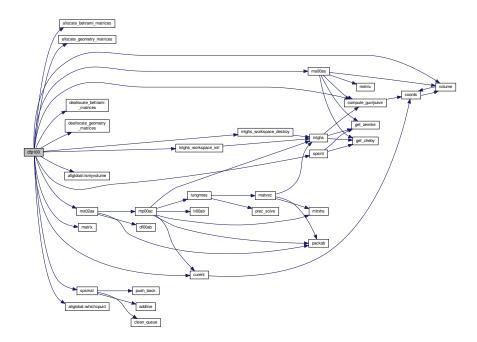
#### **Parameters**

Ndofgl	
X	
Fvec	
LComputeDerivatives	

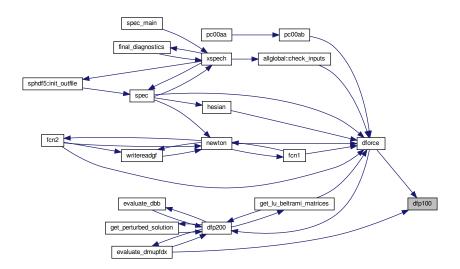
References allocate\_beltrami\_matrices(), allocate\_geometry\_matrices(), compute\_guvijsave(), allglobal ←  $\hbox{::} cpus, \ curent(), \ input list:: curpol, \ all global:: ddttcc, \ all global:: ddtt$ ::ddttss, allglobal::ddtzcc, allglobal::ddtzcs, allglobal::ddtzss, allglobal::ddtzss, allglobal::ddtzcs, al ::ddzzcs, allglobal::ddzzsc, allglobal::ddzzss, deallocate beltrami matrices(), deallocate geometry matrices(), allglobal::dma, allglobal::dmb, allglobal::dmd, allglobal::dmg, allglobal::dpflux, allglobal::dtoocc, allglobal ::dtoocs, allglobal::dtoosc, allglobal::dtooss, allglobal::guvijsave, constants::half, allglobal::iconstraintok, inputlist← ::igeometry, allglobal::imagneticok, intghs workspace destroy(), intghs workspace init(), allglobal::ipdtdpf, allglobal::iguad, allglobal::ismyvolume(), allglobal::ismyvolumevalue, inputlist::isurf, allglobal::izbs, inputlist ::lconstraint, allglobal::lcoordinatesingularity, inputlist::lfreebound, allglobal::liluprecond, allglobal::localconstraint, allglobal::lplasmaregion, inputlist::lrad, allglobal::lsavedguvij, allglobal::lvacuumregion, ma00aa(), ma02aa(), matrix(), allglobal::mbpsi, allglobal::mn, allglobal::mpi comm spec, constants::mu0, allglobal::myid, allglobal::nadof, allglobal::ncpu, allglobal::notmatrixfree, allglobal::nt, inputlist::nvol, allglobal::nz, constants::one, fileunits::ounit, constants::pi, constants::pi2, allglobal::solution, spsint(), spsmat(), allglobal::tdstcc, allglobal::tdstcs, allglobal ::tdstsc, allglobal::tdstss, allglobal::tdszcc, allglobal::tdszcs, all allglobal::ttsscs, allglobal::ttsscs, allglobal::ttsscs, constants::two, volume(), allglobal::whichcpuid(), inputlist ← ::wmacros, allglobal::xoffset, and constants::zero.

Referenced by dforce(), and evaluate dmupfdx().

Here is the call graph for this function:



Here is the caller graph for this function:



# 8.11 src/dfp200.f90 File Reference

Given the field consistent with the constraints and the geometry, computes local quantites related to the force evaluation.

#### **Functions/Subroutines**

subroutine dfp200 (LcomputeDerivatives, vvol)

Given the field consistent with the constraints and the geometry, computes local quantites related to the force evaluation.

subroutine get\_lu\_beltrami\_matrices (vvol, oBI, NN)

get LU Beltrami matrices

subroutine get\_perturbed\_solution (vvol, oBI, NN)

This routine evaluates the value of the magnetic field once the interface is perturbed using matrix perturbation theory.

• subroutine evaluate\_dmupfdx (innout, idof, ii, issym, irz)

Evaluate mu and psip derivatives and store them in dmupfdx.

 subroutine evaluate\_dbb (Ivol, idof, innout, issym, irz, ii, dBB, XX, YY, length, dRR, dZZ, dII, dLL, dPP, Ntz, LcomputeDerivatives)

Evaluate the derivative of the square of the magnetic field modulus. Add spectral constraint derivatives if required.

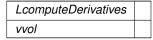
# 8.11.1 Detailed Description

Given the field consistent with the constraints and the geometry, computes local quantites related to the force evaluation.

#### 8.11.2 Function/Subroutine Documentation

Given the field consistent with the constraints and the geometry, computes local quantites related to the force evaluation.

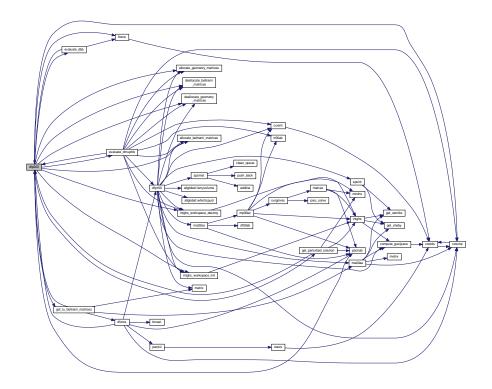
#### **Parameters**



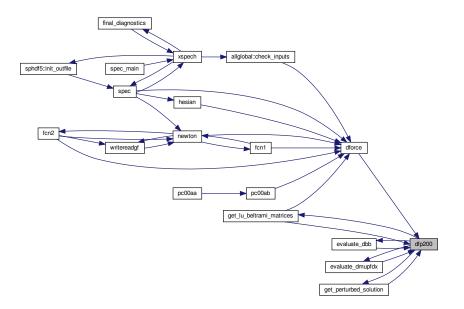
References inputlist::adiabatic, allocate\_beltrami\_matrices(), allocate\_geometry\_matrices(), allglobal::cpus, deallocate\_beltrami\_matrices(), deallocate\_geometry\_matrices(), inputlist::epsilon, evaluate\_dbb(), evaluate dumpfdx(), inputlist::gamma, get\_lu\_beltrami\_matrices(), get\_perturbed\_solution(), constants::half, inputlist::igeometry, intghs\_workspace\_destroy(), intghs\_workspace\_init(), allglobal::iquad, inputlist::lcheck, inputlist::lconstraint, allglobal::lcoordinatesingularity, inputlist::lextrap, inputlist::lfindzero, lforce(), inputlist::lfreebound, allglobal::lplasmaregion, inputlist::lrad, allglobal::lvacuumregion, allglobal::mpi\_comm\_spec, inputlist::mpol, inputlist::mu, allglobal::myid, allglobal::ncpu, inputlist::ntor, inputlist::nvol, constants::one, fileunits::ounit, packab(), inputlist::pscale, numerical::small, inputlist::tflux, constants::two, volume(), inputlist::wmacros, and constants::zero.

Referenced by dforce(), evaluate\_dbb(), evaluate\_dmupfdx(), get\_lu\_beltrami\_matrices(), and get\_perturbed\_← solution().

Here is the call graph for this function:



Here is the caller graph for this function:



**8.11.2.2 get\_lu\_beltrami\_matrices()** subroutine get\_lu\_beltrami\_matrices ( integer, intent(in) *vvol*,

```
type(matrixlu), intent(inout) oBI,
integer, intent(in) NN )
```

# get LU Beltrami matrices

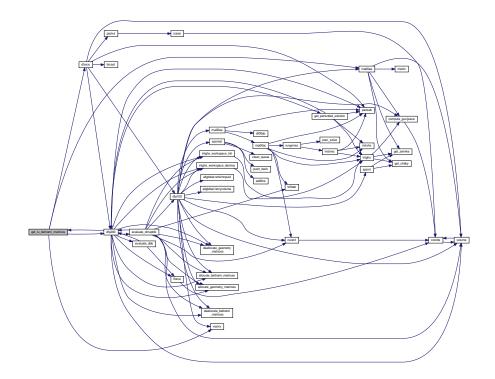
### **Parameters**

vvol	
oBI	
NN	

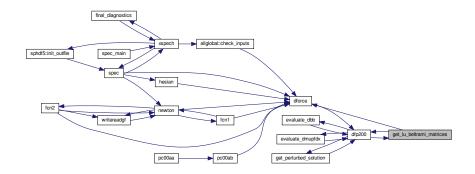
References allglobal::cpus, allglobal::dbdx, dforce(), dfp200(), allglobal::dma, allglobal::dmb, allglobal::dm

Referenced by dfp200().

Here is the call graph for this function:



Here is the caller graph for this function:



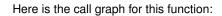
This routine evaluates the value of the magnetic field once the interface is perturbed using matrix perturbation theory.

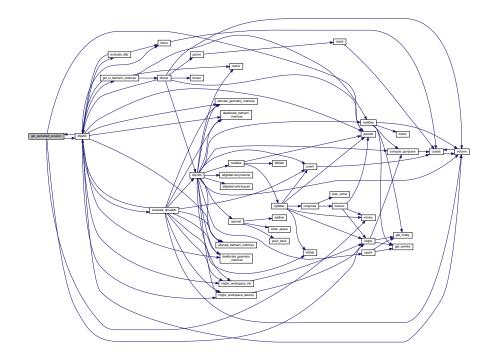
# **Parameters**

vvol	
oBI	
NN	

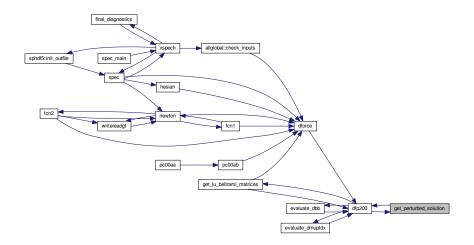
References allglobal::cpus, allglobal::dbdx, dfp200(), allglobal::dma, allglobal::dmb, allglobal::dmd, allglobal::dmd, allglobal::dmg, allglobal::dpflux, allglobal::dtflux, constants::half, intghs(), allglobal::iquad, inputlist::lconstraint, inputlist::lrad, allglobal::mn, allglobal::mpi\_comm\_spec, mtrxhs(), inputlist::mu, allglobal::myid, allglobal::nadof, allglobal::ncpu, constants::one, fileunits::ounit, packab(), allglobal::solution, constants::two, inputlist::wmacros, and constants::zero.

Referenced by dfp200().





Here is the caller graph for this function:



# 

Evaluate mu and psip derivatives and store them in dmupfdx.

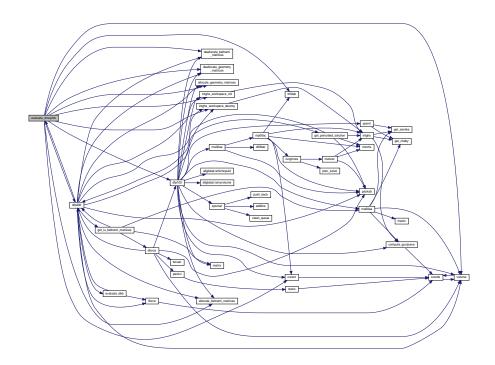
# **Parameters**

innout	
idof	
ii	
issym	
irz	

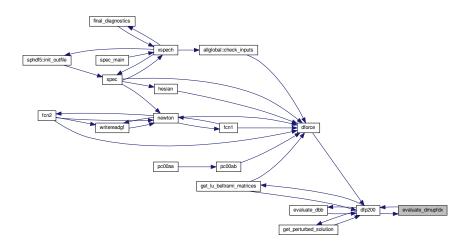
References allocate\_beltrami\_matrices(), allocate\_geometry\_matrices(), allglobal::cpus, curent(), deallocate\_deallocate\_beltrami\_matrices(), deallocate\_geometry\_matrices(), dfp100(), dfp200(), inputlist::drz, constants::half, inputlistd::igeometry, intghs\_workspace\_destroy(), intghs\_workspace\_init(), allglobal::iquad, allglobal::irbc, allglobal

Referenced by dfp200().

Here is the call graph for this function:



Here is the caller graph for this function:



```
8.11.2.5 evaluate_dbb() subroutine evaluate_dbb ( integer lvol,
```

```
integer idof,
integer innout,
integer issym,
integer irz,
integer ii,
real, dimension(1:ntz,-1:2) dBB,
real, dimension(1:ntz) XX,
real, dimension(1:ntz) YY,
real, dimension(1:ntz) length,
real, dimension(1:ntz,-1:2) dRR,
real, dimension(1:ntz,-1:2) dZZ,
real, dimension(1:ntz) dII,
real, dimension(1:ntz) dLL,
real, dimension(1:ntz) dPP,
integer Ntz,
logical, intent(in) LcomputeDerivatives )
```

Evaluate the derivative of the square of the magnetic field modulus. Add spectral constraint derivatives if required.

#### **Parameters**

Ivol	
idof	
innout	
issym	
irz	
ii	
dBB	
XX	
YY	
length	

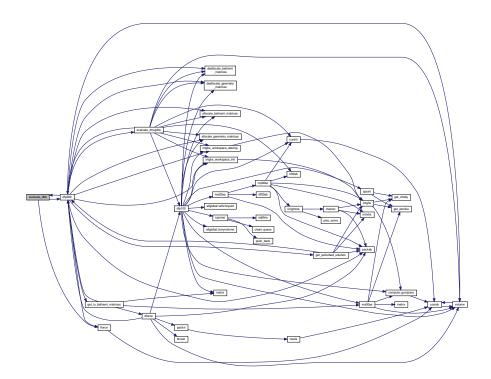
### **Parameters**

dRR	
dZZ	
dII	
dLL	
dPP	
Ntz	
LcomputeDerivatives	

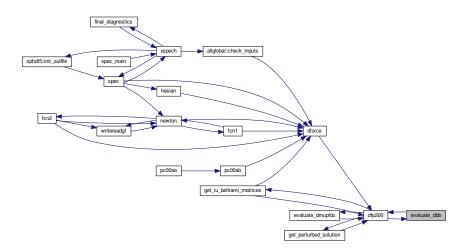
References inputlist::adiabatic, allglobal::cpus, dfp200(), allglobal::dpflux, inputlist::drz, inputlist::epsilon, inputlist:::gamma, constants::half, inputlist::igeometry, allglobal::irbc, allglobal::irbc, allglobal::izbc, allglobal::izbs, inputlist::lcheck, inputlist::lconstraint, allglobal::lcoordinatesingularity, lforce(), allglobal::localconstraint, allglobal::lplasmaregion, inputlist::lrad, allglobal::lvacuumregion, allglobal::mpi\_comm\_spec, allglobal::myid, allglobal::ncpu, inputlist::ntor, inputlist::nvol, constants::one, fileunits::ounit, inputlist::pscale, numerical::small, constants::two, inputlist::wmacros, and constants::zero.

Referenced by dfp200().

Here is the call graph for this function:



Here is the caller graph for this function:



# 8.12 src/global.f90 File Reference

Defines input namelists and global variables, and opens some output files.

# **Data Types**

- type typedefns::subgrid
   used for quantities which have different resolutions in different volumes, e.g. the vector potential More...
- type typedefns::matrixlu
- type typedefns::derivative

 $\mathrm{d}\mathbf{B}/\mathrm{d}\mathbf{X}$  (?) More...

### **Modules**

module constants

some constants used throughout the code

· module numerical

platform-dependant numerical resolution

module fileunits

central definition of file units to avoid conflicts

· module cputiming

timing variables

· module typedefns

type definitions for custom datatypes

· module allglobal

global variable storage used as "workspace" throughout the code

· module fftw\_interface

Interface to FFTW library.

### **Functions/Subroutines**

- subroutine fileunits::mute (action)
- subroutine allglobal::build\_vector\_potential (Ivol, iocons, aderiv, tderiv)
- subroutine allglobal::set\_mpi\_comm (comm)
- subroutine allglobal::read\_inputlists\_from\_file ()
- subroutine allglobal::check\_inputs ()
- subroutine allglobal::broadcast\_inputs
- · subroutine allglobal::wrtend

The restart file is written.

• subroutine allglobal::ismyvolume (vvol)

Check if volume vvol is associated to the corresponding MPI node.

subroutine allglobal::whichcpuid (vvol, cpu\_id)

Returns which MPI node is associated to a given volume.

#### **Variables**

```
• real, parameter constants::zero = 0.0
  real, parameter constants::one = 1.0
• real, parameter constants::two = 2.0
• real, parameter constants::three = 3.0
• real, parameter constants::four = 4.0
  real, parameter constants::five = 5.0
• real, parameter constants::six = 6.0
  real, parameter constants::seven = 7.0
• real, parameter constants::eight = 8.0
• real, parameter constants::nine = 9.0
• real, parameter constants::ten = 10.0
• real, parameter constants::eleven = 11.0
• real, parameter constants::twelve = 12.0

    real, parameter constants::hundred = 100.0

    real, parameter constants::thousand = 1000.0

    real, parameter constants::half = one / two

• real, parameter constants::third = one / three
```

1/3

```
    real, parameter constants::quart = one / four

• real, parameter constants::fifth = one / five
  real, parameter constants::sixth = one / six

    real, parameter constants::pi2 = 6.28318530717958623

  real, parameter constants::pi = pi2 / two
• real, parameter constants::mu0 = 2.0E-07 * pi2
     4\pi \cdot 10^{-7}
• real, parameter constants::goldenmean = 1.618033988749895
     golden mean = (1+\sqrt{5})/2 ;
• real, parameter constants::version = 3.10
      version of SPEC
• real, parameter numerical::machprec = 1.11e-16
     machine precision: 0.5*epsilon(one) for 64 bit double precision
• real, parameter numerical::vsmall = 100*machprec
      very small number
• real, parameter numerical::small = 10000*machprec
     small number

    real, parameter numerical::sqrtmachprec = sqrt(machprec)

     square root of machine precision

    real, parameter numerical::logtolerance = 1.0e-32

     this is used to avoid taking alog10(zero); see e.g. dforce;
• integer fileunits::iunit = 10
     input; used in global/readin:ext.sp, global/wrtend:ext.sp.end
• integer fileunits::ounit = 6
     screen output;
integer fileunits::gunit = 13
      wall geometry; used in wa00aa
• integer fileunits::aunit = 11
      vector potential; used in ra00aa:.ext.AtAzmn;
• integer fileunits::dunit = 12
     derivative matrix; used in newton:.ext.GF;
• integer fileunits::hunit = 14
     eigenvalues of Hessian; under re-construction;
• integer fileunits::munit = 14
     matrix elements of Hessian;

    integer fileunits::lunit = 20

     local unit; used in lunit+myid: pp00aa:.ext.poincare,.ext.transform;
• integer fileunits::vunit = 15
     for examination of adaptive quadrature; used in casing:.ext.vcint;
  real cputiming::tmanual = 0.0
  real cputiming::manualt = 0.0
• real cputiming::trzaxis = 0.0
real cputiming::rzaxist = 0.0
• real cputiming::tpackxi = 0.0
real cputiming::packxit = 0.0
• real cputiming::tvolume = 0.0
```

- real cputiming::volumet = 0.0
- real cputiming::tcoords = 0.0
- real cputiming::coordst = 0.0
- real cputiming::tbasefn = 0.0
- real cputiming::basefnt = 0.0
- real cputiming::tmemory = 0.0
- real cputiming::memoryt = 0.0
- real cputiming::tmetrix = 0.0
- real cputiming::metrixt = 0.0
- real cputiming::tma00aa = 0.0
- real cputiming::ma00aat = 0.0
- real cputiming::tmatrix = 0.0
- real cputiming::matrixt = 0.0
- real cputiming::tspsmat = 0.0
- real cputiming::spsmatt = 0.0
- real cputiming::tspsint = 0.0
- real cputiming::spsintt = 0.0
- real cputiming::tmp00ac = 0.0
- real cputiming::mp00act = 0.0
- real cputiming::tma02aa = 0.0
- Todi oputining itinaozaa o.c
- real cputiming::ma02aat = 0.0
  real cputiming::tpackab = 0.0
- real cputiming::packabt = 0.0
- real cputiming::ttr00ab = 0.0
- real cputiming::tr00abt = 0.0
- real cputiming::tcurent = 0.0
- real cputiming::curentt = 0.0
- real cputiming::tdf00ab = 0.0
- real cputiming::df00abt = 0.0
- real cputiming::tlforce = 0.0
- real cputiming::Iforcet = 0.0
- real cputiming::tintghs = 0.0
- real cputiming::intghst = 0.0
- real cputiming::tmtrxhs = 0.0
- real cputiming::mtrxhst = 0.0
- real cputiming::tlbpol = 0.0
- real cputiming::lbpolt = 0.0
- real cputiming::tbrcast = 0.0
- real cputiming::brcastt = 0.0
- real cputiming::tdfp100 = 0.0
- real cputiming::dfp100t = 0.0
- real cputiming::tdfp200 = 0.0
- real cputiming::dfp200t = 0.0
- real cputiming::tdforce = 0.0
- real cputiming::dforcet = 0.0
- real cputiming::tnewton = 0.0
- real cputiming::newtont = 0.0
- real cputiming::tcasing = 0.0
- real cputiming::casingt = 0.0
- real cputiming::tbnorml = 0.0
- real cputiming::bnormlt = 0.0
- real cputiming::tjo00aa = 0.0
- real cputiming::jo00aat = 0.0
- real cputiming::tpp00aa = 0.0
- real cputiming::pp00aat = 0.0

```
real cputiming::tpp00ab = 0.0
  real cputiming::pp00abt = 0.0
  real cputiming::tbfield = 0.0
  real cputiming::bfieldt = 0.0
  real cputiming::tstzxvz = 0.0
  real cputiming::stzxyzt = 0.0
  real cputiming::thesian = 0.0
  real cputiming::hesiant = 0.0
  real cputiming::tra00aa = 0.0
  real cputiming::ra00aat = 0.0
  real cputiming::tnumrec = 0.0
  real cputiming::numrect = 0.0
  real cputiming::tdcuhre = 0.0
  real cputiming::dcuhret = 0.0
  real cputiming::tminpack = 0.0
  real cputiming::minpackt = 0.0
  real cputiming::tiqpack = 0.0
  real cputiming::iqpackt = 0.0
  real cputiming::trksuite = 0.0
  real cputiming::rksuitet = 0.0
  real cputiming::ti1mach = 0.0
  real cputiming::i1macht = 0.0
  real cputiming::td1mach = 0.0
  real cputiming::d1macht = 0.0
  real cputiming::tilut = 0.0
  real cputiming::ilutt = 0.0
  real cputiming::titers = 0.0
  real cputiming::iterst = 0.0
  real cputiming::tsphdf5 = 0.0
  real cputiming::sphdf5t = 0.0
  real cputiming::tpreset = 0.0
  real cputiming::presett = 0.0
  real cputiming::tglobal = 0.0
  real cputiming::globalt = 0.0
  real cputiming::txspech = 0.0
  real cputiming::xspecht = 0.0
  real cputiming::tinputlist = 0.0
  real cputiming::inputlistt = 0.0
  real cputiming::treadin = 0.0
  real cputiming::twrtend = 0.0
  integer allglobal::myid
     MPI rank of current CPU.
· integer allglobal::ncpu
     number of MPI tasks
· integer allglobal::ismyvolumevalue
     flag to indicate if a CPU is operating on its assigned volume
· real allglobal::cpus
     initial time
· integer allglobal::mpi_comm_spec
```

SPEC MPI communicator.
logical allglobal::skip\_write = .false.
real allglobal::pi2nfp
real allglobal::pi2pi2nfp
real allglobal::pi2pi2nfphalf

```
    real allglobal::pi2pi2nfpquart
```

character(len=1000) allglobal::ext

· real allglobal::forceerr

total force-imbalance

real allglobal::energy

MHD energy.

- real, dimension(:), allocatable allglobal::ipdt
- real, dimension(:,:), allocatable allglobal::ipdtdpf

Toroidal pressure-driven current.

- · integer allglobal::mvol
- · logical allglobal::yesstellsym

internal shorthand copies of Istellsym, which is an integer input;

· logical allglobal::notstellsym

internal shorthand copies of Istellsym, which is an integer input;

- logical allglobal::yesmatrixfree
- · logical allglobal::notmatrixfree

to use matrix-free method or not

real, dimension(:,:), allocatable allglobal::cheby

local workspace for evaluation of Chebychev polynomials

real, dimension(:,:,:), allocatable allglobal::zernike

local workspace for evaluation of Zernike polynomials

• real, dimension(:,:,:), allocatable allglobal::tt

derivatives of Chebyshev polynomials at the inner and outer interfaces;

• real, dimension(:,:,:), allocatable allglobal::rtt

derivatives of Zernike polynomials at the inner and outer interfaces;

• real, dimension(:,:), allocatable allglobal::rtm

 $\boldsymbol{r}^{m}$  term of Zernike polynomials at the origin

· real, dimension(:), allocatable allglobal::zernikedof

Zernike degree of freedom for each m.

· integer allglobal::mne

enhanced resolution for metric elements

• integer, dimension(:), allocatable allglobal::ime

enhanced poloidal mode numbers for metric elements

• integer, dimension(:), allocatable allglobal::ine

enhanced toroidal mode numbers for metric elements

integer allglobal::mns

enhanced resolution for straight field line transformation

integer, dimension(:), allocatable allglobal::ims

enhanced poloidal mode numbers for straight field line transformation

• integer, dimension(:), allocatable allglobal::ins

enhanced toroidal mode numbers for straight field line transformation

integer allglobal::Impol

what is this?

· integer allglobal::Intor

what is this?

· integer allglobal::smpol

what is this?

· integer allglobal::sntor

what is this?

• real allglobal::xoffset = 1.0

used to normalize NAG routines (which ones exacly where?)

· logical, dimension(:), allocatable allglobal::imagneticok

used to indicate if Beltrami fields have been correctly constructed;

```
logical allglobal::iconstraintok
      Used to break iteration loops of slaves in the global constraint minimization.

    real, dimension(:,:), allocatable allglobal::beltramierror

      to store the integral of |curlB-mu*B| computed by jo00aa;
· integer allglobal::mn
      total number of Fourier harmonics for coordinates/fields; calculated from Mpol, Ntor in readin()

    integer, dimension(:), allocatable allglobal::im

      poloidal mode numbers for Fourier representation

    integer, dimension(:), allocatable allglobal::in

      toroidal mode numbers for Fourier representation

    real, dimension(:), allocatable allglobal::halfmm

      I saw this already somewhere...

    real, dimension(:), allocatable allglobal::regumm

      I saw this already somewhere...
· real allglobal::rscale
      no idea

    real, dimension(:,:), allocatable allglobal::psifactor

• real, dimension(:,:), allocatable allglobal::inifactor
      no idea

    real, dimension(:), allocatable allglobal::bbweight

      weight on force-imbalance harmonics; used in dforce()

    real, dimension(:), allocatable allglobal::mmpp

      spectral condensation factors

    real, dimension(:,:), allocatable allglobal::irbc

      cosine R harmonics of interface surface geometry; stellarator symmetric

    real, dimension(:,:), allocatable allglobal::izbs

      sine Z harmonics of interface surface geometry; stellarator symmetric
• real, dimension(:,:), allocatable allglobal::irbs
      sine R harmonics of interface surface geometry; non-stellarator symmetric
• real, dimension(:,:), allocatable allglobal::izbc
      cosine Z harmonics of interface surface geometry; non-stellarator symmetric

    real, dimension(:,:), allocatable allglobal::drbc

      cosine R harmonics of interface surface geometry; stellarator symmetric; linear deformation

    real, dimension(:,:), allocatable allglobal::dzbs

      sine Z harmonics of interface surface geometry; stellarator symmetric; linear deformation

    real, dimension(:,:), allocatable allglobal::drbs

      sine R harmonics of interface surface geometry; non-stellarator symmetric; linear deformation

    real, dimension(:,:), allocatable allglobal::dzbc

      cosine Z harmonics of interface surface geometry; non-stellarator symmetric; linear deformation

    real, dimension(:,:), allocatable allglobal::irij

      interface surface geometry; real space
• real, dimension(:,:), allocatable allglobal::izij
      interface surface geometry; real space

    real, dimension(:,:), allocatable allglobal::drij

      interface surface geometry; real space

    real, dimension(:,:), allocatable allglobal::dzij

      interface surface geometry; real space

    real, dimension(:,:), allocatable allglobal::trij
```

```
interface surface geometry; real space

    real, dimension(:,:), allocatable allglobal::tzij

      interface surface geometry; real space

    real, dimension(:), allocatable allglobal::ivns

      sine harmonics of vacuum normal magnetic field on interfaces; stellarator symmetric
• real, dimension(:), allocatable allglobal::ibns
      sine harmonics of plasma normal magnetic field on interfaces; stellarator symmetric
• real, dimension(:), allocatable allglobal::ivnc
      cosine harmonics of vacuum normal magnetic field on interfaces; non-stellarator symmetric
· real, dimension(:), allocatable allglobal::ibnc
      cosine harmonics of plasma normal magnetic field on interfaces; non-stellarator symmetric

    real, dimension(:), allocatable allglobal::lrbc

      local workspace
• real, dimension(:), allocatable allglobal::lzbs
      local workspace

    real, dimension(:), allocatable allglobal::lrbs

      local workspace

    real, dimension(:), allocatable allglobal::lzbc

      local workspace
integer allglobal::num_modes
• integer, dimension(:), allocatable allglobal::mmrzrz
• integer, dimension(:), allocatable allglobal::nnrzrz
• real, dimension(:,:,:), allocatable allglobal::allrzrz

    integer allglobal::nt

      discrete resolution along \theta of grid in real space
· integer allglobal::nz
      discrete resolution along \zeta of grid in real space

    integer allglobal::ntz

      discrete resolution; Ntz=Nt*Nz shorthand
· integer allglobal::hnt
      discrete resolution; Ntz=Nt*Nz shorthand
· integer allglobal::hnz
      discrete resolution; Ntz=Nt*Nz shorthand
· real allglobal::sontz
      one / sqrt (one*Ntz); shorthand

    real, dimension(:,:,:), allocatable allglobal::rij

      real-space grid; R

    real, dimension(:,:,:), allocatable allglobal::zij

      real-space grid; Z

    real, dimension(:,:,:), allocatable allglobal::xij

      what is this?

    real, dimension(:,:,:), allocatable allglobal::yij

      what is this?

    real, dimension(:,:), allocatable allglobal::sg

      real-space grid; jacobian and its derivatives

    real, dimension(:,:,:,:), allocatable allglobal::guvij

      real-space grid; metric elements

    real, dimension(:,:,:), allocatable allglobal::gvuij

      real-space grid; metric elements (?); 10 Dec 15;

    real, dimension(:,:,:,:), allocatable allglobal::guvijsave
```

what is this?

- integer, dimension(:,:), allocatable allglobal::ki identification of Fourier modes
- integer, dimension(:,:,:), allocatable allglobal::kijs identification of Fourier modes
- integer, dimension(:,:,:), allocatable allglobal::kija identification of Fourier modes
- integer, dimension(:), allocatable allglobal::iotakkii identification of Fourier modes
- integer, dimension(:,:), allocatable allglobal::iotaksub identification of Fourier modes
- integer, dimension(:,:), allocatable allglobal::iotakadd identification of Fourier modes
- integer, dimension(:,:), allocatable allglobal::iotaksgn identification of Fourier modes
- real, dimension(:), allocatable allglobal::efmn
   Fourier harmonics; dummy workspace.
- real, dimension(:), allocatable allglobal::ofmn
   Fourier harmonics; dummy workspace.
- real, dimension(:), allocatable allglobal::cfmn Fourier harmonics; dummy workspace.
- real, dimension(:), allocatable allglobal::sfmn
- Fourier harmonics; dummy workspace.
   real, dimension(:), allocatable allglobal::evmn
  Fourier harmonics; dummy workspace.
- real, dimension(:), allocatable allglobal::odmn

  Fourier harmonics: dummy workspace.
- real, dimension(:), allocatable allglobal::comn Fourier harmonics; dummy workspace.
- real, dimension(:), allocatable allglobal::simn Fourier harmonics; dummy workspace.
- real, dimension(:), allocatable allglobal::ijreal what is this?
- real, dimension(:), allocatable allglobal::ijimag
   what is this?
- real, dimension(:), allocatable allglobal::jireal what is this?
- real, dimension(:), allocatable allglobal::jiimag
   what is this?
- real, dimension(:), allocatable allglobal::jkreal what is this?
- real, dimension(:), allocatable allglobal::jkimag
   what is this?
- real, dimension(:), allocatable allglobal::kjreal what is this?
- real, dimension(:), allocatable allglobal::kjimag
   what is this?
- real, dimension(:,:,:), allocatable allglobal::bsupumn
   tangential field on interfaces; θ-component; required for virtual casing construction of field; 11 Oct 12
- tangential field on interfaces; θ-component; required for virtual casing construction of field; 11 Oct 12
  real, dimension(:,:,:), allocatable allglobal::bsupvmn
  - tangential field on interfaces;  $\zeta$  -component; required for virtual casing construction of field; 11 Oct 12
- real, dimension(:,:), allocatable allglobal::goomne

- described in preset()
- real, dimension(:,:), allocatable allglobal::goomno described in preset()
- real, dimension(:,:), allocatable allglobal::gssmne described in preset()
- real, dimension(:,:), allocatable allglobal::gssmno described in preset()
- real, dimension(:,:), allocatable allglobal::gstmne described in preset()
- real, dimension(:,:), allocatable allglobal::gstmno described in preset()
- real, dimension(:,:), allocatable allglobal::gszmne described in preset()
- real, dimension(:,:), allocatable allglobal::gszmno described in preset()
- real, dimension(:,:), allocatable allglobal::gttmne described in preset()
- real, dimension(:,:), allocatable allglobal::gttmno described in preset()
- real, dimension(:,:), allocatable allglobal::gtzmne described in preset()
- real, dimension(:,:), allocatable allglobal::gtzmno described in preset()
- real, dimension(:,:), allocatable allglobal::gzzmne described in preset()
- real, dimension(:,:), allocatable allglobal::gzzmno described in preset()
- real, dimension(:,:,:,:), allocatable allglobal::dtoocc volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::dtoocs
   volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::dtoosc
   volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:), allocatable allglobal::dtooss
   volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::ttsscc
   volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::ttsscs
   volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::ttsssc volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::ttssss
   volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:), allocatable allglobal::tdstcc
- volume-integrated Chebychev-metrics; see matrix()real, dimension(:,:,:,:), allocatable allglobal::tdstcs
- volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::tdstsc
   volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::tdstss
   volume-integrated Chebychev-metrics; see matrix()

- real, dimension(:,:,:,:), allocatable allglobal::tdszcc volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:), allocatable allglobal::tdszcs
   volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::tdszsc volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::tdszss
   volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::ddttcc volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::ddttcs
   volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:), allocatable allglobal::ddttsc volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::ddttss
   volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::ddtzcc
   volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::ddtzcs
   volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::ddtzsc volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:), allocatable allglobal::ddtzss volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:), allocatable allglobal::ddzzcc
   volume-integrated Chebychev-metrics: see matrix()
- real, dimension(:,:,:), allocatable allglobal::ddzzcs
   volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:), allocatable allglobal::ddzzsc volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:,:,:), allocatable allglobal::ddzzss
   volume-integrated Chebychev-metrics; see matrix()
- real, dimension(:,:), allocatable allglobal::tsc
   what is this?
- real, dimension(:,:), allocatable allglobal::tss
   what is this?
- real, dimension(:,:), allocatable allglobal::dtc what is this?
- real, dimension(:,:), allocatable allglobal::dts what is this?
- real, dimension(:,:), allocatable allglobal::dzc what is this?
- real, dimension(:,:), allocatable allglobal::dzs what is this?
- real, dimension(:,:), allocatable allglobal::ttc
   what is this?
- real, dimension(:,:), allocatable allglobal::tzc what is this?
- real, dimension(:,:), allocatable allglobal::tts what is this?
- real, dimension(:,:), allocatable allglobal::tzs

```
what is this?

    real, dimension(:), allocatable allglobal::dtflux

      \delta \psi_{toroidal} in each annulus

    real, dimension(:), allocatable allglobal::dpflux

      \delta\psi_{poloidal} in each annulus
• real, dimension(:), allocatable allglobal::sweight
      minimum poloidal length constraint weight

    integer, dimension(:), allocatable allglobal::nadof

      degrees of freedom in Beltrami fields in each annulus

    integer, dimension(:), allocatable allglobal::nfielddof

      degrees of freedom in Beltrami fields in each annulus, field only, no Lagrange multipliers

    type(subgrid), dimension(:,:,:), allocatable allglobal::ate

      magnetic vector potential cosine Fourier harmonics; stellarator-symmetric
• type(subgrid), dimension(:,:,:), allocatable allglobal::aze
      magnetic vector potential cosine Fourier harmonics; stellarator-symmetric

    type(subgrid), dimension(:,:,:), allocatable allglobal::ato

      magnetic vector potential sine Fourier harmonics; non-stellarator-symmetric

    type(subgrid), dimension(:,:,:), allocatable allglobal::azo

      magnetic vector potential sine Fourier harmonics; non-stellarator-symmetric

    integer, dimension(:,:), allocatable allglobal::lma

      Lagrange multipliers (?)

    integer, dimension(:,:), allocatable allglobal::lmb

      Lagrange multipliers (?)

    integer, dimension(:,:), allocatable allglobal::lmc

      Lagrange multipliers (?)
• integer, dimension(:,:), allocatable allglobal::Imd
      Lagrange multipliers (?)
• integer, dimension(:,:), allocatable allglobal::lme
      Lagrange multipliers (?)

    integer, dimension(:,:), allocatable allglobal::lmf

      Lagrange multipliers (?)

    integer, dimension(:,:), allocatable allglobal::lmg

      Lagrange multipliers (?)

    integer, dimension(:,:), allocatable allglobal::lmh

      Lagrange multipliers (?)

    real, dimension(:,:), allocatable allglobal::lmavalue

      what is this?
• real, dimension(:,:), allocatable allglobal::Imbvalue
      what is this?

    real, dimension(:,:), allocatable allglobal::lmcvalue

      what is this?

    real, dimension(:,:), allocatable allglobal::lmdvalue

      what is this?

    real, dimension(:,:), allocatable allglobal::lmevalue

      what is this?

    real, dimension(:,:), allocatable allglobal::Imfvalue

      what is this?
• real, dimension(:,:), allocatable allglobal::Imgvalue
      what is this?
```

what is this?

real, dimension(:,:), allocatable allglobal::lmhvalue

```
• integer, dimension(:,:), allocatable allglobal::fso
      what is this?

    integer, dimension(:,:), allocatable allglobal::fse

      what is this?

    logical allglobal::lcoordinatesingularity

      set by LREGION macro; true if inside the innermost volume
· logical allglobal::lplasmaregion
      set by LREGION macro; true if inside the plasma region

    logical allglobal::lvacuumregion

      set by LREGION macro; true if inside the vacuum region
· logical allglobal::lsavedguvij
      flag used in matrix free

    logical allglobal::localconstraint

      what is this?

    real, dimension(:,:), allocatable allglobal::dma

      energy and helicity matrices; quadratic forms

    real, dimension(:,:), allocatable allglobal::dmb

      energy and helicity matrices; quadratic forms

    real, dimension(:,:), allocatable allglobal::dmd

      energy and helicity matrices; quadratic forms
• real, dimension(:), allocatable allglobal::dmas
      sparse version of dMA, data

    real, dimension(:), allocatable allglobal::dmds

      sparse version of dMD, data
• integer, dimension(:), allocatable allglobal::idmas
      sparse version of dMA and dMD, indices
• integer, dimension(:), allocatable allglobal::jdmas
      sparse version of dMA and dMD, indices

    integer, dimension(:), allocatable allglobal::ndmasmax

      number of elements for sparse matrices
• integer, dimension(:), allocatable allglobal::ndmas
      number of elements for sparse matrices
· real, dimension(:), allocatable allglobal::dmg
      what is this?
• real, dimension(:), allocatable allglobal::adotx
      the matrix-vector product

    real, dimension(:), allocatable allglobal::ddotx

      the matrix-vector product
• real, dimension(:,:), allocatable allglobal::solution
      this is allocated in dforce; used in mp00ac and ma02aa; and is passed to packab

    real, dimension(:,:,:), allocatable allglobal::gmreslastsolution

      used to store the last solution for restarting GMRES
• real, dimension(:), allocatable allglobal::mbpsi
      matrix vector products

    logical allglobal::liluprecond

      whether to use ILU preconditioner for GMRES

    real, dimension(:,:), allocatable allglobal::beltramiinverse

      Beltrami inverse matrix.

    real, dimension(:,:,:), allocatable allglobal::diotadxup

      measured rotational transform on inner/outer interfaces for each volume; d(transform)/dx; (see dforce)
```

real, dimension(:,:,:), allocatable allglobal::ditgpdxtp

```
measured toroidal and poloidal current on inner/outer interfaces for each volume; d(ltor,Gpol)/dx; (see dforce)
• real, dimension(:,:,:,:), allocatable allglobal::glambda
      save initial guesses for iterative calculation of rotational-transform
· integer allglobal::lmns
      what is this?
• real, dimension(:,:,:), allocatable allglobal::bemn
      force vector; stellarator-symmetric (?)

    real, dimension(:,:), allocatable allglobal::iomn

      force vector; stellarator-symmetric (?)

    real, dimension(:,:,:), allocatable allglobal::somn

      force vector; non-stellarator-symmetric (?)

    real, dimension(:,:,:), allocatable allglobal::pomn

      force vector; non-stellarator-symmetric (?)
• real, dimension(:,:,:), allocatable allglobal::bomn
      force vector; stellarator-symmetric (?)

    real, dimension(:,:), allocatable allglobal::iemn

      force vector; stellarator-symmetric (?)

    real, dimension(:,:,:), allocatable allglobal::semn

      force vector; non-stellarator-symmetric (?)

    real, dimension(:,:,:), allocatable allglobal::pemn

      force vector; non-stellarator-symmetric (?)

    real, dimension(:), allocatable allglobal::bbe

      force vector (?); stellarator-symmetric (?)

    real, dimension(:), allocatable allglobal::iio

      force vector (?); stellarator-symmetric (?)
• real, dimension(:), allocatable allglobal::bbo
      force vector (?); non-stellarator-symmetric (?)
• real, dimension(:), allocatable allglobal::iie
      force vector (?); non-stellarator-symmetric (?)

    real, dimension(:,:,:), allocatable allglobal::btemn

      covariant \theta cosine component of the tangential field on interfaces; stellarator-symmetric

    real, dimension(:,:,:), allocatable allglobal::bzemn

      covariant \zeta cosine component of the tangential field on interfaces; stellarator-symmetric

    real, dimension(:,:,:), allocatable allglobal::btomn

      covariant \theta sine component of the tangential field on interfaces; non-stellarator-symmetric

    real, dimension(:,:,:), allocatable allglobal::bzomn

      covariant ζ sine component of the tangential field on interfaces; non-stellarator-symmetric
• real, dimension(:,:), allocatable allglobal::bloweremn
      covariant field for Hessian computation

    real, dimension(:,:), allocatable allglobal::bloweromn

      covariant field for Hessian computation

    integer allglobal::lgdof

      geometrical degrees of freedom associated with each interface

    integer allglobal::ngdof

      total geometrical degrees of freedom

    real, dimension(:,:,:), allocatable allglobal::dbbdrz

      derivative of magnetic field w.r.t. geometry (?)
• real, dimension(:,:), allocatable allglobal::diidrz
      derivative of spectral constraints w.r.t. geometry (?)

    real, dimension(:,:,:,:), allocatable allglobal::dffdrz
```

derivatives of B^2 at the interfaces wrt geometry

real allglobal::gbzeta

```
    real, dimension(:,:,:,:), allocatable allglobal::dbbdmp

      derivatives of B^2 at the interfaces wrt mu and dpflux
• real, dimension(:,:,:,:), allocatable allglobal::dmupfdx
      derivatives of mu and dpflux wrt geometry at constant interface transform

    logical allglobal::lhessianallocated

      flag to indicate that force gradient matrix is allocated (?)
• real, dimension(:,:), allocatable allglobal::hessian
      force gradient matrix (?)

    real, dimension(:,:), allocatable allglobal::dessian

      derivative of force gradient matrix (?)
• real, dimension(:,:), allocatable allglobal::cosi
      some precomputed cosines

    real, dimension(:,:), allocatable allglobal::sini

      some precomputed sines

    real, dimension(:), allocatable allglobal::gteta

      something related to \sqrt{g} and \theta ?

    real, dimension(:), allocatable allglobal::gzeta

      something related to \sqrt{g} and \zeta?

    real, dimension(:), allocatable allglobal::ajk

      definition of coordinate axis
• real, dimension(:,:,:,:), allocatable allglobal::dradr
      derivatives of coordinate axis

    real, dimension(:,:,:,:), allocatable allglobal::dradz

      derivatives of coordinate axis

    real, dimension(:,:,:,:), allocatable allglobal::dzadr

      derivatives of coordinate axis

    real, dimension(:,:,:,:), allocatable allglobal::dzadz

      derivatives of coordinate axis
• real, dimension(:,:,:), allocatable allglobal::drodr
      derivatives of coordinate axis
• real, dimension(:,:,:), allocatable allglobal::drodz
      derivatives of coordinate axis
• real, dimension(:,:,:), allocatable allglobal::dzodr
      derivatives of coordinate axis

    real, dimension(:,:,:), allocatable allglobal::dzodz

      derivatives of coordinate axis

    integer, dimension(:,:), allocatable allglobal::djkp

      for calculating cylindrical volume

    integer, dimension(:,:), allocatable allglobal::djkm

      for calculating cylindrical volume

    real, dimension(:), allocatable allglobal::lbbintegral

      B.B integral.
• real, dimension(:), allocatable allglobal::labintegral
      A.B integral.
• real, dimension(:), allocatable allglobal::vvolume
      volume integral of \sqrt{g}; computed in volume

    real allglobal::dvolume

      derivative of volume w.r.t. interface geometry

    integer allglobal::ivol

      labels volume; some subroutines (called by NAG) are fixed argument list but require the volume label
```

toroidal (contravariant) field; calculated in bfield; required to convert  $\dot{\theta}$  to  $B^{\theta}$ ,  $\dot{s}$  to  $B^{s}$ • integer, dimension(:), allocatable allglobal::iquad internal copy of Nguad • real, dimension(:,:), allocatable allglobal::gaussianweight weights for Gaussian quadrature • real, dimension(:,:), allocatable allglobal::gaussianabscissae abscissae for Gaussian quadrature logical allglobal::lblinear controls selection of Beltrami field solver; depends on LBeltrami logical allglobal::lbnewton controls selection of Beltrami field solver; depends on LBeltrami · logical allglobal::lbsequad controls selection of Beltrami field solver; depends on LBeltrami real, dimension(1:3) allglobal::orzp used in mg00aa() to determine  $(s, \theta, \zeta)$  given  $(R, Z, \varphi)$  type(derivative) allglobal::dbdx  $d\mathbf{B}/d\mathbf{X}$  (?) · integer allglobal::globaljk labels position real, dimension(:,:), allocatable allglobal::dxyz computational boundary; position real, dimension(:,:), allocatable allglobal::nxyz computational boundary; normal real, dimension(:,:), allocatable allglobal::jxyz plasma boundary; surface current real, dimension(1:2) allglobal::tetazeta real allglobal::virtualcasingfactor = -one / (four\*pi) this agrees with diagno · integer allglobal::iberror for computing error in magnetic field • integer allglobal::nfreeboundaryiterations number of free-boundary iterations already performed integer, parameter allglobal::node = 2 best to make this global for consistency between calling and called routines • logical allglobal::first\_free\_bound = .false. flag to indicate that this is the first free-boundary iteration type(c\_ptr) fftw\_interface::planf FFTW-related (?) • type(c\_ptr) fftw\_interface::planb FFTW-related (?) • complex(c\_double\_complex), dimension(:,:,:), allocatable fftw\_interface::cplxin

• complex(c\_double\_complex), dimension(:,:,:), allocatable fftw\_interface::cplxout

FFTW-related (?)

FFTW-related (?)

### 8.12.1 Detailed Description

Defines input namelists and global variables, and opens some output files.

Note that all variables in namelist need to be broadcasted in readin.

## Input geometry

• The geometry of the l-th interface, for l=0,N where  $N\equiv {\sf Nvol},$  is described by a set of Fourier harmonics, using an arbitrary poloidal angle,

$$R_l(\theta,\zeta) = \sum_j R_{j,l} \cos(m_j \theta - n_j \zeta), \qquad (259)$$

$$Z_l(\theta,\zeta) = \sum_{j}^{3} Z_{j,l} \sin(m_j \theta - n_j \zeta). \tag{260}$$

• These harmonics are read from the ext.sp file and come directly after the namelists described above. The required format is as follows:

- The coordinate axis corresponds to j=0 and the outermost boundary corresponds to  $j=\mathsf{Nvol}.$
- An arbitrary selection of harmonics may be inluded in any order, but only those within the range specified by Mpol and Ntor will be used.
- The geometry of all the interfaces, i.e. l=0,N, including the degenerate "coordinate-axis" interface, must be given.

# 8.12.2 Data Type Documentation

**8.12.2.1 type typedefns::subgrid** used for quantities which have different resolutions in different volumes, e.g. the vector potential

# Class Members

real, dimension(:), allocatable		
integer, dimension(:), allocatable	i	indices

## **Class Members**

real, dimension(:,:), allocatable	mat	
integer, dimension(:), allocatable	ipivot	

### 8.12.2.2 type typedefns::matrixlu

# 8.12.2.3 type typedefns::derivative ${\rm d}{\bf B}/{\rm d}{\bf X}$ (?)

#### **Class Members**

logical	1	what is this?
integer	vol	Used in coords(); required for global constraint force gradient evaluation.
integer	innout	what is this?
integer	ii	what is this?
integer	irz	what is this?
integer	issym	what is this?

### 8.13 src/hesian.f90 File Reference

Computes eigenvalues and eigenvectors of derivative matrix,  $\nabla_{\xi} \mathbf{F}$ .

### **Functions/Subroutines**

• subroutine hesian (NGdof, position, Mvol, mn, LGdof) Computes eigenvalues and eigenvectors of derivative matrix,  $\nabla_{\varepsilon} \mathbf{F}$ .

# 8.13.1 Detailed Description

Computes eigenvalues and eigenvectors of derivative matrix,  $\nabla_{\xi} \mathbf{F}$ .

# 8.14 src/inputlist.f90 File Reference

Input namelists.

#### **Functions/Subroutines**

• subroutine inputlist::initialize\_inputs

# **Variables**

• integer, parameter inputlist::mnvol = 256

The maximum value of Nvol is MNvol=256.

• integer, parameter inputlist::mmpol = 64

The maximum value of Mpol is MNpol=64.

• integer, parameter inputlist::mntor = 64

The maximum value of Ntor is MNtor=64.

• integer inputlist::igeometry = 3

selects Cartesian, cylindrical or toroidal geometry;

• integer inputlist::istellsym = 1

stellarator symmetry is enforced if Istellsym==1

• integer inputlist::lfreebound = 0

compute vacuum field surrounding plasma

• real inputlist::phiedge = 1.0

```
total enclosed toroidal magnetic flux;
• real inputlist::curtor = 0.0
      total enclosed (toroidal) plasma current;
• real inputlist::curpol = 0.0
      total enclosed (poloidal) linking current;
• real inputlist::gamma = 0.0
      adiabatic index; cannot set |\gamma| = 1
• integer inputlist::nfp = 1
      field periodicity
• integer inputlist::nvol = 1
      number of volumes
integer inputlist::mpol = 0
      number of poloidal Fourier harmonics
• integer inputlist::ntor = 0
      number of toroidal Fourier harmonics

    integer, dimension(1:mnvol+1) inputlist::lrad = 4

       Chebyshev resolution in each volume.
• integer inputlist::lconstraint = -1
      selects constraints; primarily used in ma02aa() and mp00ac().

    real, dimension(1:mnvol+1) inputlist::tflux = 0.0

      toroidal flux, \psi_t, enclosed by each interface

    real, dimension(1:mnvol+1) inputlist::pflux = 0.0

      poloidal flux, \psi_p, enclosed by each interface

    real, dimension(1:mnvol) inputlist::helicity = 0.0

      helicity, \mathcal{K}, in each volume, \mathcal{V}_i
• real inputlist::pscale = 0.0
      pressure scale factor
real, dimension(1:mnvol+1) inputlist::pressure = 0.0
      pressure in each volume

    integer inputlist::ladiabatic = 0

      logical flag

    real, dimension(1:mnvol+1) inputlist::adiabatic = 0.0

      adiabatic constants in each volume
real, dimension(1:mnvol+1) inputlist::mu = 0.0
      helicity-multiplier, \mu, in each volume
• real, dimension(1:mnvol+1) inputlist::ivolume = 0.0
       Toroidal current constraint normalized by \mu_0 (I_{volume} = \mu_0 \cdot [A]), in each volume. This is a cumulative quantity:
      I_{\mathcal{V},i} = \int_0^{\psi_{t,i}} \mathbf{J} \cdot \mathbf{dS}. Physically, it represents the sum of all non-pressure driven currents.
• real, dimension(1:mnvol) inputlist::isurf = 0.0
       Toroidal current normalized by \mu_0 at each interface (cumulative). This is the sum of all pressure driven currents.
• integer, dimension(0:mnvol) inputlist::pl = 0
       "inside" interface rotational-transform is \iota=(p_l+\gamma p_r)/(q_l+\gamma q_r), where \gamma is the golden mean, \gamma=(1+\sqrt{5})/2.

    integer, dimension(0:mnvol) inputlist::ql = 0

       "inside" interface rotational-transform is \iota=(p_l+\gamma p_r)/(q_l+\gamma q_r), where \gamma is the golden mean, \gamma=(1+\sqrt{5})/2.
• integer, dimension(0:mnvol) inputlist::pr = 0
       "inside" interface rotational-transform is \,\iota=(p_l+\gamma p_r)/(q_l+\gamma q_r), where \gamma is the golden mean, \gamma=(1+\sqrt{5})/2.

    integer, dimension(0:mnvol) inputlist::qr = 0

       "inside" interface rotational-transform is \iota=(p_l+\gamma p_r)/(q_l+\gamma q_r), where \gamma is the golden mean, \gamma=(1+\sqrt{5})/2.

    real, dimension(0:mnvol) inputlist::iota = 0.0

      rotational-transform, t, on inner side of each interface

    integer, dimension(0:mnvol) inputlist::lp = 0
```

```
"outer" interface rotational-transform is \,\iota=(p_l+\gamma p_r)/(q_l+\gamma q_r), where \gamma is the golden mean, \gamma=(1+\sqrt{5})/2.

    integer, dimension(0:mnvol) inputlist::lq = 0

      "outer" interface rotational-transform is \,\iota=(p_l+\gamma p_r)/(q_l+\gamma q_r), where \gamma is the golden mean, \gamma=(1+\sqrt{5})/2.

    integer, dimension(0:mnvol) inputlist::rp = 0

      "outer" interface rotational-transform is \iota=(p_l+\gamma p_r)/(q_l+\gamma q_r), where \gamma is the golden mean, \gamma=(1+\sqrt{5})/2.

    integer, dimension(0:mnvol) inputlist::rq = 0

      "outer" interface rotational-transform is \,\iota=(p_l+\gamma p_r)/(q_l+\gamma q_r), where \gamma is the golden mean, \gamma=(1+\sqrt{5})/2.

    real, dimension(0:mnvol) inputlist::oita = 0.0

      rotational-transform, t, on outer side of each interface
• real inputlist::mupftol = 1.0e-14
      accuracy to which \mu and \Delta \psi_n are required
integer inputlist::mupfits = 8
      an upper limit on the transform/helicity constraint iterations;
• real inputlist::rpol = 1.0
      poloidal extent of slab (effective radius)
real inputlist::rtor = 1.0
      toroidal extent of slab (effective radius)

    integer inputlist::lreflect = 0

      =1 reflect the upper and lower bound in slab, =0 do not reflect

    real, dimension(0:mntor) inputlist::rac = 0.0

      stellarator symmetric coordinate axis;

    real, dimension(0:mntor) inputlist::zas = 0.0

      stellarator symmetric coordinate axis;

    real, dimension(0:mntor) inputlist::ras = 0.0

      non-stellarator symmetric coordinate axis;
• real, dimension(0:mntor) inputlist::zac = 0.0
      non-stellarator symmetric coordinate axis;

    real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::rbc = 0.0

      stellarator symmetric boundary components;

    real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::zbs = 0.0

      stellarator symmetric boundary components;

    real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::rbs = 0.0

      non-stellarator symmetric boundary components;

    real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::zbc = 0.0

      non-stellarator symmetric boundary components;

    real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::rwc = 0.0

      stellarator symmetric boundary components of wall;
• real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::zws = 0.0
      stellarator symmetric boundary components of wall;

    real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::rws = 0.0

      non-stellarator symmetric boundary components of wall;

    real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::zwc = 0.0

      non-stellarator symmetric boundary components of wall;

    real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::vns = 0.0

      stellarator symmetric normal field at boundary; vacuum component;

    real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::bns = 0.0

      stellarator symmetric normal field at boundary; plasma component;

    real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::vnc = 0.0

      non-stellarator symmetric normal field at boundary; vacuum component;

    real, dimension(-mntor:mntor,-mmpol:mmpol) inputlist::bnc = 0.0
```

non-stellarator symmetric normal field at boundary; plasma component;

• integer inputlist::linitialize = 0

```
Used to initialize geometry using a regularization / extrapolation method.
• integer inputlist::lautoinitbn = 1
      Used to initialize B_{ns} using an initial fixed-boundary calculation.
integer inputlist::lzerovac = 0
      Used to adjust vacuum field to cancel plasma field on computational boundary.
• integer inputlist::ndiscrete = 2
      resolution of the real space grid on which fast Fourier transforms are performed is given by Ndiscrete*Mpol*4
integer inputlist::nquad = -1
      Resolution of the Gaussian quadrature.
• integer inputlist::impol = -4
      Fourier resolution of straight-fieldline angle on interfaces.
• integer inputlist::intor = -4
      Fourier resolution of straight-fieldline angle on interfaces;.
• integer inputlist::lsparse = 0
      controls method used to solve for rotational-transform on interfaces
• integer inputlist::lsvdiota = 0
      controls method used to solve for rotational-transform on interfaces; only relevant if Lsparse = 0
integer inputlist::imethod = 3
      controls iterative solution to sparse matrix arising in real-space transformation to the straight-fieldline angle; only
      relevant if Lsparse.eq.2;
• integer inputlist::iorder = 2
      controls real-space grid resolution for constructing the straight-fieldline angle; only relevant if Lsparse>0
• integer inputlist::iprecon = 0
      controls iterative solution to sparse matrix arising in real-space transformation to the straight-fieldline angle; only
      relevant if Lsparse.eq. 2;
• real inputlist::iotatol = -1.0
      tolerance required for iterative construction of straight-fieldline angle; only relevant if Lsparse.ge.2
integer inputlist::lextrap = 0
      geometry of innermost interface is defined by extrapolation
integer inputlist::mregular = -1
      maximum regularization factor
integer inputlist::lrzaxis = 1
      controls the guess of geometry axis in the innermost volume or initialization of interfaces
integer inputlist::ntoraxis = 3
      the number of n harmonics used in the Jacobian m=1 harmonic elimination method; only relevant if Lrzaxis. \leftarrow
• integer inputlist::lbeltrami = 4
      Control flag for solution of Beltrami equation.
integer inputlist::linitgues = 1
      controls how initial guess for Beltrami field is constructed
• integer inputlist::lposdef = 0
      redundant:
• real inputlist::maxrndgues = 1.0
      the maximum random number of the Beltrami field if Linitgues = 3
• integer inputlist::Imatsolver = 3
      1 for LU factorization, 2 for GMRES, 3 for GMRES matrix-free

    integer inputlist::nitergmres = 200

      number of max iteration for GMRES

    real inputlist::epsgmres = 1e-14

      the precision of GMRES
```

```
integer inputlist::lgmresprec = 1
      type of preconditioner for GMRES, 1 for ILU sparse matrix
• real inputlist::epsilu = 1e-12
      the precision of incomplete LU factorization for preconditioning
• integer inputlist::lfindzero = 0
      use Newton methods to find zero of force-balance, which is computed by dforce()
• real inputlist::escale = 0.0
      controls the weight factor, BBweight, in the force-imbalance harmonics

    real inputlist::opsilon = 1.0

      weighting of force-imbalance
• real inputlist::pcondense = 2.0
      spectral condensation parameter

    real inputlist::epsilon = 0.0

      weighting of spectral-width constraint

    real inputlist::wpoloidal = 1.0

       "star-like" poloidal angle constraint radial exponential factor used in preset() to construct sweight

    real inputlist::upsilon = 1.0

      weighting of "star-like" poloidal angle constraint used in preset() to construct sweight
• real inputlist::forcetol = 1.0e-10
      required tolerance in force-balance error; only used as an initial check
• real inputlist::c05xmax = 1.0e-06
      required tolerance in position, \mathbf{x} \equiv \{R_{i,v}, Z_{i,v}\}
real inputlist::c05xtol = 1.0e-12
      required tolerance in position, \mathbf{x} \equiv \{R_{i,v}, Z_{i,v}\}
real inputlist::c05factor = 1.0e-02
      used to control initial step size in CO5NDF and CO5PDF

    logical inputlist::lreadgf = .true.

      \operatorname{\textit{read}} \nabla_{\mathbf{x}} \mathbf{F} from file ext . GF
integer inputlist::mfreeits = 0
      maximum allowed free-boundary iterations
• real inputlist::bnstol = 1.0e-06
      redundant;
• real inputlist::bnsblend = 0.666
      redundant;
• real inputlist::gbntol = 1.0e-06
      required tolerance in free-boundary iterations
real inputlist::gbnbld = 0.666
      normal blend

    real inputlist::vcasingeps = 1.e-12

      regularization of Biot-Savart; see bnorml(), casing()

    real inputlist::vcasingtol = 1.e-08

      accuracy on virtual casing integral; see bnorml(), casing()

    integer inputlist::vcasingits = 8

      minimum number of calls to adaptive virtual casing routine; see casing()
• integer inputlist::vcasingper = 1
      periods of integragion in adaptive virtual casing routine; see <a href="casing()">casing()</a>

    integer inputlist::mcasingcal = 8

      minimum number of calls to adaptive virtual casing routine; see casing(); redundant;
real inputlist::odetol = 1.0e-07
      o.d.e. integration tolerance for all field line tracing routines
real inputlist::absreq = 1.0e-08
```

```
redundant
• real inputlist::relreq = 1.0e-08
      redundant
• real inputlist::absacc = 1.0e-04
      redundant
real inputlist::epsr = 1.0e-08
      redundant
• integer inputlist::nppts = 0
      number of toroidal transits used (per trajectory) in following field lines for constructing Poincaré plots; if nPpts<1,
      no Poincaré plot is constructed;
• real inputlist::ppts = 0.0
      stands for Poincare plot theta start. Chose at which angle (normalized over \pi) the Poincare field-line tracing start.
• integer, dimension(1:mnvol+1) inputlist::nptrj = -1
      number of trajectories in each annulus to be followed in constructing Poincaré plot
• logical inputlist::lhevalues = .false.
      to compute eigenvalues of 
abla \mathbf{F}
• logical inputlist::lhevectors = .false.
      to compute eigenvectors (and also eigenvalues) of \nabla \mathbf{F}
• logical inputlist::lhmatrix = .false.
      to compute and write to file the elements of \nabla \mathbf{F}
• integer inputlist::lperturbed = 0
      to compute linear, perturbed equilibrium
integer inputlist::dpp = -1
      perturbed harmonic
• integer inputlist::dqq = -1
      perturbed harmonic
• integer inputlist::lerrortype = 0
      the type of error output for Lcheck=1
• integer inputlist::ngrid = -1
      the number of points to output in the grid, -1 for Lrad(vvol)
• real inputlist::drz = 1E-5
      difference in geometry for finite difference estimate (debug only)
• integer inputlist::lcheck = 0
      implement various checks
• logical inputlist::ltiming = .false.
      to check timing
real inputlist::fudge = 1.0e-00
      redundant
• real inputlist::scaling = 1.0e-00
      redundant
• logical inputlist::wmanual = .false.
• logical inputlist::wrzaxis = .false.
• logical inputlist::wpackxi = .false.
• logical inputlist::wvolume = .false.
• logical inputlist::wcoords = .false.
• logical inputlist::wbasefn = .false.
• logical inputlist::wmemory = .false.
• logical inputlist::wmetrix = .false.
• logical inputlist::wma00aa = .false.
• logical inputlist::wmatrix = .false.
```

logical inputlist::wspsmat = .false.
logical inputlist::wspsint = .false.

- logical inputlist::wmp00ac = .false.
- logical inputlist::wma02aa = .false.
- logical inputlist::wpackab = .false.
- logical inputlist::wtr00ab = .false.
- logical inputlist::wcurent = .false.
- logical inputlist::wdf00ab = .false.
- logical inputlist::wlforce = .false.
- logical inputlist::wintghs = .false.
- logical inputlist::wmtrxhs = .false.
- logical inputlist::wlbpol = .false.
- logical inputlist::wbrcast = .false.
- logical inputlist::wdfp100 = .false.
- logical inputlist::wdfp200 = .false.
- logical inputlist::wdforce = .false.
- logical inputlist::wnewton = .false.
- logical inputlist::wcasing = .false.
- logical inputlist::wbnorml = .false.
- logical inputlist::wjo00aa = .false.
- logical inputlist::wpp00aa = .false.
- logical inputlist::wpp00ab = .false.
- logical inputlist::wbfield = .false.
- logical inputlist::wstzxyz = .false.
- logical inputlist::whesian = .false.
- logical inputlist::wra00aa = .false.
- logical inputlist::wnumrec = .false.
- logical inputlist::wdcuhre = .false.
- logical inputlist::wminpack = .false.
- logical inputlist::wiqpack = .false.
- logical inputlist::wrksuite = .false.
- logical inputlist::wi1mach = .false.
- logical inputlist::wd1mach = .false.
- logical inputlist::wilut = .false.
- logical inputlist::witers = .false.
- logical inputlist::wsphdf5 = .false.
- logical inputlist::wpreset = .false.
- logical inputlist::wglobal = .false.
- logical inputlist::wxspech = .false.
- logical inputlist::wbuild\_vector\_potential = .false.
- logical inputlist::wreadin = .false.

write screen output of readin()

• logical inputlist::wwrtend = .false.

write screen output of wrtend()

• logical inputlist::wmacros = .false.

write screen output from expanded macros

#### 8.14.1 Detailed Description

Input namelists.

## 8.15 src/intghs.f90 File Reference

Calculates volume integrals of Chebyshev-polynomials and covariant field for Hessian computation.

#### **Data Types**

• type intghs\_module::intghs\_workspace

This calculates the integral of something related to matrix-vector-multiplication.

#### **Functions/Subroutines**

• subroutine intghs (Iquad, mn, Ivol, Irad, idx)

Calculates volume integrals of Chebyshev polynomials and covariant field products.

subroutine intghs\_workspace\_init (Ivol)
 init workspace

• subroutine intghs\_workspace\_destroy ()

free workspace

#### Variables

type(intghs\_workspace) intghs\_module::wk

This is an instance of the intghs\_workspace type.

#### 8.15.1 Detailed Description

Calculates volume integrals of Chebyshev-polynomials and covariant field for Hessian computation.

#### 8.15.2 Function/Subroutine Documentation

Calculates volume integrals of Chebyshev polynomials and covariant field products.

## **Parameters**

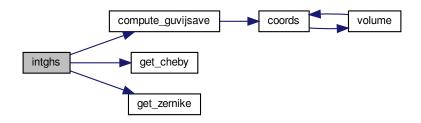
lquad	
mn	
Ivol	
Irad	
idx	

References allglobal::ate, allglobal::ate, allglobal::aze, allglobal::aze, compute\_guvijsave(), allglobal::cpus, allglobal::dbdx, allglobal::dtc, allglobal::dtc, allglobal::dzc, allglobal::dzc, allglobal::gaussianabscissae, allglobal::gaussianabscissae, allglobal::guvijsave, constants::half, allglobal:-

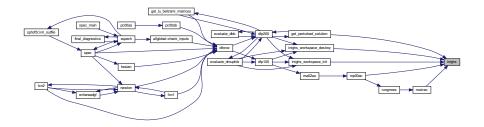
::im, allglobal::in, allglobal::lcoordinatesingularity, allglobal::lsavedguvij, allglobal::mne, allglobal::mpi\_comm\_ spec, inputlist::mpol, allglobal::myid, allglobal::ncpu, allglobal::notstellsym, allglobal::nt, allglobal::ntz, allglobal::ntz, allglobal::ntz, allglobal::ntz, allglobal::ntz, allglobal::ntz, allglobal::g, numerical::small, numerical-::sqrtmachprec, allglobal::tsc, allglobal::tsc,

Referenced by get\_perturbed\_solution(), intghs\_workspace\_destroy(), intghs\_workspace\_init(), matvec(), and mp00ac().

Here is the call graph for this function:



Here is the caller graph for this function:



```
8.15.2.2 intghs_workspace_init() subroutine intghs_workspace_init ( integer, intent(in) lvol )
```

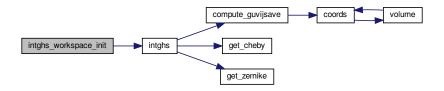
init workspace

**Parameters** 

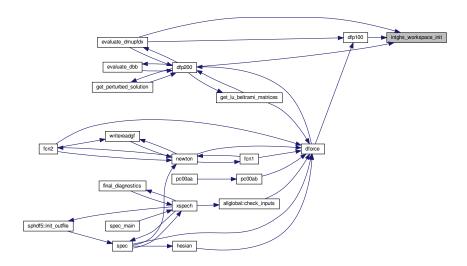
Ivol

References allglobal::cpus, intghs(), allglobal::iquad, inputlist::lrad, allglobal::mn, allglobal::mpi\_comm\_spec, inputlist::mpol, allglobal::myid, allglobal::ncpu, allglobal::ntz, fileunits::ounit, inputlist::wmacros, and constants::zero.

Here is the call graph for this function:



Here is the caller graph for this function:



## **8.15.2.3 intghs\_workspace\_destroy()** subroutine intghs\_workspace\_destroy

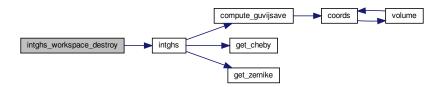
free workspace

**Parameters** 

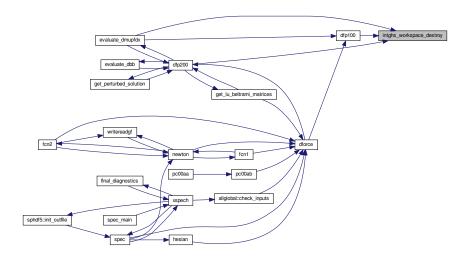
Ivol

References allglobal::cpus, intghs(), allglobal::mpi\_comm\_spec, allglobal::myid, allglobal::ncpu, fileunits::ounit, and inputlist::wmacros.

Here is the call graph for this function:



Here is the caller graph for this function:



## 8.16 src/jo00aa.f90 File Reference

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

## **Functions/Subroutines**

• subroutine jo00aa (Ivol, Ntz, Iquad, mn) Measures error in Beltrami equation,  $\nabla imes {f B} - \mu {f B}.$ 

## 8.16.1 Detailed Description

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

## 8.17 src/lforce.f90 File Reference

Computes  $B^2$ , and the spectral condensation constraints if required, on the interfaces,  $\mathcal{I}_i$ .

#### **Functions/Subroutines**

subroutine Iforce (Ivol, iocons, ideriv, Ntz, dBB, XX, YY, length, DDI, MMI, iflag)
 Computes B<sup>2</sup>, and the spectral condensation constraints if required, on the interfaces, \( \mathcal{I}\_i \).

## 8.17.1 Detailed Description

Computes  $B^2$ , and the spectral condensation constraints if required, on the interfaces,  $\mathcal{I}_i$ .

#### 8.18 src/ma00aa.f90 File Reference

Calculates volume integrals of Chebyshev polynomials and metric element products.

#### **Functions/Subroutines**

subroutine ma00aa (Iquad, mn, Ivol, Irad)
 Calculates volume integrals of Chebyshev polynomials and metric element products.

## 8.18.1 Detailed Description

Calculates volume integrals of Chebyshev polynomials and metric element products.

## 8.19 src/ma02aa.f90 File Reference

Constructs Beltrami field in given volume consistent with flux, helicity, rotational-transform and/or parallel-current constraints.

#### **Functions/Subroutines**

• subroutine ma02aa (Ivol, NN)

Constructs Beltrami field in given volume consistent with flux, helicity, rotational-transform and/or parallel-current constraints.

#### 8.19.1 Detailed Description

Constructs Beltrami field in given volume consistent with flux, helicity, rotational-transform and/or parallel-current constraints.

## 8.20 src/matrix.f90 File Reference

Constructs energy and helicity matrices that represent the Beltrami linear system.

#### **Functions/Subroutines**

- subroutine matrix (Ivol, mn, Irad)
   Constructs energy and helicity matrices that represent the Beltrami linear system. gauge conditions
- subroutine matrixbg (Ivol, mn, Irad)

#### 8.20.1 Detailed Description

Constructs energy and helicity matrices that represent the Beltrami linear system.

## 8.21 src/memory.f90 File Reference

memory management module

#### **Functions/Subroutines**

- subroutine allocate\_beltrami\_matrices (vvol, LcomputeDerivatives) allocate Beltrami matrices
- subroutine deallocate\_beltrami\_matrices (LcomputeDerivatives)

deallocate Beltrami matrices

- subroutine allocate\_geometry\_matrices (vvol, LcomputeDerivatives)
  - allocate geometry matrices
- subroutine deallocate\_geometry\_matrices (LcomputeDerivatives) deallocate geometry matrices

#### 8.21.1 Detailed Description

memory management module

## 8.21.2 Function/Subroutine Documentation

```
8.21.2.1 allocate_beltrami_matrices() subroutine allocate_beltrami_matrices ( integer, intent(in) vvol, logical, intent(in) LcomputeDerivatives )
```

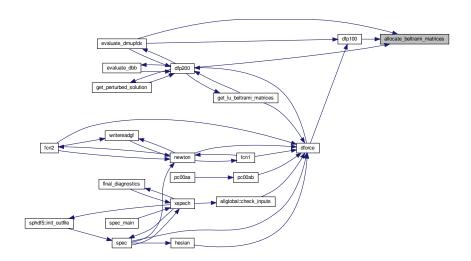
allocate Beltrami matrices

**Parameters** 

vvol LcomputeDerivatives References allglobal::adotx, allglobal::dma, allglobal::dmas, allglobal::dmas, allglobal::dmb, allglobal::dmb, allglobal::dmb, allglobal::dmb, allglobal::dmb, allglobal::dmb, allglobal::dmb, allglobal::dmb, allglobal::dmb, allglobal::mbpsi, allglobal::mbpsi, allglobal::ndmasmax, allglobal::ndmasmax.

Referenced by dfp100(), dfp200(), and evaluate\_dmupfdx().

Here is the caller graph for this function:



## **8.21.2.2 deallocate\_beltrami\_matrices()** subroutine deallocate\_beltrami\_matrices ( logical, intent(in) *LcomputeDerivatives* )

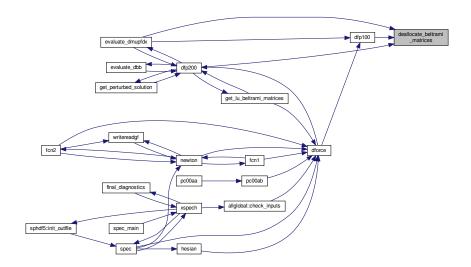
deallocate Beltrami matrices

#### **Parameters**

LcomputeDerivatives

References allglobal::adotx, allglobal::dmax, allglobal::dmax, allglobal::dmax, allglobal::dmbx, allglobal::

Here is the caller graph for this function:



# **8.21.2.3 allocate\_geometry\_matrices()** subroutine allocate\_geometry\_matrices ( integer *vvol*, logical, intent(in) *LcomputeDerivatives* )

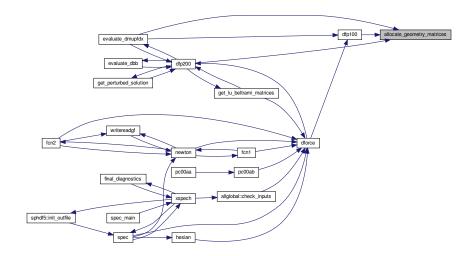
allocate geometry matrices

#### **Parameters**

vvol	
LcomputeDerivatives	

References allglobal::ddttcc, allglobal::ddttcs, allglobal::ddttsc, allglobal::dtsc, allglobal::dtsc, allglobal::dtsc, allglobal::dtsc, allglobal::dtsc, allglobal::dtsc, allglobal::mot, inputlist::mpol, allglobal::notstellsym, allglobal::ntt, allglobal::tdstcc, allglobal::tdstcs, allglobal::tdstcs, allglobal::tdstcs, allglobal::tssc, allglobal::tssc, allglobal::tssc, allglobal::tssc, allglobal::tssc, allglobal::tssc, allglobal::tssc, allglobal::ttssc, allglobal::

Here is the caller graph for this function:



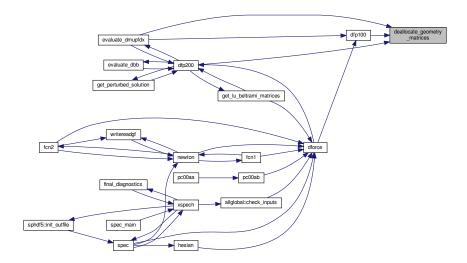
## **8.21.2.4 deallocate\_geometry\_matrices()** subroutine deallocate\_geometry\_matrices ( logical, intent(in) *LcomputeDerivatives* )

deallocate geometry matrices

#### **Parameters**

LcomputeDerivatives

Here is the caller graph for this function:



## 8.22 src/metrix.f90 File Reference

Calculates the metric quantities,  $\sqrt{g}\,g^{\mu\nu}$ , which are required for the energy and helicity integrals.

## **Functions/Subroutines**

- subroutine metrix (Iquad, IvoI)

  Calculates the metric quantities,  $\sqrt{g} g^{\mu\nu}$ , which are required for the energy and helicity integrals.
- subroutine compute\_guvijsave (lquad, vvol, ideriv, Lcurvature)

  compute guvijsave

## 8.22.1 Detailed Description

Calculates the metric quantities,  $\sqrt{g}\,g^{\mu\nu}$ , which are required for the energy and helicity integrals.

## 8.22.2 Function/Subroutine Documentation

compute guvijsave

#### **Parameters**

lquad	
vvol	
ideriv	
Lcurvature	

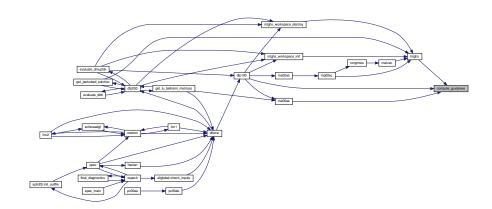
References coords(), allglobal::gaussianabscissae, allglobal::guvij, allglobal::guvijsave, allglobal::mn, allglobal::ntz, and allglobal::sg.

Referenced by dfp100(), intghs(), and ma00aa().

Here is the call graph for this function:



Here is the caller graph for this function:



## 8.23 src/mp00ac.f90 File Reference

Solves Beltrami/vacuum (linear) system, given matrices.

#### **Functions/Subroutines**

- subroutine mp00ac (Ndof, Xdof, Fdof, Ddof, Ldfjac, iflag)
   Solves Beltrami/vacuum (linear) system, given matrices.
   unpacking fluxes, helicity multiplier
- subroutine rungmres (n, nrestart, mu, vvol, rhs, sol, ipar, fpar, wk, nw, guess, a, au, jau, ju, iperm, ierr) run GMRES
- subroutine matvec (n, x, ax, a, mu, vvol)

  compute a.x by either by coumputing it directly, or using a matrix free method
- subroutine prec\_solve (n, vecin, vecout, au, jau, ju, iperm)
   apply the preconditioner

#### 8.23.1 Detailed Description

Solves Beltrami/vacuum (linear) system, given matrices.

#### 8.23.2 Function/Subroutine Documentation

```
8.23.2.1 rungmres() subroutine rungmres (
             integer n,
             integer nrestart,
             real mu,
             integer vvol,
             real, dimension(1:n) rhs,
             real, dimension(1:n) sol,
             integer, dimension(16) ipar,
             real, dimension(16) fpar,
             real, dimension(1:nw) wk,
             integer nw,
             real, dimension(n) guess,
             real, dimension(*) a,
             real, dimension(*) au,
             integer, dimension(*) jau,
             integer, dimension(*) ju,
             integer, dimension(*) iperm,
             integer ierr )
```

## run GMRES

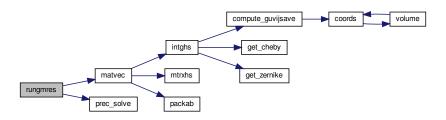
#### **Parameters**

n	
nrestart	
ти	
vvol	
rhs	
sol	
ipar	
fpar	
wk	
nw	
guess	
а	
au	
jau	
ju	
iperm	
ierr	

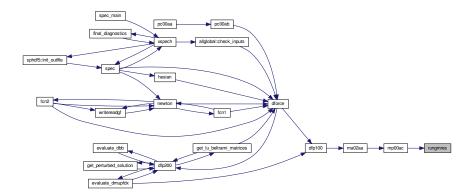
References inputlist::epsgmres, allglobal::liluprecond, matvec(), inputlist::nitergmres, constants::one, prec\_solve(), and constants::zero.

Referenced by mp00ac().

Here is the call graph for this function:



Here is the caller graph for this function:



compute a.x by either by coumputing it directly, or using a matrix free method

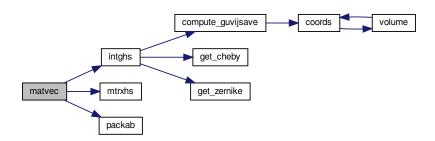
#### **Parameters**

n	
X	
ax	
а	
ти	
vvol	

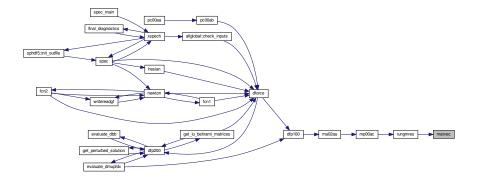
References allglobal::dmd, intghs(), allglobal::quad, inputlist::lrad, allglobal::mn, mtrxhs(), allglobal::notmatrixfree, constants::one, packab(), and constants::zero.

Referenced by rungmres().

Here is the call graph for this function:



Here is the caller graph for this function:



apply the preconditioner

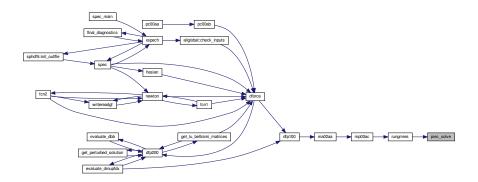
#### **Parameters**

iperm

n		
vecin		
vecout		
au		
Generated or	ı We	d Oct 6 2021 10:03:38 for SPEC by Doxygen
iu		

Referenced by rungmres().

Here is the caller graph for this function:



## 8.24 src/mtrxhs.f90 File Reference

Constructs matrices that represent the Beltrami linear system, matrix-free.

#### **Functions/Subroutines**

subroutine mtrxhs (Ivol, mn, Irad, resultA, resultD, idx)
 Constructs matrices that represent the Beltrami linear system, matrix-free.

## 8.24.1 Detailed Description

Constructs matrices that represent the Beltrami linear system, matrix-free.

## 8.25 src/newton.f90 File Reference

Employs Newton method to find  $\mathbf{F}(\mathbf{x}) = 0$ , where  $\mathbf{x} \equiv \{\text{geometry}\}\$ and  $\mathbf{F}$  is defined in dforce() .

## Modules

• module newtontime timing of Newton iterations

## Functions/Subroutines

- subroutine newton (NGdof, position, ihybrd) Employs Newton method to find  $\mathbf{F}(\mathbf{x}) = 0$ , where  $\mathbf{x} \equiv \{\text{geometry}\}\$ and  $\mathbf{F}$  is defined in dforce() .
- subroutine writereadgf (readorwrite, NGdof, ireadhessian)

read or write force-derivative matrix

• subroutine fcn1 (NGdof, xx, fvec, irevcm)

 subroutine fcn2 (NGdof, xx, fvec, fjac, Ldfjac, irevcm) fcn2

#### **Variables**

· integer newtontime::nfcalls

number of calls to get function values (?)

· integer newtontime::ndcalls

number of calls to get derivative values (?)

· real newtontime::lastcpu

last CPU that called this (?)

## 8.25.1 Detailed Description

Employs Newton method to find  $\mathbf{F}(\mathbf{x}) = 0$ , where  $\mathbf{x} \equiv \{\text{geometry}\}\$  and  $\mathbf{F}$  is defined in dforce().

## 8.26 src/packab.f90 File Reference

Packs, and unpacks, Beltrami field solution vector;  $\mathbf{a} \equiv \{A_{\theta,e,i,l}, A_{\zeta,e,i,l}, \text{etc.}\}.$ 

#### **Functions/Subroutines**

subroutine packab (packorunpack, Ivol, NN, solution, ideriv)
 Packs and unpacks Beltrami field solution vector.

#### 8.26.1 Detailed Description

Packs, and unpacks, Beltrami field solution vector;  $\mathbf{a} \equiv \{A_{\theta,e,i,l}, A_{\zeta,e,i,l}, \text{etc.}\}.$ 

## 8.27 src/packxi.f90 File Reference

Packs, and unpacks, geometrical degrees of freedom; and sets coordinate axis.

## **Functions/Subroutines**

 subroutine packxi (NGdof, position, Mvol, mn, iRbc, iZbs, iRbs, iZbc, packorunpack, LComputeDerivatives, LComputeAxis)

Packs, and unpacks, geometrical degrees of freedom; and sets coordinate axis.

#### 8.27.1 Detailed Description

Packs, and unpacks, geometrical degrees of freedom; and sets coordinate axis.

## 8.28 src/pc00aa.f90 File Reference

Use preconditioned conjugate gradient method to find minimum of energy functional.

#### **Functions/Subroutines**

subroutine pc00aa (NGdof, position, Nvol, mn, ie04dgf)
 Use preconditioned conjugate gradient method to find minimum of energy functional.

#### 8.28.1 Detailed Description

Use preconditioned conjugate gradient method to find minimum of energy functional.

## 8.29 src/pc00ab.f90 File Reference

Returns the energy functional and it's derivatives with respect to geometry.

#### **Functions/Subroutines**

• subroutine pc00ab (mode, NGdof, Position, Energy, Gradient, nstate, iuser, ruser)

Returns the energy functional and it's derivatives with respect to geometry.

## 8.29.1 Detailed Description

Returns the energy functional and it's derivatives with respect to geometry.

## 8.30 src/pp00aa.f90 File Reference

Constructs Poincaré plot and "approximate" rotational-transform (driver).

## Functions/Subroutines

• subroutine pp00aa

Constructs Poincaré plot and "approximate" rotational-transform (driver).

#### 8.30.1 Detailed Description

Constructs Poincaré plot and "approximate" rotational-transform (driver).

## 8.31 src/pp00ab.f90 File Reference

Follows magnetic fieldline using ode-integration routine from rksuite.f .

## **Functions/Subroutines**

• subroutine pp00ab (Ivol, sti, Nz, nPpts, poincaredata, fittedtransform, utflag)

Constructs Poincaré plot and "approximate" rotational-transform (for single field line).

#### 8.31.1 Detailed Description

Follows magnetic fieldline using ode-integration routine from rksuite.f .

## 8.32 src/preset.f90 File Reference

Allocates and initializes internal arrays.

#### **Functions/Subroutines**

· subroutine preset

Allocates and initializes internal arrays.

## 8.32.1 Detailed Description

Allocates and initializes internal arrays.

## 8.33 src/ra00aa.f90 File Reference

Writes vector potential to .ext.sp.A .

#### **Functions/Subroutines**

• subroutine ra00aa (writeorread)

Writes vector potential to .ext.sp.A .

## 8.33.1 Detailed Description

Writes vector potential to .ext.sp.A .

## 8.34 src/rzaxis.f90 File Reference

The coordinate axis is assigned via a poloidal average over an arbitrary surface.

#### **Functions/Subroutines**

- subroutine rzaxis (Mvol, mn, inRbc, inZbs, inRbs, inZbc, ivol, LcomputeDerivatives)

  The coordinate axis is assigned via a poloidal average over an arbitrary surface.
- subroutine **fndiff\_rzaxis** (Mvol, mn, ivol, jRbc, jRbs, jZbc, JZbs, imn, irz, issym)

## 8.34.1 Detailed Description

The coordinate axis is assigned via a poloidal average over an arbitrary surface.

## 8.35 src/sphdf5.f90 File Reference

Writes all the output information to ext.sp.h5.

#### Modules

· module sphdf5

writing the HDF5 output file

#### Functions/Subroutines

• subroutine sphdf5::init outfile

Initialize the interface to the HDF5 library and open the output file.

subroutine sphdf5::mirror\_input\_to\_outfile

Mirror input variables into output file.

subroutine sphdf5::init\_convergence\_output

Prepare convergence evolution output.

subroutine sphdf5::write\_convergence\_output (nDcalls, ForceErr)

Write convergence output (evolution of interface geometry, force, etc).

• subroutine sphdf5::write\_grid

Write the magnetic field on a grid.

subroutine sphdf5::init\_flt\_output (numTrajTotal)

Initialize field line tracing output group and create array datasets.

subroutine sphdf5::write\_poincare (offset, data, success)

Write a hyperslab of Poincare data corresponding to the output of one parallel worker.

• subroutine sphdf5::write\_transform (offset, length, lvol, diotadxup, fiota)

Write the rotational transform output from field line following.

• subroutine sphdf5::finalize\_flt\_output

Finalize Poincare output.

• subroutine sphdf5::write\_vector\_potential (sumLrad, allAte, allAze, allAto, allAzo)

Write the magnetic vector potential Fourier harmonics to the output file group  $/ vector\_potential$ .

• subroutine sphdf5::hdfint

Write the final state of the equilibrium to the output file.

· subroutine sphdf5::finish\_outfile

Close all open HDF5 objects (we know of) and list any remaining still-open objects.

#### **Variables**

• logical, parameter sphdf5::hdfdebug = .false.

global flag to enable verbal diarrhea commenting HDF5 operations

• integer, parameter sphdf5::internalhdf5msg = 0

1: print internal HDF5 error messages; 0: only error messages from sphdf5

integer sphdf5::hdfier

error flag for HDF5 library

integer sphdf5::rank

rank of data to write using macros

• integer(hid t) sphdf5::file id

default file ID used in macros

integer(hid\_t) sphdf5::space\_id

default dataspace ID used in macros

integer(hid\_t) sphdf5::dset\_id

default dataset ID used in macros

integer(hsize\_t), dimension(1:1) sphdf5::onedims

dimension specifier for one-dimensional data used in macros

integer(hsize t), dimension(1:2) sphdf5::twodims

dimension specifier for two-dimensional data used in macros

integer(hsize t), dimension(1:3) sphdf5::threedims

dimension specifier for three-dimensional data used in macros

· logical sphdf5::grp\_exists

flags used to signal if a group already exists

logical sphdf5::var\_exists

flags used to signal if a variable already exists

• integer(hid\_t) sphdf5::iteration\_dset\_id

Dataset identifier for "iteration".

• integer(hid t) sphdf5::dataspace

dataspace for extension by 1 iteration object

integer(hid\_t) sphdf5::memspace

memspace for extension by 1 iteration object

integer(hsize t), dimension(1) sphdf5::old data dims

current dimensions of "iterations" dataset

integer(hsize\_t), dimension(1) sphdf5::data\_dims

new dimensions for "iterations" dataset

integer(hsize\_t), dimension(1) sphdf5::max\_dims

maximum dimensions for "iterations" dataset

• integer(hid\_t) sphdf5::plist\_id

Property list identifier used to activate dataset transfer property.

integer(hid\_t) sphdf5::dt\_ndcalls\_id

Memory datatype identifier (for "nDcalls" dataset in "/grid")

integer(hid t) sphdf5::dt energy id

Memory datatype identifier (for "Energy" dataset in "/grid")

integer(hid t) sphdf5::dt forceerr id

Memory datatype identifier (for "ForceErr" dataset in "/grid")

integer(hid\_t) sphdf5::dt\_irbc\_id

Memory datatype identifier (for "iRbc" dataset in "/grid")

• integer(hid\_t) sphdf5::dt\_izbs\_id

Memory datatype identifier (for "iZbs" dataset in "/grid")

integer(hid\_t) sphdf5::dt\_irbs\_id

Memory datatype identifier (for "iRbs" dataset in "/grid")

integer(hid\_t) sphdf5::dt\_izbc\_id

Memory datatype identifier (for "iZbc" dataset in "/grid")

integer, parameter sphdf5::rankp =3

rank of Poincare data

integer, parameter sphdf5::rankt =2

rank of rotational transform data

• integer(hid\_t) sphdf5::grppoincare

group for Poincare data

integer(hid\_t) sphdf5::dset\_id\_t

Dataset identifier for  $\theta$  coordinate of field line following.

integer(hid\_t) sphdf5::dset\_id\_s

Dataset identifier for s coordinate of field line following.

```
integer(hid_t) sphdf5::dset_id_r
      Dataset identifier for R coordinate of field line following.
  integer(hid t) sphdf5::dset id z
      Dataset identifier for Z coordinate of field line following.
  integer(hid_t) sphdf5::dset_id_success
      Dataset identifier for success flag of trajectories to follow.
• integer(hid t) sphdf5::filespace t
      Dataspace identifier in file for \theta coordinate of field line following.
integer(hid_t) sphdf5::filespace_s
      Dataspace identifier in file for s coordinate of field line following.

    integer(hid t) sphdf5::filespace r

      Dataspace identifier in file for R coordinate of field line following.
integer(hid_t) sphdf5::filespace_z
      Dataspace identifier in file for Z coordinate of field line following.

    integer(hid t) sphdf5::filespace success

      Dataspace identifier in file for success flag of trajectories to follow.
integer(hid_t) sphdf5::memspace_t
      Dataspace identifier in memory for \theta coordinate of field line following.
integer(hid_t) sphdf5::memspace_s
      Dataspace identifier in memory for s coordinate of field line following.
integer(hid_t) sphdf5::memspace_r
      Dataspace identifier in memory for R coordinate of field line following.
  integer(hid t) sphdf5::memspace z
      Dataspace identifier in memory for {\cal Z} coordinate of field line following.
integer(hid_t) sphdf5::memspace_success
      Dataspace identifier in memory for success flag of trajectories to follow.

    integer(hid t) sphdf5::grptransform

      group for rotational transform data
integer(hid_t) sphdf5::dset_id_diotadxup
      Dataset identifier for diotadxup (derivative of rotational transform ?)
integer(hid_t) sphdf5::dset_id_fiota
      Dataset identifier for fiota ( rotational transform ?)
• integer(hid_t) sphdf5::filespace_diotadxup
      Dataspace identifier in file for diotadxup.

    integer(hid_t) sphdf5::filespace_fiota

      Dataspace identifier in file for fiota.

    integer(hid t) sphdf5::memspace diotadxup

      Dataspace identifier in memory for diotadxup.
• integer(hid_t) sphdf5::memspace_fiota
      Dataspace identifier in memory for fiota.

    character(len=15), parameter sphdf5::aname = "description"

      Attribute name for descriptive info.
integer(hid_t) sphdf5::attr_id
      Attribute identifier.
integer(hid_t) sphdf5::aspace_id
      Attribute Dataspace identifier.
integer(hid_t) sphdf5::atype_id
      Attribute Datatype identifier.
  integer, parameter sphdf5::arank = 1
      Attribure rank.
  integer(hsize_t), dimension(arank) sphdf5::adims = (/1/)
```

Attribute dimension.

• integer(size\_t) sphdf5::attrlen

Length of the attribute string.

• character(len=:), allocatable sphdf5::attr\_data

Attribute data.

#### 8.35.1 Detailed Description

Writes all the output information to ext.sp.h5.

If the output file already exists, it will be deleted and replaced by an empty one, which gets filled in with the updated data. All calls to the HDF5 API are filtered to only happen from MPI rank-0 to be able to use the serial HDF5 library. Parallel HDF5 was considered in the past, but abandoned due to very subtle and irreproducible errors.

## 8.36 src/spsint.f90 File Reference

Calculates volume integrals of Chebyshev-polynomials and metric elements for preconditioner.

#### **Functions/Subroutines**

subroutine spsint (Iquad, mn, Ivol, Irad)
 Calculates volume integrals of Chebyshev-polynomials and metric elements for preconditioner.

#### 8.36.1 Detailed Description

Calculates volume integrals of Chebyshev-polynomials and metric elements for preconditioner.

## 8.37 src/spsmat.f90 File Reference

Constructs matrices for the precondtioner.

#### **Functions/Subroutines**

• subroutine spsmat (Ivol, mn, Irad)

Constructs matrices for the precondtioner.

• subroutine push\_back (iq, nq, NN, vA, vD, vjA, qA, qD, qjA)

push a new element at the back of the queue

subroutine clean\_queue (nq, NN, qA, qD, qjA)

clean the queue

subroutine addline (ng, NN, qA, qD, qjA, ns, nrow, dMAS, dMDS, jdMAS, idMAS)

add the content from the queue to the real matrices

#### 8.37.1 Detailed Description

Constructs matrices for the precondtioner.

## 8.37.2 Function/Subroutine Documentation

push a new element at the back of the queue

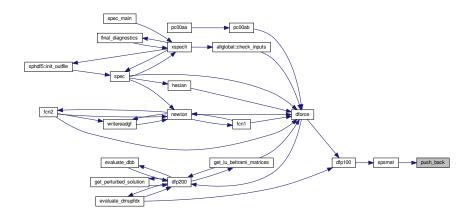
#### **Parameters**

iq	
nq	
NN	
vΑ	
νD	
vjA	
qΑ	
qD	
qjA	

References constants::zero.

Referenced by spsmat().

Here is the caller graph for this function:



#### clean the queue

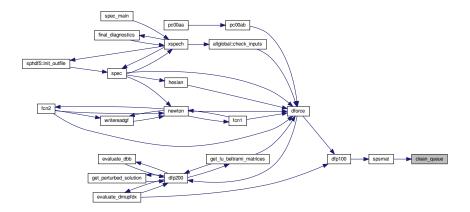
#### **Parameters**

nq	
NN	
qΑ	
qD	
qjA	

References constants::zero.

Referenced by spsmat().

Here is the caller graph for this function:



```
8.37.2.3 addline() subroutine addline (
    integer, dimension(4), intent(inout) nq,
    integer, intent(inout) NN,
    real, dimension(nn,4), intent(inout) qA,
    real, dimension(nn,4), intent(inout) qD,
    integer, dimension(nn,4), intent(inout) qjA,
    integer, intent(inout) ns,
    integer, intent(inout) nrow,
    real, dimension(*) dMAS,
    real, dimension(*) dMDS,
    integer, dimension(*) jdMAS,
    integer, dimension(*) idMAS)
```

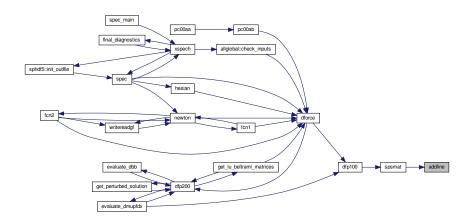
add the content from the queue to the real matrices

#### **Parameters**

nq	
NN	
qΑ	
qD	
qjA	
ns	
nrow	
dMAS	
dMDS	
jdMAS	
idMAS	

Referenced by spsmat().

Here is the caller graph for this function:



## 8.38 src/stzxyz.f90 File Reference

Calculates coordinates,  $\mathbf{x}(s,\theta,\zeta) \equiv R \, \mathbf{e}_R + Z \, \mathbf{e}_Z$ , and metrics, at given  $(s,\theta,\zeta)$ .

## **Functions/Subroutines**

• subroutine stzxyz (Ivol, stz, RpZ)  $\textit{Calculates coordinates, } \mathbf{x}(s,\theta,\zeta) \equiv R\,\mathbf{e}_R + Z\,\mathbf{e}_Z, \textit{and metrics, at given } (s,\theta,\zeta).$ 

## 8.38.1 Detailed Description

Calculates coordinates,  $\mathbf{x}(s, \theta, \zeta) \equiv R \mathbf{e}_R + Z \mathbf{e}_Z$ , and metrics, at given  $(s, \theta, \zeta)$ .

## 8.39 src/tr00ab.f90 File Reference

Calculates rotational transform given an arbitrary tangential field.

#### **Functions/Subroutines**

subroutine tr00ab (Ivol, mn, NN, Nt, Nz, iflag, Idiota)
 Calculates rotational transform given an arbitrary tangential field.

## 8.39.1 Detailed Description

Calculates rotational transform given an arbitrary tangential field.

#### 8.40 src/volume.f90 File Reference

Computes volume of each region; and, if required, the derivatives of the volume with respect to the interface geometry.

#### **Functions/Subroutines**

• subroutine volume (Ivol, vflag)

Computes volume of each region; and, if required, the derivatives of the volume with respect to the interface geometry.

#### 8.40.1 Detailed Description

Computes volume of each region; and, if required, the derivatives of the volume with respect to the interface geometry.

#### 8.41 src/wa00aa.f90 File Reference

Constructs smooth approximation to wall.

#### **Modules**

module laplaces

...todo...

#### **Functions/Subroutines**

• subroutine wa00aa (iwa00aa)

Constructs smooth approximation to wall.

• subroutine vacuumphi (Nconstraints, rho, fvec, iflag)

Compute vacuum magnetic scalar potential (?)

#### **Variables**

```
• logical laplaces::stage1
      what is this?
· logical laplaces::exterior
      what is this?

    logical laplaces::dorm

      what is this?

    integer laplaces::nintervals

      what is this?

    integer laplaces::nsegments

      what is this?

    integer laplaces::ic

      what is this?
• integer laplaces::np4
      what is this?
integer laplaces::np1
      what is this?
• integer, dimension(:), allocatable laplaces::icint
      what is this?
• real laplaces::originalalpha
      what is this?

    real, dimension(:), allocatable laplaces::xpoly

      what is this?

    real, dimension(:), allocatable laplaces::ypoly

      what is this?
• real, dimension(:), allocatable laplaces::phi
      what is this?
• real, dimension(:), allocatable laplaces::phid
      what is this?
• real, dimension(:,:), allocatable laplaces::cc
      what is this?

    integer laplaces::ilength

      what is this?
• real laplaces::totallength
      what is this?

    integer laplaces::niterations

     counter; eventually redundant; 24 Oct 12;
· integer laplaces::iangle
     angle; eventually redundant; 24 Oct 12;

    real laplaces::rmid

     used to define local polar coordinate; eventually redundant; 24 Oct 12;
· real laplaces::zmid
      used to define local polar coordinate; eventually redundant; 24 Oct 12;
· real laplaces::alpha
      eventually redundant; 24 Oct 12;
```

## 8.41.1 Detailed Description

Constructs smooth approximation to wall.

## 8.42 src/xspech.f90 File Reference

Main program.

#### **Functions/Subroutines**

• program spec\_main

Main program of SPEC.

• subroutine xspech

Main subroutine of SPEC.

• subroutine read\_command\_args

Read command-line arguments; in particular, determine input file (name or extension).

subroutine spec

This is the main "driver" for the physics part of SPEC.

subroutine final\_diagnostics

Final diagnostics.

· subroutine ending

Closes output files, writes screen summary.

## 8.42.1 Detailed Description

Main program.

#### 8.42.2 Function/Subroutine Documentation

```
8.42.2.1 spec_main() program spec_main
```

Main program of SPEC.

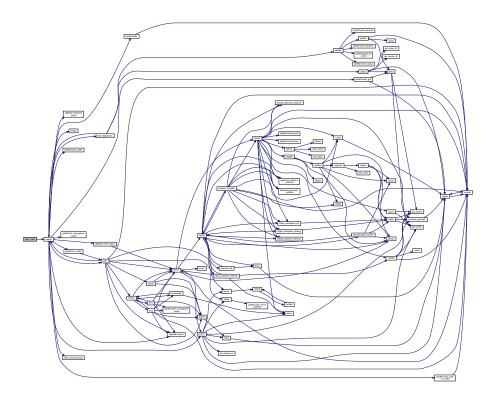
This only calls the xpech() subroutine to do a stand-alone SPEC run.

Returns

none

References xspech().

Here is the call graph for this function:



## 8.42.2.2 xspech() subroutine xspech

Main subroutine of SPEC.

This orchestrates a stand-alone SPEC run:

- · read the input file
- solve the MRxMHD equilibrium (see spec())
- run some diagnostics on the results
- write the output file(s)

## reading input, allocating global variables

- The input namelists and geometry are read in via a call to readin() . A full description of the required input is given in global.f90 .
- Most internal variables, global memory etc., are allocated in preset() .
- All quantities in the input file are mirrored into the output file's group  $/ { input}$  .

## preparing output file group iterations

• The group /iterations is created in the output file. This group contains the interface geometry at each iteration, which is useful for constructing movies illustrating the convergence. The data structure in use is an unlimited array of the following compound datatype:

```
DATATYPE H5T_COMPOUND {
   H5T_NATIVE_INTEGER "nDcalls";
   H5T_NATIVE_DOUBLE "Energy";
   H5T_NATIVE_DOUBLE "ForceErr";
   H5T_ARRAY { [Mvol+1] [mn] H5T_NATIVE_DOUBLE } "iRbc";
   H5T_ARRAY { [Mvol+1] [mn] H5T_NATIVE_DOUBLE } "iZbs";
   H5T_ARRAY { [Mvol+1] [mn] H5T_NATIVE_DOUBLE } "iRbs";
   H5T_ARRAY { [Mvol+1] [mn] H5T_NATIVE_DOUBLE } "iZbc";
}
```

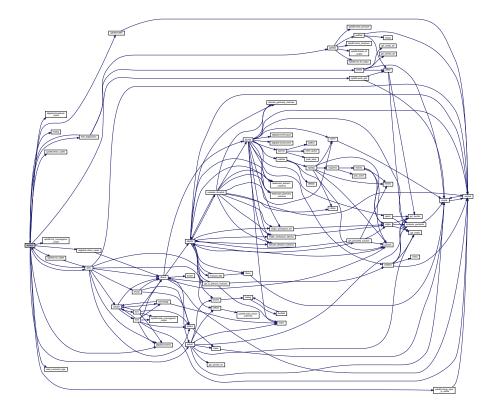
#### restart files

wrtend() is called to write the restart files.

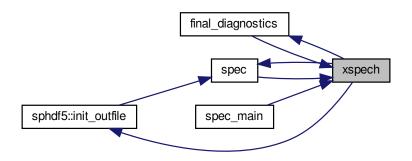
References allglobal::broadcast\_inputs(), allglobal::check\_inputs(), allglobal::cpus, ending(), final\_diagnostics(), sphdf5::finish\_outfile(), sphdf5::init\_convergence\_output(), sphdf5::init\_outfile(), numerical::machprec, sphdf5::mirror\_input\_to\_outfile(), allglobal::mpi\_comm\_spec, allglobal::myid, allglobal::ncpu, fileunits ::ounit, preset(), read\_command\_args(), numerical::small, spec(), numerical::vsmall, sphdf5::write\_grid(), and allglobal::wrtend().

Referenced by final diagnostics(), spec(), and spec main().

Here is the call graph for this function:



Here is the caller graph for this function:



# **8.42.2.3 read\_command\_args()** subroutine read\_command\_args

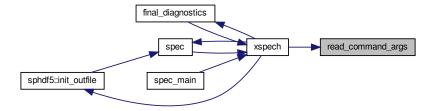
Read command-line arguments; in particular, determine input file (name or extension).

- The input file name, ext, is given as the first command line input, and the input file itself is then ext.sp.
- Alternatively, you can directly specify the input file itself as  ${\tt ext.sp}$  .
- Additional command line inputs recognized are:
  - help or -h will give help information to user
  - -readin will immediately set Wreadin=T; this may be over-ruled when the namelist screenlist is read

 $References\ all global:: mpi\_comm\_spec,\ all global:: myid,\ file units:: ounit,\ and\ input list:: wreadin.$ 

Referenced by xspech().

Here is the caller graph for this function:



8.42.2.4 spec() subroutine spec

This is the main "driver" for the physics part of SPEC.

Picard iterations are performed (if in free-boundary mode) and within each Picard iteration, the fixed-boundary problem is solved (also iteratively). **packing geometrical degrees-of-freedom into vector** 

• If NGdof.gt.0, where NGdof counts the geometrical degrees-of-freedom, i.e. the  $R_{bc}$ ,  $Z_{bs}$ , etc., then packxi() is called to "pack" the geometrical degrees-of-freedom into position (0:NGdof).

#### initialize adiabatic constants

• If Ladiabatic.eq.0, then the "adiabatic constants" in each region,  $P_v$ , are calculated as

$$P_v \equiv p_v V_v^{\gamma},\tag{262}$$

where  $p_v \equiv \texttt{pressure}$  (vvol) , the volume  $V_v$  of each region is computed by volume() , and the adiabatic index  $\gamma \equiv \texttt{gamma}$  .

#### solving force-balance

- If there are geometrical degress of freedom, i.e. if NGdof.gt.0, then
  - Todo If Lminimize.eq.1, call pc00aa() to find minimum of energy functional using quasi-Newton, preconditioned conjugate gradient method, E04DGF
  - If Lfindzero.gt.0, call newton() to find extremum of constrained energy functional using a Newton method, C05PDF.

# post diagnostics

- The pressure is computed from the adiabatic constants from Eqn. (262), i.e.  $p = P/V^{\gamma}$ .
- The Beltrami/vacuum fields in each region are re-calculated using dforce() .
- If Lcheck.eq.5.or. LHevalues.or. LHevectors.or. Lperturbed.eq.1, then the force-gradient matrix is examined using hesian().

## free-boundary: re-computing normal field

- If Lfreebound.eq.1 and Lfindzero.gt.0 and mfreeits.ne.0, then the magnetic field at the computational boundary produced by the plasma currents is computed using bnorml().
- The "new" magnetic field at the computational boundary produced by the plasma currents is updated using a Picard scheme:

$$\operatorname{Bns}_{i}^{j} = \lambda \operatorname{Bns}_{i}^{j-1} + (1 - \lambda) \operatorname{Bns}_{i}, \tag{263}$$

where j labels free-boundary iterations, the "blending parameter" is  $\lambda \equiv \mathtt{gBnbld}$ , and  $\mathtt{Bns}_i$  is computed by virtual casing. The subscript "\$i\$" labels Fourier harmonics.

• If the new (unblended) normal field is *not* sufficiently close to the old normal field, as quantified by gBntol, then the free-boundary iterations continue. This is quantified by

$$\sum_{i} |\operatorname{Bns}_{i}^{j-1} - \operatorname{Bns}_{i}|/N, \tag{264}$$

where N is the total number of Fourier harmonics.

- There are several choices that are available:
  - if mfreeits=-2: the vacuum magnetic field (really, the normal component of the field produced by the external currents at the computational boundary) required to hold the given equlibrium is written to file. This information is required as input by FOCUS [8] for example. (This option probably needs to revised.)
  - if mfreeits=-1: after the plasma field is computed by virtual casing, the vacuum magnetic field is set to exactly balance the plasma field (again, we are really talking about the normal component at the computational boundary.) This will ensure that the computational boundary itself if a flux surface of the total magnetic field.
  - if mfreeits=0: the plasma field at the computational boundary is not updated; no "free-boundary" iterations take place.
  - if mfreeits>0: the plasma field at the computational boundary is updated according to the above blending Eqn. (263), and the free-boundary iterations will continue until either the tolerance condition is met (see gBntol and Eqn. (264)) or the maximum number of free-boundary iterations, namely mfreeits, is reached. For this case, Lzerovac is relevant: if Lzerovac=1, then the vacuum field is set equal to the normal field at every iteration, which results in the computational boundary being a flux surface. (I am not sure if this is identical to setting mfreeits=-1; the logic etc. needs to be revised.)

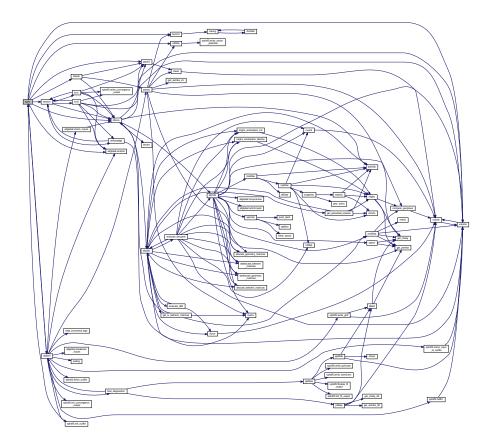
### output files: vector potential

• The vector potential is written to file using ra00aa().

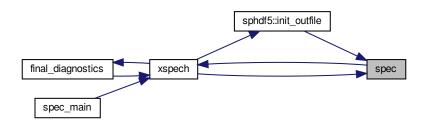
References inputlist::adiabatic, allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::bbe, allglobal::bbe, allglobal::bbe, bnorml(), allglobal::cfmn, allglobal::cpus, dforce(), allglobal::dpflux, allglobal::dfflux, allglobal::efmn, allglobal::forceerr, inputlist::gamma, inputlist::gbnbld, inputlist::gbntol, inputlist::helicity, hesian(), allglobal::ibnc, allglobal::ibns, inputlist::igeometry, allglobal::iie, allglobal::iio, allglobal::im, allglobal::imagneticok, allglobal::ibns, inputlist::isurf, allglobal::ivns, inputlist::ivolume, allglobal::izbc, allglobal::izbc, allglobal::izbs, inputlist::ladiabatic, inputlist::ladiabatic, inputlist::ladiabatic, inputlist::lfreebound, allglobal::lgdof, inputlist::lhevalues, inputlist::lhevalues, inputlist::lhevalues, inputlist::lrad, fileunits::lunit, allglobal::lvacuumregion, inputlist::lzerovac, inputlist::mfreeits, allglobal::mn, inputlist::mu, constants::mu0, allglobal::myid, allglobal::ncpu, newton(), inputlist::nfp, allglobal::ngdof, allglobal::notstellsym, inputlist::nppts, inputlist::nptrj, allglobal::ntz, inputlist::nvol, inputlist::odetol, allglobal::ofmn, constants::one, fileunits::ounit, packxi(), inputlist::pflux, inputlist::phiedge, constants::pi2, inputlist::pressure, inputlist::pscale, ra00aa(), inputlist::rbc, inputlist::rbs, allglobal::sfmn, inputlist::tflux, inputlist::vcasingtol, volume(), numerical::vsmall, allglobal::vvolume, inputlist::wmacros, allglobal::wrtend(), xspech(), allglobal::yesstellsym, inputlist::zbc, inputlist::zbs, and constants::zero.

Referenced by sphdf5::init\_outfile(), and xspech().

Here is the call graph for this function:



Here is the caller graph for this function:



# **8.42.2.5** final\_diagnostics() subroutine final\_diagnostics

Final diagnostics.

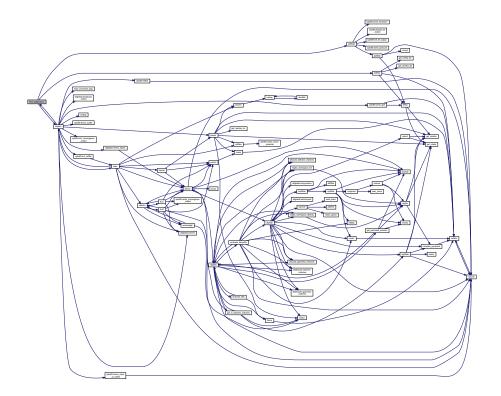
• sc00aa() is called to compute the covariant components of the magnetic field at the interfaces; these are related to the singular currents

- if Lcheck=1, jo00aa() is called to compute the error in the Beltrami equation
- pp00aa() is called to construct the Poincare plot by field-line following.

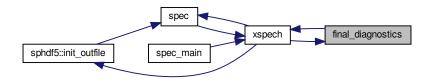
References allglobal::beltramierror, allglobal::btemn, allglobal::btemn, allglobal::bzemn, allglobal::bzemn, allglobal::bzemn, allglobal::bzemn, allglobal::bzemn, allglobal::bzemn, allglobal::bzemn, allglobal::imagneticok, allglobal::iquad, inputlist::isurf, inputlist::ivolume, jo00aa(), inputlist::lcheck, allglobal::lcoordinatesingularity, allglobal::lplasmaregion, allglobal::lvacuumregion, allglobal::mn, allglobal::mpi\_comm\_spec, inputlist::mpt, allglobal::mtz, inputlist::nvol, inputlist::odetol, allglobal::ofmn, fileunits::ounit, pp00aa(), allglobal::sfmn, inputlist::wmacros, xspech(), and constants::zero.

Referenced by xspech().

Here is the call graph for this function:



Here is the caller graph for this function:



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# References

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