SPEC

3.10

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1 The Stepped Pressure Equilibrium Code

A PDF version of this manual is available: `SPEC_manual.pdf`

- `Github pages`
- `Subroutine documentations`
- `SPEC on PPPL Theory Dept.`
- `MRxMHD website`

2 Compilation hints for SPEC

In order to run SPEC, you need a copy of the HDF5 libraries installed which has both the Fortran interface and the parallel (MPI I/O) enabled.

2.1 Mac

See e.g. this document for more detailed instructions: `https://support.hdfgroup.org/ftp/↩ HDF5/current/src/unpacked/release_docs/INSTALL_CMake.txt`

In short:

1. download `hdf5-1.10.5.tar.gz` from `https://www.hdfgroup.org/downloads/hdf5/source-code/`
2. extract

```
tar xzf hdf5-1.10.5.tar.gz
```

1. cd into source folder

```
cd hdf5-1.10.5
```

1. make a build folder

```
mkdir build
```

1. cd into build folder

```
cd build
```

1. run cmake with options for parallel support and Fortran interface (parallel support and C++ interface are not compatible; so we have to disable the C++ interface)

```
cmake -DHDF5_BUILD_FORTRAN:BOOL=ON -DHDF5_ENABLE_PARALLEL:BOOL=ON -DHDF5_↩
BUILD_CPP_LIB:BOLL=OFF ..
```

1. actually build the HDF5 library

```
make
```

This should leave you with a file "hdf5-1.10.5.dmg" or similar, which you can install just as any other Mac application. During the build process of SPEC, you then only need to specify the HDF5 folder in the Makefile, which will likely be `/Applications/HDF_Group/HDF5/1.10.5`.

3 Manual / Documentation

3.1 Poloidal flux and rotational transform

Given the canonical integrable form, $\mathbf{A} = \psi\nabla\theta - \chi(\psi)\nabla\zeta$, we can derive $\mathbf{B} = \nabla\psi\times\nabla\theta + \nabla\zeta\times\nabla\psi\ \chi'$. The poloidal flux is given by

$$\Psi_p = \int\int \mathbf{B}\cdot\mathbf{e}_\zeta\times\mathbf{e}_\psi\ d\zeta d\psi = 2\pi\int\chi' d\psi. \tag{1}$$

The rotational-transform is

$$\iota\!\!\!- = \frac{\mathbf{B}\cdot\nabla\theta}{\mathbf{B}\cdot\nabla\zeta} = \chi'. \tag{2}$$

The rotational-transform has the same sign as the poloidal flux.

The SPEC representation for the magnetic vector potential is

$$\mathbf{A} = A_\theta\nabla\theta + A_\zeta\nabla\zeta, \tag{3}$$

where we can see that $A_\zeta = -\chi$. The poloidal flux is

$$\int \mathbf{B}\cdot d\mathbf{s} = \oint A_\zeta d\zeta. \tag{4}$$

It would seem that the rotational-transform has opposite sign to A_ζ. To be honest, I am a little confused regarding the sign.

3.2 Outline

This document is intended to organise the different potentially valuable improvements to the SPEC code, which could make it more robust, faster, and increase its capabilities.

The document is divided in two categories:

Numerical Improvements : independent improvements that are of numerical importance but have no added physics value *per se*, although they may allow new or better physics investigations.

Physics Applications : research topics that could be addressed with the code, either in its present form or after the completion of one or more topics listed in Numerical Improvements .

3.3 Numerical Improvements

3.3.1 Compile code with GCC for error checking

Has been implemented in Makefile for most platforms. Checks against Intel version show small differences on the order of 10^{-15} relative deviation, which are likely due so slighly different optimization strategies.

3.3.2 Profile code with gprof to find inefficient lines of code

3.3.3 Run code with Valgrind to identify memory leaks

3.3.4 De-NAG-ification

Compilation of SPEC does not rely on NAG anymore; some functionality (e.g. SQP in ma02aa.f90) might need replacements for the NAG routines to be re-enabled.

3.3.5 Revision of spectral-constraints

This is bit of a mess. All the mathematics is standard, and all that is required is for someone to calmly go through lots of algebra. This task should be high priority, as SRH suspects that the spectral constraints as presently enforced result in an ill-conditioned force vector, which means that the code is overly sensitive to the initial guess and does not converge robustly. Potential speed improvements are tremendous.

3.3.6 Extension to arbitrary toroidal angle

This can further reduce the required Fourier resolution, and so this can reduce the computation. SRH is particularly interested in this as it will allow for exotic configurations (knots, figure-8, etc.) that cannot presently be computed.

3.3.7 Exploit symmetry of the metric

This is easy, but somewhat tedious. Take a look at ma00aa() to see what is required. Potential speed improvement is considerable.

3.3.8 symmetry of "local" Beltrami matrices

This is easy. Take a look at matrix(), which constructs the Beltrami matrices, and mp00ac(), which performs the inversion. Potential speed improvement is considerable.

3.3.9 Exploit block tri-diagonal structure of "global" linearized force balance matrix

This requires an efficient subroutine. SRH believes that Hirshman constructed such a routine (Hirshman et al. (2010) [4]). The potential speed improvement is tremendous. See newton() for where the tri-diagonal, linearized force-balance matrix is inverted.

3.3.10 Enforce Helicity constraint

This will allow investigation of different, arguably more-physical classes of equilibria. See ma02aa() .

3.3.11 Establish test-cases

A suite of test cases should be constructed, with different geometries etc., that run fast, and that can be benchmarked to machine precision. In the InputFiles/TestCases directory, some input files for SPEC are available for this purpose. One should write routines which execute these input files and compare the output data against a publicy-available set of output files to check SPEC before a new release is made.

3.3.12 Verify free-boundary

This is almost complete. The corresponding publication is being written. The virtual casing routines need to be investigated and made more efficient. The virtual casing routine in slab geometry needs revision (because of an integral over an infinite domain).

3.3.13 Enforcement of toroidal current profile

Adjust μ's, fluxes and/or rotational transform to obtain desired current profile (without singular currents). This is implemented and needs to be merged into the master branch. An additional routine is required to iterate on the helicity multipliers etc. as required *after* the local Beltrami fields have been calculated and *before* the global force balance iterations proceed.

3.3.14 Interpret eigenvectors and eigenvalues of Hessian

This is already completed: see hesian(). However, this actually computes the force gradient matrix. For toroidal geometry there is a complication; namely that the hessian matrix includes the derivatives of the spectral constraints. For Cartesian geometry, it is ready to go. SRH will begin writing a paper on the stability of slab MRxMHD equilibria.

3.4 Physics Applications

3.4.1 Calculate high-resolution equilibria, e.g. W7-X

requires: Exploit symmetry of the metric , symmetry of "local" Beltrami matrices , and other improvements that can make the code faster at high Fourier resolution

3.4.2 Calculate equilibria by conserving helicity and fluxes

Applications to saturated island studies, sawteeth, etc. requires: Calculate equilibria by conserving helicity and fluxes

3.4.3 Calculate free-boundary stellarator equilibria

to predict scrape-off-layer (SOL) topologies and β-limits. requires: Verify free-boundary Mostly complete.

3.4.4 Evaluate stability of MRxMHD equilibria

perhaps starting from simplest system (slab tearing). requires: Interpret eigenvectors and eigenvalues of Hessian

3.5 Revision of coordinate singularity: axisymmetric; polar coordinates

- Consider a general, magnetic vector potential given in Cartesian coordinates,

$$\mathbf{A} = A_x \nabla x + A_y \nabla y + A_z \nabla z + \nabla g \tag{5}$$

where A_x, A_y, A_z, and the as-yet-arbitrary gauge function, g, are regular at $(x, y) = (0, 0)$, i.e. they can be expanded as a Taylor series, e.g.

$$A_x = \sum_{i,j} \alpha_{i,j} x^i y^j, \qquad A_y = \sum_{i,j} \beta_{i,j} x^i y^j, \qquad A_z = \sum_{i,j} \gamma_{i,j} x^i y^j, \qquad g = \sum_{i,j} \delta_{i,j} x^i y^j, \tag{6}$$

for small x and small y.

- Note that we have restricted attention to the "axisymmetric" case, as there is no dependence on z.
- The "polar" coordinate transformation,

$$\begin{aligned} x &= r\cos\theta, \\ y &= r\sin\theta, \\ z &= \zeta, \end{aligned} \tag{7}$$

induces the vector transformation

$$\begin{array}{ccccccc} \nabla x & = & \cos\theta\,\nabla r & - & r\sin\theta\,\nabla\theta & & , \\ \nabla y & = & \sin\theta\,\nabla r & + & r\cos\theta\,\nabla\theta & & , \\ \nabla z & = & & & & \nabla\zeta & . \end{array} \tag{8}$$

- By repeated applications of the double-angle formula, the expressions for A_x, A_y and g can be cast as functions of (r, θ),

$$A_x = \sum_m r^m [a_{m,0} + a_{m,1}\, r^2 + a_{m,2}\, r^4 + ...] \sin(m\theta), \tag{9}$$

$$A_y = \sum_m r^m [b_{m,0} + b_{m,1}\, r^2 + b_{m,2}\, r^4 + ...] \cos(m\theta), \tag{10}$$

$$A_z = \sum_m r^m [c_{m,0} + c_{m,1}\, r^2 + c_{m,2}\, r^4 + ...] \cos(m\theta), \tag{11}$$

$$g = \sum_m r^m [g_{m,0} + g_{m,1}\, r^2 + g_{m,2}\, r^4 + ...] \sin(m\theta), \tag{12}$$

where attention is restricted to stellarator symmetric geometry, but similar expressions hold for the non-stellarator symmetric terms.

- Collecting these expressions, the vector potential can be expressed

$$\mathbf{A} = A_r \nabla r + A_\theta \nabla\theta + A_\zeta \nabla\zeta + \partial_r g\, \nabla r + \partial_\theta g\, \nabla\theta, \tag{13}$$

where

$$\begin{array}{cclcccccccccc} A_r & = & r^0 & [& (& & & b_{0,0} & + & g_{1,0} &) & + & (...)r^2 + (...)r^4 + ... &] & \sin\theta \\ & + & r^1 & [& (& a_{1,0}/2 & + & b_{1,0}/2 & + & 2g_{2,0} &) & + & (...)r^2 + (...)r^4 + ... &] & \sin 2\theta \\ & + & r^2 & [& (& a_{2,0}/2 & + & b_{2,0}/2 & + & 3g_{3,0} &) & + & (...)r^2 + (...)r^4 + ... &] & \sin 3\theta \\ & + & ... \end{array} \tag{14}$$

(Note: Mathematica was used to perform the algebraic manipulations, and the relevant notebook was included as part of the SPEC CVS repository.)

- There is precisely enough gauge freedom so that we may choose $A_r = 0$. For example, the choice

$$\begin{array}{rclcccccccc} g_{1,0} & = & - & & & & b_{0,0} & & & & , \\ g_{2,0} & = & - & (& a_{1,0}/2 & + & b_{1,0}/2 &) & / & 2 & , \\ g_{3,0} & = & - & (& a_{2,0}/2 & + & b_{2,0}/2 &) & / & 3 & , \\ \ldots & = & \ldots & & & & & & & & \end{array} \tag{15}$$

eliminates the lowest order r dependence in each harmonic.

- By working through the algebra (again, using Mathematica) the expressions for A_θ and A_ζ become

$$A_\theta = r^2 f_0(\rho) + r^3 f_1(\rho)\cos(\theta) + r^4 f_2(\rho)\cos(2\theta) + r^5 f_3(\rho)\cos(3\theta) + \ldots \tag{16}$$
$$A_\zeta = g_0(\rho) + r^1 g_1(\rho)\cos(\theta) + r^2 g_2(\rho)\cos(2\theta) + r^3 g_3(\rho)\cos(3\theta) + \ldots \tag{17}$$

where $\rho \equiv r^2$ and the $f_m(\rho)$ and $g_m(\rho)$ are abitrary polynomials in ρ. [The expression for A_ζ is unchanged from Eqn. (11).]

3.5.1 somewhat generally, ...

- For stellarator-symmetric configurations,

$$\mathbf{A} = \sum_{m,n} A_{\theta,m,n}\cos(m\theta - n\zeta)\nabla\theta + \sum_{m,n} A_{\zeta,m,n}\cos(m\theta - n\zeta)\nabla\zeta, \tag{18}$$

where now the dependence on ζ is included, and the angles are arbitrary.

- The near-origin behaviour of A_θ and A_ζ given in Eqn. (16) and Eqn. (17) are flippantly generalized to

$$A_{\theta,m,n} = r^{m+2} f_{m,n}(\rho), \tag{19}$$
$$A_{\zeta,m,n} = r^{m} \; g_{m,n}(\rho), \tag{20}$$

where the $f_{m,n}(\rho)$ and $g_{m,n}(\rho)$ are arbitrary polynomials in ρ.

- Additional gauge freedom can be exploited: including an additional gauge term ∇h where h only depends on ζ, e.g.

$$h(\zeta) = h_{0,0}\,\zeta + \sum h_{0,n}\sin(-n\zeta), \tag{21}$$

does not change the magnetic field and does not change any of the above discussion.

- The representation for the $A_{\theta,m,n}$ does not change, but we must clarify that Eqn. (20) holds for only the $m \neq 0$ harmonics:

$$A_{\zeta,m,n} = r^m \; g_{m,n}(\rho), \quad \text{for} \quad m \neq 0. \tag{22}$$

- For the $m = 0$, $n \neq 0$ harmonics of A_ζ, including the additional gauge gives $A_{\zeta,0,n} = g_{0,n}(\rho) + n\,h_{0,n}$. Recall that $g_{0,n}(\rho) = g_{0,n,0} + g_{0,n,1}\rho + g_{0,n,2}\rho^2 + \ldots$, and we can choose $h_{0,n} = -g_{0,n,0}/n$ to obtain

$$A_{\zeta,m,n} = r^m \; g_{m,n}(\rho), \quad \text{for} \;\; m = 0, n \neq 0, \;\; \text{with} \;\; g_{m,n}(0) = 0. \tag{23}$$

- For the $m = 0$, $n = 0$ harmonic of A_ζ, we have $A_{\zeta,0,0} = g_{0,0}(\rho) + h_{0,0}$. Similarly, choose $h_{0,0} = -g_{0,n,0}$ to obtain

$$A_{\zeta,m,m} = r^m \; g_{m,n}(\rho), \quad \text{for} \;\; m = 0, n = 0, \;\; \text{with} \;\; g_{m,n}(0) = 0. \tag{24}$$

- To simplify the algorithmic implementation of these conditions, we shall introduce a "regularization" factor, $\rho^{m/2} = r^m$.

- Note that the representation for $A_{\theta,m,n}$ given in Eqn. (19), with an arbitrary polynomial $f_{m,n}(\rho) = f_{m,n,0} + f_{m,n,1}\rho + f_{m,n,2}\rho^2 + \ldots$, is equivalent to $A_{\theta,m,n} = \rho^{m/2}\alpha_{m,n}(\rho)$ where $\alpha_{m,n}(\rho)$ is an arbitrary polynomial with the constraint $\alpha_{m,n}(0) = 0$.

- We can write the vector potential as

$$A_{\theta,m,n} = \rho^{m/2}\alpha_{m,n}(\rho), \quad \text{with} \;\; \alpha_{m,n}(0) = 0 \;\; \text{for all} \;\; (m,n), \tag{25}$$
$$A_{\zeta,m,n} = \rho^{m/2}\beta_{m,n}(\rho), \quad \text{with} \;\; \beta_{m,n}(0) = 0 \;\; \text{for} \;\; m = 0. \tag{26}$$

3.5.2 non-stellarator symmetric terms

- Just guessing, for the non-stellarator-symmetric configurations,

$$A_{\theta,m,n} = \rho^{m/2}\alpha_{m,n}(\rho), \quad \text{with } \alpha_{m,n}(0) = 0 \text{ for all } (m,n), \tag{27}$$
$$A_{\zeta,m,n} = \rho^{m/2}\beta_{m,n}(\rho), \quad \text{with } \beta_{m,n}(0) = 0 \text{ for } m = 0. \tag{28}$$

4 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 (lvol, mn, Nt, Nz, iflag, ldItGp)

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 (lvol, NN)

If `Lconstraint` = 2, then $\mu = \boldsymbol{\mu}_1$ is varied in order to satisfy the helicity constraint, and $\Delta\psi_p = \boldsymbol{\mu}_2$ 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 (lvol, stz, RpZ)

Please see co01aa() for documentation.

5 Module Index

5.1 Modules

Here is a list of all modules:

6 Data Type Index

6.1 Data Types List

Here are the data types with brief descriptions:

7 File Index

7.1 File List

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

8 Module Documentation

8.1 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 (lvol, Ntz, lquad, 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 (lvol, sti, Nz, nPpts, poincaredata, fittedtransform, utflag)

  Constructs Poincaré plot and "approximate" rotational-transform (for single field line).
- subroutine stzxyz (lvol, stz, RpZ)

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

8.1.1 Detailed Description

8.1.2 Function/Subroutine Documentation

8.1.2.1 bfield()

```
subroutine bfield (
        real, intent(in) zeta,
        real, dimension(1:node), intent(in) st,
        real, dimension(1:node), intent(out) Bst )
```

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.

$$\dot{s} \equiv \frac{B^s}{B^\zeta}, \qquad \dot{\theta} \equiv \frac{B^\theta}{B^\zeta}. \tag{29}$$

Representation of magnetic field

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

$$A_\theta(s,\theta,\zeta) = \sum_{i,l} A_{\theta,e,i,l}\, \overline{T}_{l,i}(s) \cos\alpha_i + \sum_{i,l} A_{\theta,o,i,l}\, \overline{T}_{l,i}(s) \sin\alpha_i, \tag{30}$$

$$A_\zeta(s,\theta,\zeta) = \sum_{i,l} A_{\zeta,e,i,l}\, \overline{T}_{l,i}(s) \cos\alpha_i + \sum_{i,l} A_{\zeta,o,i,l}\, \overline{T}_{l,i}(s) \sin\alpha_i, \tag{31}$$

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

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

$$\begin{array}{ccl}\sqrt{g}\,\mathbf{B} & = & \mathbf{e}_s \sum_{i,l}[(-m_i A_{\zeta,e,i,l} - n_i A_{\theta,e,i,l})\overline{T}_{l,i} \sin\alpha_i + (+m_i A_{\zeta,o,i,l} + n_i A_{\theta,o,i,l})\overline{T}_{l,i} \cos\alpha_i] \\ & + & \mathbf{e}_\theta \sum_{i,l}[(- A_{\zeta,e,i,l})\overline{T}'_{l,i} \cos\alpha_i + (- A_{\zeta,o,i,l})\overline{T}'_{l,i} \sin\alpha_i] \\ & + & \mathbf{e}_\zeta \sum_{i,l}[(A_{\theta,e,i,l})\overline{T}'_{l,i} \cos\alpha_i + (A_{\theta,o,i,l})\overline{T}'_{l,i} \sin\alpha_i]\end{array} \tag{32}$$

- In Eqn. (29) , 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.

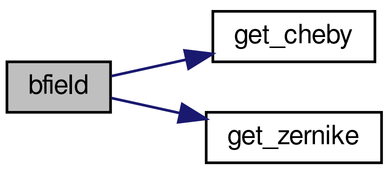
Parameters

in	*zeta*	toroidal angle ζ
in	*st*	radial coordinate s and poloidal angle θ
out	*Bst*	tangential magnetic field directions B_s, B_θ

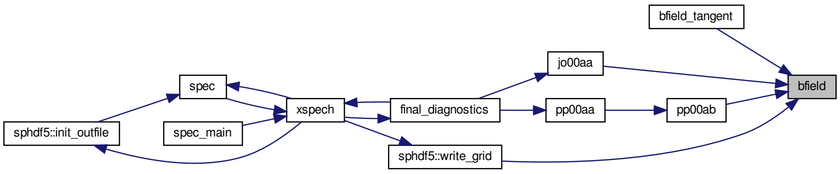
References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::cpus, allglobal::gbzeta, get_←cheby(), get_zernike(), constants::half, allglobal::halfmm, allglobal::im, allglobal::in, allglobal::ivol, allglobal←::lcoordinatesingularity, inputlist::lrad, allglobal::mn, allglobal::mpi_comm_spec, inputlist::mpol, allglobal←::myid, allglobal::ncpu, allglobal::node, allglobal::notstellsym, constants::one, fileunits::ounit, 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:



8.1.2.2 hesian()

```
subroutine hesian (
        integer, intent(in) NGdof,
        real, dimension(0:ngdof) position,
        integer, intent(in) Mvol,
        integer, intent(in) mn,
        integer, intent(in) LGdof )
```

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

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, μ, 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:

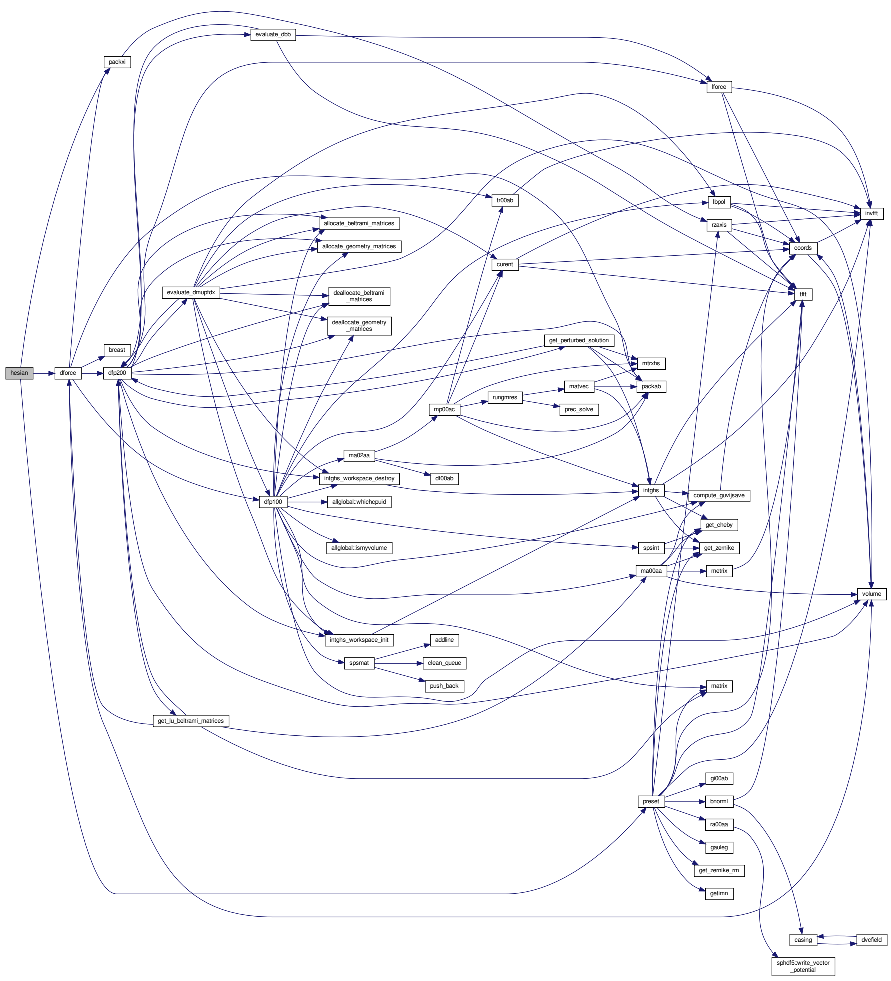
```
open(hunit,file="."//trim(ext)//".GF.ev",status="unknown",form="unformatted")
write(hunit)ngdof,ldvr,ldvi          ! integers; if only the eigenvalues were computed then Ldvr=Ldvi=1;
write(hunit)evalr(1:ngdof)           ! reals    ; real      part of eigenvalues;
write(hunit)evali(1:ngdof)      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

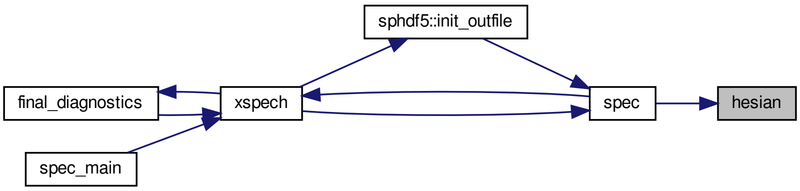
References allglobal::cpus, allglobal::dbbdmp, allglobal::dbbdrz, allglobal::dessian, allglobal::dffdrz, dforce(), allglobal::dmupfdx, inputlist::dpp, inputlist::dqq, allglobal::drbc, allglobal::drbs, allglobal::dzbc, allglobal::dzbs, allglobal::energy, constants::half, inputlist::helicity, allglobal::hessian, fileunits::hunit, inputlist::igeometry, allglobal↩ ::im, allglobal::in, allglobal::irbc, allglobal::irbs, allglobal::izbc, allglobal::izbs, allglobal::lbbintegral, inputlist::lcheck, inputlist::lfindzero, inputlist::lfreebound, allglobal::lhessianallocated, inputlist::lhevalues, inputlist::lhevectors, inputlist::lhmatrix, allglobal::localconstraint, inputlist::lperturbed, allglobal::mpi_comm_spec, inputlist::mu, fileunits↩ ::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:



8.1.2.3 jo00aa()

```
subroutine jo00aa (
        integer, intent(in) lvol,
        integer, intent(in) Ntz,
        integer, intent(in) lquad,
        integer, intent(in) mn )
```

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, j $\equiv \nabla \times \nabla \times \mathbf{A}$

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

$$
\begin{aligned}
A_\theta(s,\theta,\zeta) &= \sum_{i,l} A_{\theta,e,i,l}\, \overline{T}_{l,i}(s) \cos\alpha_i + \sum_{i,l} A_{\theta,o,i,l}\, \overline{T}_{l,i}(s) \sin\alpha_i, && (33)\\
A_\zeta(s,\theta,\zeta) &= \sum_{i,l} A_{\zeta,e,i,l}\, \overline{T}_{l,i}(s) \cos\alpha_i + \sum_{i,l} A_{\zeta,o,i,l}\, \overline{T}_{l,i}(s) \sin\alpha_i, && (34)
\end{aligned}
$$

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

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

$$
\begin{array}{rcll}
\sqrt{g}\,\mathbf{B} & = & \mathbf{e}_s & \sum_{i,l}[(-m_i A_{\zeta,e,i,l} - n_i A_{\theta,e,i,l})\overline{T}_{l,i} \sin\alpha_i + (+m_i A_{\zeta,o,i,l} + n_i A_{\theta,o,i,l})\overline{T}_{l,i} \cos\alpha_i] \\
& + & \mathbf{e}_\theta & \sum_{i,l}[(- A_{\zeta,e,i,l})\overline{T}'_{l,i} \cos\alpha_i + (- A_{\zeta,o,i,l})\overline{T}'_{l,i} \sin\alpha_i] \\
& + & \mathbf{e}_\zeta & \sum_{i,l}[(A_{\theta,e,i,l})\overline{T}'_{l,i} \cos\alpha_i + (A_{\theta,o,i,l})\overline{T}'_{l,i} \sin\alpha_i]
\end{array} \quad (35)
$$

- The current is

$$
\sqrt{g}\,\mathbf{j} = (\partial_\theta B_\zeta - \partial_\zeta B_\theta)\,\mathbf{e}_s + (\partial_\zeta B_s - \partial_s B_\zeta)\,\mathbf{e}_\theta + (\partial_s B_\theta - \partial_\theta B_s)\,\mathbf{e}_\zeta, \quad (36)
$$

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

$$
\begin{aligned}
B_s &= (\sqrt{g}B^s)\, g_{ss}/\sqrt{g} + (\sqrt{g}B^\theta)\, g_{s\theta}/\sqrt{g} + (\sqrt{g}B^\zeta)\, g_{s\zeta}/\sqrt{g}, && (37)\\
B_\theta &= (\sqrt{g}B^s)\, g_{s\theta}/\sqrt{g} + (\sqrt{g}B^\theta)\, g_{\theta\theta}/\sqrt{g} + (\sqrt{g}B^\zeta)\, g_{\theta\zeta}/\sqrt{g}, && (38)\\
B_\zeta &= (\sqrt{g}B^s)\, g_{s\zeta}/\sqrt{g} + (\sqrt{g}B^\theta)\, g_{\theta\zeta}/\sqrt{g} + (\sqrt{g}B^\zeta)\, g_{\zeta\zeta}/\sqrt{g}. && (39)
\end{aligned}
$$

quantification of the error

- The measures of the error are

$$
\begin{aligned}
||\,(\mathbf{j}-\mu\mathbf{B})\cdot\nabla s|| &\equiv \int ds \oint\!\!\oint d\theta d\zeta \;\; |\sqrt{g}\,\mathbf{j}\cdot\nabla s-\mu\,\sqrt{g}\,\mathbf{B}\cdot\nabla s|\,, && (40)\\
||\,(\mathbf{j}-\mu\mathbf{B})\cdot\nabla \theta|| &\equiv \int ds \oint\!\!\oint d\theta d\zeta \;\; |\sqrt{g}\,\mathbf{j}\cdot\nabla \theta-\mu\,\sqrt{g}\,\mathbf{B}\cdot\nabla \theta|\,, && (41)\\
||\,(\mathbf{j}-\mu\mathbf{B})\cdot\nabla \zeta|| &\equiv \int ds \oint\!\!\oint d\theta d\zeta \;\; |\sqrt{g}\,\mathbf{j}\cdot\nabla \zeta-\mu\,\sqrt{g}\,\mathbf{B}\cdot\nabla \zeta|\,. && (42)
\end{aligned}
$$

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. (41)?
- What is the predicted scaling of the error in the Chebyshev-Fourier representation scale with numerical resolution? Note that the predicted error scaling for E^s, E^θ and E^ζ may not be standard, as various radial derivatives are taken to compute the components of $\mathbf{j}$. (See for example the discussion in Sec.IV.C in Hudson et al. (2011) [5] , 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	*lvol*	in which volume should the Beltrami error be computed
in	*Ntz*	number of grid points in θ and ζ
in	*lquad*	degree of Gaussian quadrature
in	*mn*	number of Fourier harmonics

details of the numerics

- The integration over s is performed using Gaussian integration, e.g., $\displaystyle\int f(s)ds \approx \sum_k \omega_k f(s_k)$; with the abscissae, s_k, and the weights, ω_k, for $k=1,$ `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, $g_{\mu,\nu}\equiv$ `gij(1:6,0,1:Ntz)`, and the Jacobian, $\sqrt{g}\equiv$ `sg(0,1:Ntz)`, are calculated on a regular angular grid, (θ_i,ζ_j), in coords(). The derivatives $\partial_i g_{\mu,\nu}\equiv$ `gij(1:6,i,1`↩ `:Ntz)` and $\partial_i\sqrt{g}\equiv$ `sg(i,1:Ntz)`, with respect to $i\in\{s,\theta,\zeta\}$ are also returned.
  - The Fourier components of the vector potential given in Eqn. (33) and Eqn. (34), 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,θ,ζ), are computed on the regular angular grid (using FFTs).

- The following quantities are then computed on the regular angular grid

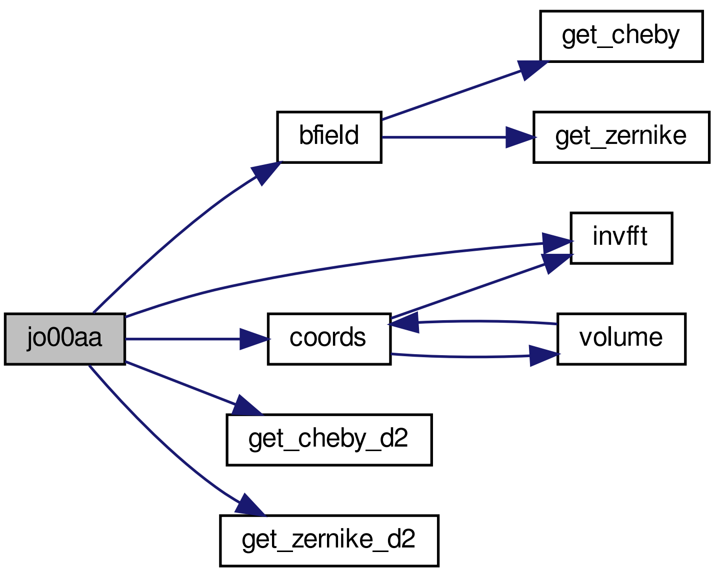
$$\begin{aligned}
\sqrt{g}j^s &= \sum_u \left[\partial_\theta(\sqrt{g}B^u)\; g_{u,\zeta} + (\sqrt{g}B^u)\; \partial_\theta g_{u,\zeta} - (\sqrt{g}B^u) g_{u,\zeta}\; \partial_\theta \sqrt{g}/\sqrt{g}\right] / \sqrt{g} \\
&- \sum_u \left[\partial_\zeta(\sqrt{g}B^u)\; g_{u,\theta} + (\sqrt{g}B^u)\; \partial_\zeta g_{u,\theta} - (\sqrt{g}B^u) g_{u,\theta}\; \partial_\zeta \sqrt{g}/\sqrt{g}\right] / \sqrt{g}, \qquad (43) \\
\sqrt{g}j^\theta &= \sum_u \left[\partial_\zeta(\sqrt{g}B^u)\; g_{u,s} + (\sqrt{g}B^u)\; \partial_\zeta g_{u,s} - (\sqrt{g}B^u) g_{u,s}\; \partial_\zeta \sqrt{g}/\sqrt{g}\right] / \sqrt{g} \\
&- \sum_u \left[\partial_s(\sqrt{g}B^u)\; g_{u,\zeta} + (\sqrt{g}B^u)\; \partial_s g_{u,\zeta} - (\sqrt{g}B^u) g_{u,\zeta}\; \partial_s \sqrt{g}/\sqrt{g}\right] / \sqrt{g}, \qquad (44) \\
\sqrt{g}j^\zeta &= \sum_u \left[\partial_s(\sqrt{g}B^u)\; g_{u,\theta} + (\sqrt{g}B^u)\; \partial_s g_{u,\theta} - (\sqrt{g}B^u) g_{u,\theta}\; \partial_s \sqrt{g}/\sqrt{g}\right] / \sqrt{g} \\
&- \sum_u \left[\partial_\theta(\sqrt{g}B^u)\; g_{u,s} + (\sqrt{g}B^u)\; \partial_\theta g_{u,s} - (\sqrt{g}B^u) g_{u,s}\; \partial_\theta \sqrt{g}/\sqrt{g}\right] / \sqrt{g}. \qquad (45)
\end{aligned}$$

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

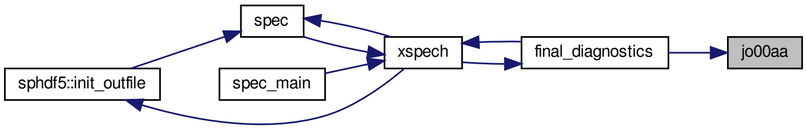
References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::beltramierror, bfield(), allglobal↩ ::cfmn, allglobal::cheby, coords(), allglobal::cpus, allglobal::dpflux, allglobal::dtflux, allglobal::efmn, allglobal::gbzeta, get_cheby_d2(), get_zernike_d2(), allglobal::guvij, constants::half, inputlist::igeometry, allglobal::im, allglobal::in, invfft(), 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::nz, 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:



8.1.2.4 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`

  - $\theta \equiv$ `data(1,k,j)` is the poloidal angle,
  - $s \equiv$ `data(2,k,j)` is the radial coordinate,
  - $R \equiv$ `data(3,k,j)` is the cylindrical R,
  - $Z \equiv$ `data(4,k,j)` is the cylindrical Z,
- The integer `k=0`,Nz-1 labels toroidal planes, so that $\phi = (2\pi/\mathtt{Nfp})(k/\mathtt{Nz})$,
- 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

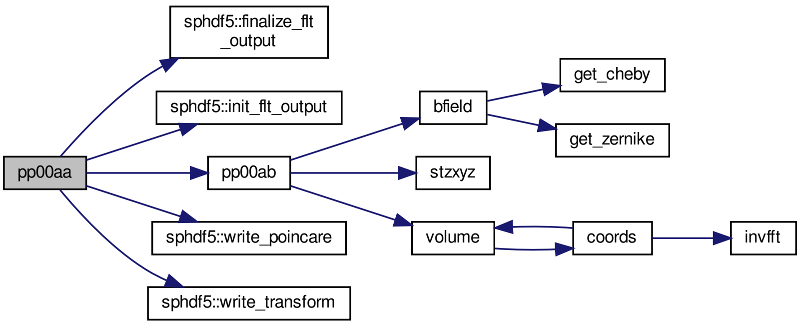
- The rotational-transform data is written to .ext.transform:xxxx , where `xxxx` is an integer indicating the volume. The format of this file is as follows:

```
open(lunit+myid,file="."//trim(ext)//".sp.t."//svol,status="unknown",form="unformatted")
write(lunit+myid) lnptrj-ioff+1                               ! integer
write(lunit+myid) diotadxup(0:1,0,lvol)                       ! doubles
write(lunit+myid) ( fiota(itrj,1:2), itrj = ioff, lnptrj ) ! doubles
close(lunit+myid)
```

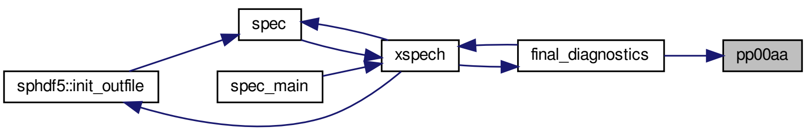
References allglobal::cpus, allglobal::diotadxup, sphdf5::finalize_flt_output(), constants::half, inputlist::igeometry, sphdf5::init_flt_output(), inputlist::iota, allglobal::ivol, inputlist::lconstraint, allglobal::lcoordinatesingularity, allglobal::lplasmaregion, inputlist::lrad, allglobal::lvacuumregion, 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:



8.1.2.5 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.

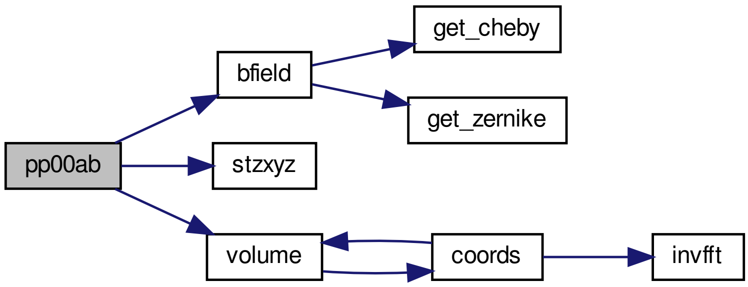
Parameters

in	*lvol*	
	sti	
in	*Nz*	
in	*nPpts*	
	poincaredata	
	fittedtransform	
out	*utflag*	

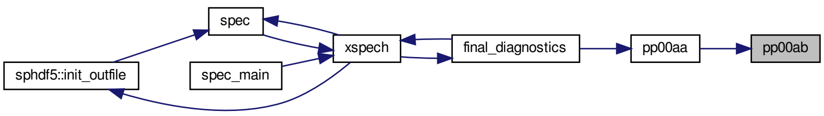
References bfield(), allglobal::cpus, allglobal::ivol, allglobal::mpi_comm_spec, allglobal::myid, allglobal::ncpu, allglobal::node, inputlist::nvol, inputlist::odetol, constants::one, fileunits::ounit, constants::pi2, numerical::small, stzxyz(), constants::two, volume(), and constants::zero.

Referenced by pp00aa().

Here is the call graph for this function:



Here is the caller graph for this function:



8.1.2.6 stzxyz()

```
subroutine stzxyz (
    integer, intent(in) lvol,
    real, dimension(1:3), intent(in) stz,
    real, dimension(1:3), intent(out) RpZ )
```

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

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

Parameters

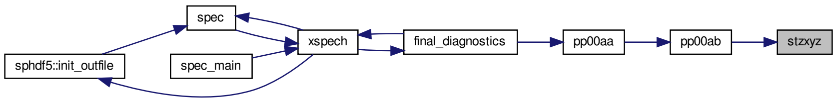
in	*lvol*	
in	*stz*	
out	*RpZ*	

References allglobal::cpus, constants::half, allglobal::halfmm, inputlist::igeometry, allglobal::im, allglobal::in, allglobal::irbc, allglobal::irbs, allglobal::izbc, allglobal::izbs, allglobal::lcoordinatesingularity, 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:



8.2 Free-Boundary Computation

Functions/Subroutines

- subroutine bnorml (mn, Ntz, efmn, ofmn)

    Computes $\mathbf{B}_{Plasma} \cdot \mathbf{e}_\theta \times \mathbf{e}_\zeta$ 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.

8.2.1 Detailed Description

8.2.2 Function/Subroutine Documentation

8.2.2.1 bnorml()

```
subroutine bnorml (
        integer, intent(in) mn,
        integer, intent(in) Ntz,
        real, dimension(1:mn), intent(out) efmn,
        real, dimension(1:mn), intent(out) ofmn )
```

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 compuational 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

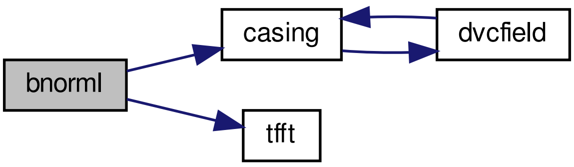
Parameters

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

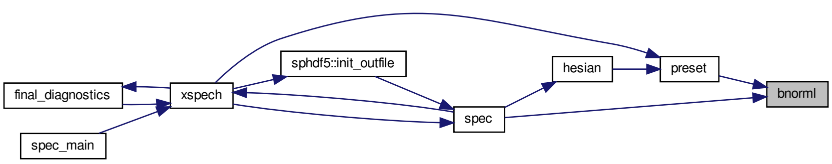
References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, casing(), allglobal::cfmn, allglobal::cpus, allglobal::dxyz, allglobal::globaljk, allglobal::gteta, allglobal::guvij, allglobal::gzeta, constants::half, inputlist::igeometry, allglobal::ijimag, allglobal::ijreal, allglobal::im, allglobal::in, 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, tfft(), 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:



8.2.2.2 casing()

```
subroutine casing (
    real, intent(in) teta,
    real, intent(in) zeta,
    real, intent(out) gBn,
    integer, intent(out) icasing )
```

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,

$$\mathbf{x}(\theta,\zeta) \equiv x(\theta,\zeta)\mathbf{i} + y(\theta,\zeta)\mathbf{j} + z(\theta,\zeta)\mathbf{k}, \tag{46}$$

  and the tangential field on this boundary,

$$\mathbf{B}_s = B^\theta \mathbf{e}_\theta + B^\zeta \mathbf{e}_\zeta, \tag{47}$$

  where θ and ζ 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) [8], Lazerson (2012) [6] 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,

$$\mathbf{j} = \mathbf{B}_s \times \mathbf{n}, \tag{48}$$

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

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

$$\mathbf{B}(\bar{\mathbf{x}}) = -\frac{1}{4\pi}\int_{\mathcal{S}} \frac{(\mathbf{B}_s \times d\mathbf{s})\times\hat{\mathbf{r}}}{r^2}, \tag{49}$$

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

- For ease of notation introduce

$$\mathbf{J} \equiv \mathbf{B}_s \times d\mathbf{s} = \alpha\,\mathbf{e}_\theta - \beta\,\mathbf{e}_\zeta, \tag{50}$$

  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 $\mathbf{J} = j_x\,\mathbf{i} + j_y\,\mathbf{j} + j_z\,\mathbf{k}$, where

$$j_x = \alpha\,x_\theta - \beta\,x_\zeta \tag{51}$$
$$j_y = \alpha\,y_\theta - \beta\,y_\zeta \tag{52}$$
$$j_z = \alpha\,z_\theta - \beta\,z_\zeta. \tag{53}$$

- Requiring that the current,

$$\mathbf{j} \equiv \nabla\times\mathbf{B} = \sqrt{g}^{-1}(\partial_\theta B_\zeta - \partial_\zeta B_\theta)\,\mathbf{e}_s + \sqrt{g}^{-1}(\partial_\zeta B_s - \partial_s B_\zeta)\,\mathbf{e}_\theta + \sqrt{g}^{-1}(\partial_s B_\theta - \partial_\theta B_s)\,\mathbf{e}_\zeta, \tag{54}$$

  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

$$\mathbf{r} \equiv r_x\,\mathbf{i} + r_y\,\mathbf{j} + r_z\,\mathbf{k} = (X-x)\,\mathbf{i} + (Y-y)\,\mathbf{j} + (Z-z)\,\mathbf{k}. \tag{55}$$

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

$$B^x = \oint\oint d\theta d\zeta \; (j_y r_z - j_z r_y)/r^3, \quad (56)$$

$$B^y = \oint\oint d\theta d\zeta \; (j_z r_x - j_x r_z)/r^3, \quad (57)$$

$$B^z = \oint\oint d\theta d\zeta \; (j_x r_y - j_y r_x)/r^3 \quad (58)$$

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

- When all is said and done, this routine calculates

$$\int_0^{2\pi}\int_0^{2\pi} \texttt{vcintegrand} \; d\theta d\zeta \quad (59)$$

for a given (X, Y, Z), where `vcintegrand` is given in Eqn. (61).

- 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 $\epsilon \equiv$`inputvar vcasingeps`. Let the "distance" be

$$D \equiv \sqrt{(X-x)^2 + (Y-y)^2 + (Z-Z)^2 + \epsilon^2}. \quad (60)$$

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

$$\texttt{vcintegrand} \equiv (B_x n_x + B_y n_y + B_z n_z)(1 + 3\epsilon^2/D^2)/D^3, \quad (61)$$

  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.

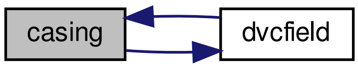
Parameters

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

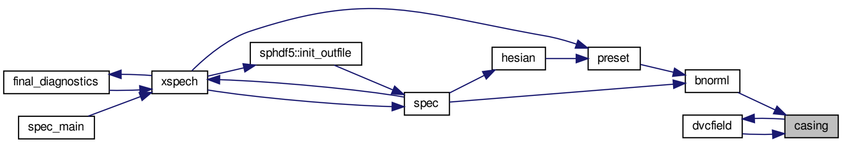
References allglobal::cpus, dvcfield(), allglobal::dxyz, allglobal::globaljk, allglobal::mpi_comm_spec, allglobal↩ ::myid, allglobal::ncpu, allglobal::nxyz, fileunits::ounit, constants::pi, constants::pi2, inputlist::vcasingits, inputlist↩ ::vcasingper, inputlist::vcasingtol, fileunits::vunit, inputlist::wmacros,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

Referenced by bnorml(), and dvcfield().

Here is the call graph for this function:



Here is the caller graph for this function:



8.2.2.3 dvcfield()

```
subroutine dvcfield (
        integer, intent(in) Ndim,
        real, dimension(1:ndim), intent(in) tz,
        integer, intent(in) Nfun,
        real, dimension(1:nfun), intent(out) vcintegrand )
```

Differential virtual casing integrand.

Differential virtual casing integrand

Parameters

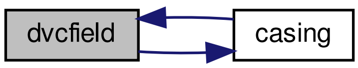
in	*Ndim*	number of parameters (==2)
in	*tz*	θ and ζ
in	*Nfun*	number of function values (==3)
out	*vcintegrand*	cartesian components of magnetic field

References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, casing(), allglobal::cpus, allglobal::dxyz, allglobal::first_free_bound, constants::four, allglobal::globaljk, constants::half, inputlist::igeometry, allglobal::im, allglobal::in, allglobal::irbc, allglobal::irbs, allglobal::izbc, allglobal::izbs, inputlist::lrad, allglobal::mn, allglobal::mpi↩ _comm_spec, allglobal::myid, allglobal::ncpu, allglobal::notstellsym, inputlist::nvol, allglobal::nxyz, constants::one,

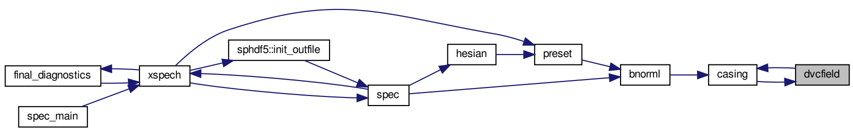
fileunits::ounit, numerical::small, constants::three, allglobal::tt, inputlist::vcasingeps, fileunits::vunit, allglobal↩
::yesstellsym, and constants::zero.

Referenced by casing().

Here is the call graph for this function:



Here is the caller graph for this function:



8.3 Parallelization

Functions/Subroutines

- subroutine brcast (lvol)

  Broadcasts Beltrami fields, profiles, . . .

8.3.1 Detailed Description

8.3.2 Function/Subroutine Documentation

8.3.2.1 brcast()

```
subroutine brcast (
        integer, intent(in) lvol )
```

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,

$$\mathbf{F}_i \equiv [[p + B^2/2]]_i = (p + B^2/2)_{v,i} - (p + B^2/2)_{v-1,i} \tag{62}$$

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

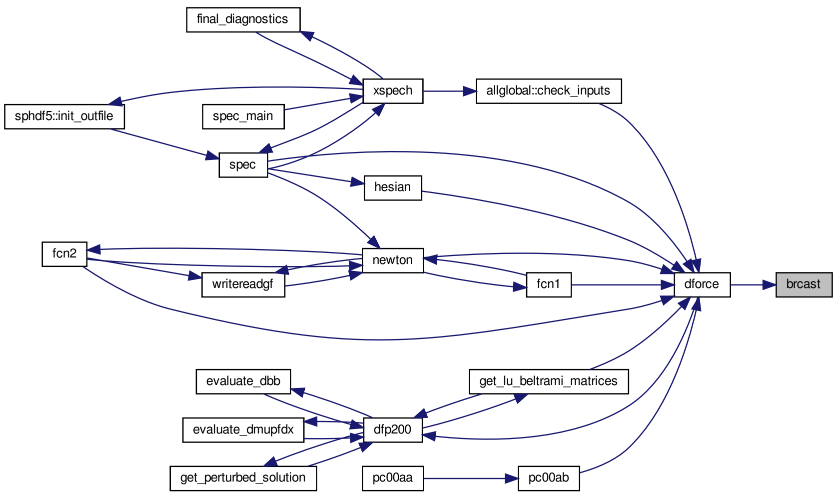
Parameters

in	*lvol*	index of nested volume

References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::bemn, allglobal::bomn, allglobal::cpus, inputlist::curpol, inputlist::curtor, 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::somn, inputlist::wmacros, and constants::zero.

Referenced by dforce().

Here is the caller graph for this function:



8.4 Geometry

Functions/Subroutines

- subroutine coords (lvol, lss, Lcurvature, Ntz, mn)

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

8.4.1 Detailed Description

8.4.2 Function/Subroutine Documentation

8.4.2.1 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,θ,ζ), which are be defined *inversely* via a transformation *to* Cartesian coordinates, (x,y,z).
- The toroidal angle, ζ, 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, θ, 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

$$\mathbf{x} \equiv r_{pol}\theta\,\hat{\mathbf{i}} + r_{tor}\zeta\,\hat{\mathbf{j}} + R\,\hat{\mathbf{k}} \tag{63}$$

    where r_{pol} and r_{tor} are inputs and $r_{pol} = r_{tor} = 1$ by default.
  - `Igeometry=2` : Cylindrical

$$\mathbf{x} = R\,\cos\theta\,\hat{\mathbf{i}} + R\,\sin\theta\,\hat{\mathbf{j}} + \zeta\,\hat{\mathbf{k}} \tag{64}$$

  - `Igeometry=3` : Toroidal

$$\mathbf{x} \equiv R\,\hat{\mathbf{r}} + Z\,\hat{\mathbf{k}} \tag{65}$$

    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

$$R_v(\theta,\zeta) \equiv \sum_j R_{j,v}\cos\alpha_j, \tag{66}$$

$$Z_v(\theta,\zeta) \equiv \sum_j Z_{j,v}\sin\alpha_j, \tag{67}$$

  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:

$$\begin{aligned} R(s,\theta,\zeta) &\equiv \sum_j \left[\frac{(1-s)}{2} R_{j,v-1} + \frac{(1+s)}{2} R_{j,v} \right] \cos\alpha_j, \\ Z(s,\theta,\zeta) &\equiv \sum_j \left[\frac{(1-s)}{2} Z_{j,v-1} + \frac{(1+s)}{2} Z_{j,v} \right] \sin\alpha_j, \end{aligned} \tag{68}$$

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

$$R_j(s) = R_{j,0} + (R_{j,1} - R_{j,0}) f_j, \tag{69}$$

$$Z_j(s) = Z_{j,0} + (Z_{j,1} - Z_{j,0}) f_j, \tag{70}$$

where, in toroidal geometry,

$$f_j \equiv \left\{ \begin{array}{ccc} \bar{s} & , & \text{for } m_j = 0, \\ \bar{s}^{m_j} & , & \text{otherwise.} \end{array} \right\}. \tag{71}$$

- 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

$$\mathbf{e}_\theta \times \mathbf{e}_\zeta = -r_{tor} R_\theta \, \hat{\mathbf{i}} - r_{pol} R_\zeta \, \hat{\mathbf{j}} + r_{pol} r_{tor} \hat{\mathbf{k}} \tag{72}$$

$$\boldsymbol{\xi} \cdot \mathbf{e}_\theta \times \mathbf{e}_\zeta = \delta R \tag{73}$$

$$\sqrt{g} = R_s \, r_{pol} \, r_{tor} \tag{74}$$

  - `Igeometry=2` : Cylindrical

$$\mathbf{e}_\theta \times \mathbf{e}_\zeta = (R_\theta \sin\theta + R\cos\theta) \, \hat{\mathbf{i}} + (R\sin\theta - R_\theta \cos\theta) \, \hat{\mathbf{j}} - R R_\zeta \, \hat{\mathbf{k}} \tag{75}$$

$$\boldsymbol{\xi} \cdot \mathbf{e}_\theta \times \mathbf{e}_\zeta = \delta R \, R \tag{76}$$

$$\sqrt{g} = R_s \, R \tag{77}$$

  - `Igeometry=3` : Toroidal

$$\mathbf{e}_\theta \times \mathbf{e}_\zeta = -R \, Z_\theta \, \hat{r} + (Z_\theta \, R_\zeta - R_\theta \, Z_\zeta) \hat{\phi} + R \, R_\theta \, \hat{z} \tag{78}$$

$$\boldsymbol{\xi} \cdot \mathbf{e}_\theta \times \mathbf{e}_\zeta = R(\delta Z \; R_\theta - \delta R \; Z_\theta) \tag{79}$$

$$\sqrt{g} = R(Z_s \; R_\theta - R_s \; Z_\theta) \tag{80}$$

cartesian metrics

- The cartesian metrics are

$$g_{ss} = R_s R_s, \quad g_{s\theta} = R_s R_\theta, \quad g_{s\zeta} = R_s R_\zeta, \quad g_{\theta\theta} = R_\theta R_\theta + r_{pol}^2, \quad g_{\theta\zeta} = R_\theta R_\zeta, \quad g_{\zeta\zeta} = R_\zeta R_\zeta + r_{tor}^2 \tag{81}$$

cylindrical metrics

- The cylindrical metrics are

$$g_{ss} = R_s R_s, \quad g_{s\theta} = R_s R_\theta, \quad g_{s\zeta} = R_s R_\zeta, \quad g_{\theta\theta} = R_\theta R_\theta + R^2, \quad g_{\theta\zeta} = R_\theta R_\zeta, \quad g_{\zeta\zeta} = R_\zeta R_\zeta + 1 \quad (82)$$

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()

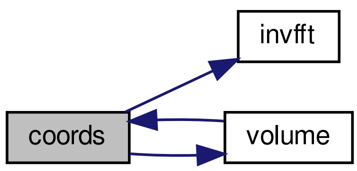
Parameters

in	*lvol*	specified in which volume to compute coordinates
in	*lss*	radial coordinate s
in	*Lcurvature*	logical control flag
in	*Ntz*	number of points in θ and ζ
in	*mn*	number of Fourier harmonics

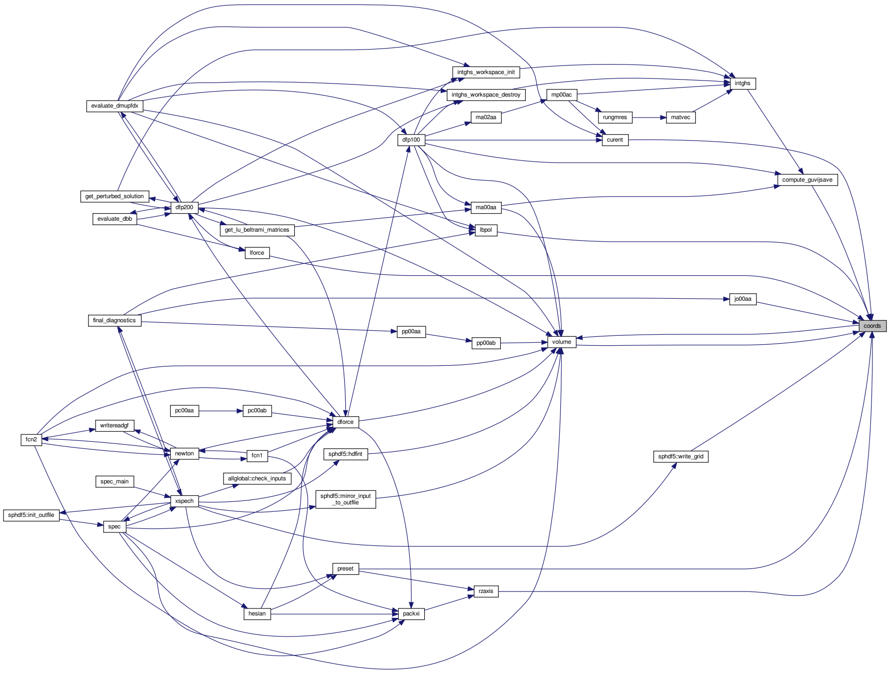
References allglobal::cosi, allglobal::cpus, allglobal::dbdx, allglobal::drodr, allglobal::drodz, allglobal::dzodr, allglobal::dzodz, allglobal::guvij, constants::half, allglobal::halfmm, inputlist::igeometry, allglobal::im, allglobal::in, invfft(), allglobal::irbc, allglobal::irbs, allglobal::izbc,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

Referenced by compute_guvijsave(), curent(), jo00aa(), lbpol(), lforce(), preset(), rzaxis(), volume(), and sphdf5::write_grid().

Here is the call graph for this function:



Here is the caller graph for this function:



8.5 Plasma Currents

Functions/Subroutines

- subroutine curent (lvol, mn, Nt, Nz, iflag, ldItGp)

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

8.5.1 Detailed Description

8.5.2 Function/Subroutine Documentation

8.5.2.1 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,

$$\int_{\mathcal{S}} \mathbf{j} \cdot d\mathbf{s} = \int_{\partial \mathcal{S}} \mathbf{B} \cdot d\mathbf{l}, \tag{83}$$

  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

$$I \equiv \int_0^{2\pi} \mathbf{B} \cdot \mathbf{e}_\theta \, d\theta = \int_0^{2\pi} \left(-\partial_s A_\zeta \; \bar{g}_{\theta\theta} + \partial_s A_\theta \; \bar{g}_{\theta\zeta} \right) \, d\theta, \tag{84}$$

  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

$$G \equiv \int_0^{2\pi} \mathbf{B} \cdot \mathbf{e}_\zeta \, d\zeta = \int_0^{2\pi} \left(-\partial_s A_\zeta \; \bar{g}_{\theta\zeta} + \partial_s A_\theta \; \bar{g}_{\zeta\zeta} \right) \, d\zeta. \tag{85}$$

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

$$I = \sum_i{}' f_i \cos(n_i \zeta) 2\pi, \tag{86}$$

  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

$$G = \sum_i{}' g_i \cos(m_i \zeta) 2\pi, \tag{87}$$

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

- The plasma current, Eqn. (86), should be independent of ζ, and the linking current, Eqn. (87), should be independent of θ.

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

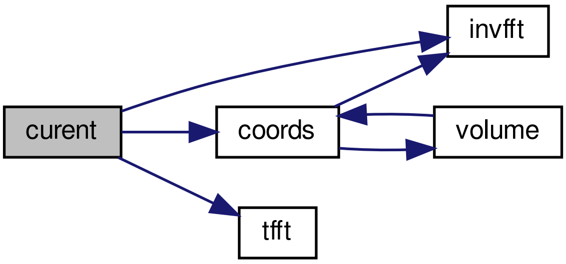
Parameters

`in`	*lvol*	index of volume
`in`	*mn*	number of Fourier harmonics
`in`	*Nt*	number of grid points along θ
`in`	*Nz*	number of grid points along ζ
`in`	*iflag*	some integer flag
`out`	*IdItGp*	plasma and linking current

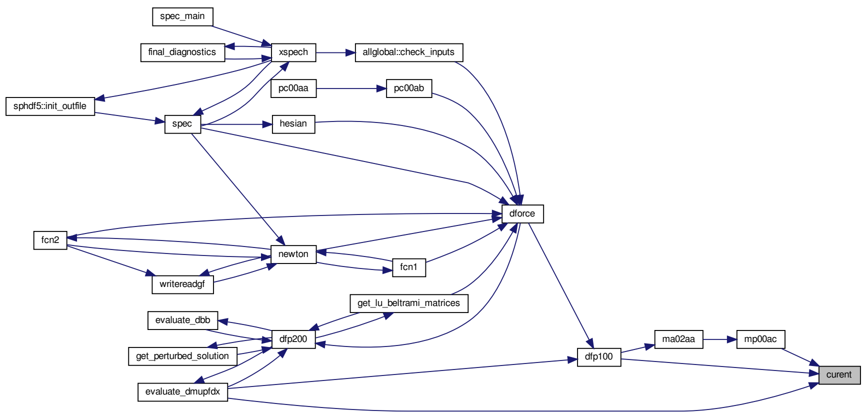
References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::cfmn, allglobal::comn, coords(), allglobal::cpus, allglobal::efmn, allglobal::evmn, allglobal::guvij, allglobal::ijimag, allglobal::ijreal, allglobal::im, allglobal::ime, allglobal::in, allglobal::ine, invfft(), allglobal::jiimag, allglobal::jireal, inputlist::lrad, allglobal::mne, allglobal::mpi_comm_spec, allglobal::myid, allglobal::ncpu, allglobal::notstellsym, allglobal::ntz, allglobal::odmn, allglobal::ofmn, constants::one, fileunits::ounit, constants::pi2, allglobal::sfmn, allglobal::sg, allglobal::simn, tfft(), 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:



8.6 "global" force

Functions/Subroutines

- subroutine dforce (NGdof, position, force, LComputeDerivatives, LComputeAxis)

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

8.6.1 Detailed Description

8.6.2 Function/Subroutine Documentation

8.6.2.1 dforce()

```
subroutine dforce (
    integer, intent(in) NGdof,
    real, dimension(0:ngdof), intent(in) position,
    real, dimension(0:ngdof), intent(out) force,
    logical, intent(in) LComputeDerivatives,
    logical LComputeAxis )
```

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 `iflag=5`.

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:

$$F_{i,v} \equiv \left[(p_{v+1} + B^2_{i,v+1}/2) - (p_v + B^2_{i,v}/2)\right] \times \texttt{BBweight}_i, \tag{88}$$

  where `BBweight_i` is defined in preset() ; and the spectral condensation constraints,

$$F_{i,v} \equiv I_{i,v} \times \texttt{epsilon} + S_{i,v,1} \times \texttt{sweight}_v - S_{i,v+1,0} \times \texttt{sweight}_{v+1}, \tag{89}$$

  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 lforce() ; and the `sweight` $_v$ are defined in preset(). All quantities local to a volume are computed in dfp200(), information is then broadcasted to the MPI node 0 in dforce() 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:

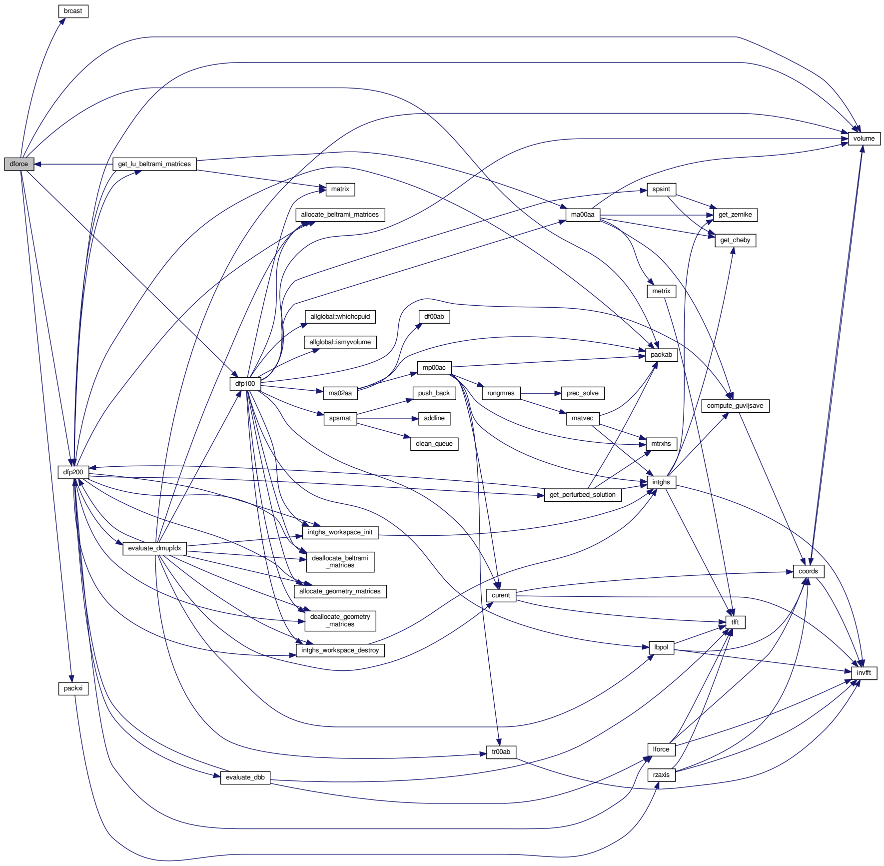
Parameters

`in`	*NGdof*	number of global degrees of freedom
`in`	*position*	
`out`	*force*	
`in`	*LComputeDerivatives*	
`in,out`	*LComputeAxis*	

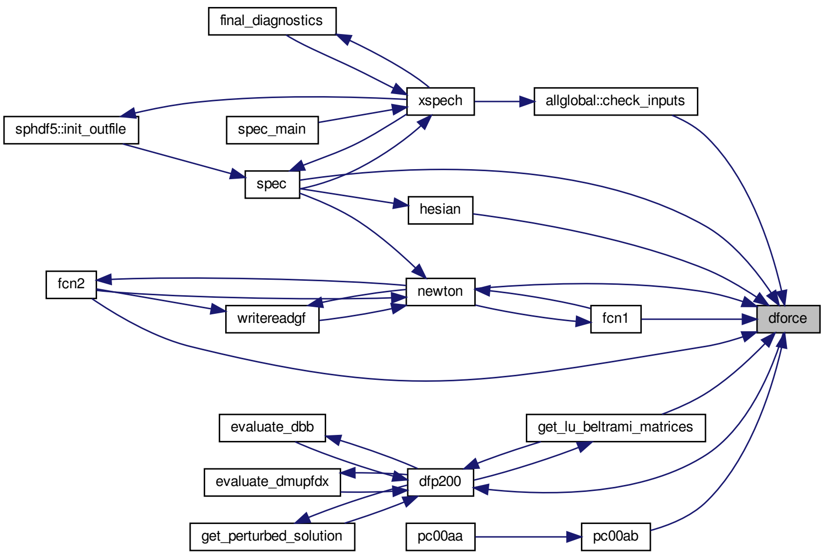
References brcast(), allglobal::cpus, allglobal::dbdx, dfp100(), dfp200(), inputlist::drz, inputlist::epsilon, constants↩ ::half, allglobal::hessian, inputlist::igeometry, allglobal::im, allglobal::in, allglobal::iquad, allglobal::irbc, allglobal↩ ::irbs, allglobal::izbc, allglobal::izbs, inputlist::lcheck, inputlist::lconstraint, 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().

Here is the call graph for this function:

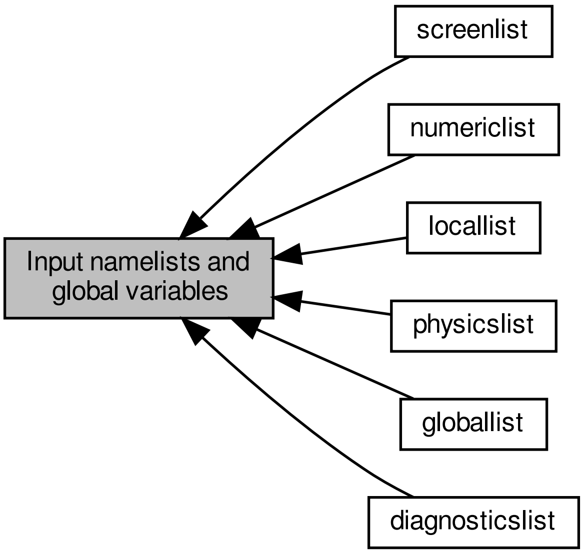


Here is the caller graph for this function:



8.7 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`.

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`.

8.7.1 Detailed Description

Input namelists.

8.8 "local" force

Functions/Subroutines

- subroutine lforce (lvol, iocons, ideriv, Ntz, dBB, XX, YY, length, DDl, MMl, iflag)

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

8.8.1 Detailed Description

8.8.2 Function/Subroutine Documentation

8.8.2.1 lforce()

```
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 MMl,
        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 $B^2 = B^s B_s + B^\theta B_\theta + B^\zeta B_\zeta$, 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

$$(\sqrt{g})^2 B^2 = A'_\zeta \, A'_\zeta \, g_{\theta\theta} - 2 \, A'_\zeta \, A'_\theta \, g_{\theta\zeta} + A'_\theta \, A'_\theta \, g_{\zeta\zeta}, \tag{90}$$

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

- The quantity returned is

$$F \equiv \texttt{pscale} \times \frac{P}{V^\gamma} + \frac{B^2}{2}, \tag{91}$$

  where $P \equiv \texttt{adiabatic}$ and $V \equiv$ 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

$$F \equiv \sum_{i=1}^{N-1} \alpha_i \underbrace{\oint\!\!\oint d\theta d\zeta \, \frac{1}{\Theta_{i,\theta}}}_{polar-angle} + \sum_{i=1}^{N-1} \beta_i \underbrace{M_i}_{spectral-width} + \sum_{i=1}^{N-1} \gamma_i \int_0^{2\pi} \frac{1}{2} \left[Z_i(0,\zeta) - Z_{i,0} \right]^2 d\zeta + \oint\!\!\oint d\theta d\zeta \sum_{i=1}^{N} \delta_i \underbrace{L_i}_{poloidal-length} \quad ($$

  where i labels the interfaces, and

$$\Theta_{i,\theta} \equiv \frac{x \, y_\theta - x_\theta \, y}{x^2 + y^2}, \tag{93}$$

$$M_i \equiv \frac{\sum_j m_j^p (R_{j,i}^2 + Z_{j,i}^2)}{\sum_j (R_{j,i}^2 + Z_{j,i}^2)}, \tag{94}$$

$$L_i \equiv \sqrt{[R_i(\theta,\zeta) - R_{i-1}(\theta,\zeta)]^2 + [Z_i(\theta,\zeta) - Z_{i-1}(\theta,\zeta)]^2}, \tag{95}$$

  and where j labels the Fourier harmonics. The α_i, β_i, γ_i and $\delta_i \equiv \texttt{sweight}$ are user-supplied weight factors.

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

$$x(\theta,\zeta) \equiv R_i(\theta,\zeta) - R_{i,0}(\zeta), \tag{96}$$

$$y(\theta,\zeta) \equiv Z_i(\theta,\zeta) - Z_{i,0}(\zeta), \tag{97}$$

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

$$R_{i,0} \equiv \int_0^{2\pi} d\theta \; R_i(\theta,\zeta) \sqrt{R_{i,\theta}(\theta,\zeta)^2 + Z_{i,\theta}(\theta,\zeta)^2}, \tag{98}$$

$$Z_{i,0} \equiv \int_0^{2\pi} d\theta \; Z_i(\theta,\zeta) \sqrt{R_{i,\theta}(\theta,\zeta)^2 + Z_{i,\theta}(\theta,\zeta)^2}, \tag{99}$$

  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

$$\delta R_i(\theta,\zeta) \equiv R_{i,\theta}(\theta,\zeta) \, \delta u_i(\theta,\zeta), \tag{100}$$

$$\delta Z_i(\theta,\zeta) \equiv Z_{i,\theta}(\theta,\zeta) \, \delta u_i(\theta,\zeta), \tag{101}$$

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

$$\delta R_{j,i} = \oint\!\!\oint d\theta d\zeta \;\; R_{i,\theta}(\theta,\zeta) \, \delta u_i(\theta,\zeta) \, \cos(m_j\theta - n_j\zeta), \tag{102}$$

$$\delta Z_{j,i} = \oint\!\!\oint d\theta d\zeta \;\; Z_{i,\theta}(\theta,\zeta) \, \delta u_i(\theta,\zeta) \, \sin(m_j\theta - n_j\zeta), \tag{103}$$

  and

$$\delta R_{i,\theta}(\theta,\zeta) \equiv R_{i,\theta\theta}(\theta,\zeta) \, \delta u_i(\theta,\zeta) + R_{i,\theta}(\theta,\zeta) \, \delta u_{i,\theta}(\theta,\zeta) \tag{104}$$

$$\delta Z_{i,\theta}(\theta,\zeta) \equiv Z_{i,\theta\theta}(\theta,\zeta) \, \delta u_i(\theta,\zeta) + Z_{i,\theta}(\theta,\zeta) \, \delta u_{i,\theta}(\theta,\zeta) \tag{105}$$

- The variation in F is

$$
\begin{aligned}
\delta F &= \sum_{i=1}^{N-1} \alpha_i \quad \oint\!\!\oint d\theta d\zeta \left(\frac{-2\Theta_{i,\theta\theta}}{\Theta_{i,\theta}^2}\right) \delta u_i \\
&+ \sum_{i=1}^{N-1} \beta_i \quad \oint\!\!\oint d\theta d\zeta \left(R_{i,\theta} X_i + Z_{i,\theta} Y_i\right) \delta u_i \\
&+ \sum_{i=1}^{N-1} \gamma_i \quad \int d\zeta \left(Z_i(0,\zeta) - Z_{i,0}\right) Z_{i,\theta}\, \delta u_i \\
&+ \sum_{i=1}^{N-1} \delta_i \quad \oint\!\!\oint d\theta d\zeta \left(\frac{\Delta R_i R_{i,\theta} + \Delta Z_i Z_{i,\theta}}{L_i}\right) \delta u_i \\
&- \sum_{i=1}^{N-1} \delta_{i+1} \oint\!\!\oint d\theta d\zeta \left(\frac{\Delta R_{i+1} R_{i,\theta} + \Delta Z_{i+1} Z_{i,\theta}}{L_{i+1}}\right) \delta u_i
\end{aligned} \tag{106}
$$

where, for the stellarator symmetric case,

$$X_i \equiv \sum_j (m_j^p - M_i)\, R_{j,i} \cos(m_j\theta - n_j\zeta), \tag{107}$$

$$Y_i \equiv \sum_j (m_j^p - M_i)\, Z_{j,i} \sin(m_j\theta - n_j\zeta), \tag{108}$$

and

$$\Delta R_i \equiv R_i(\theta,\zeta) - R_{i-1}(\theta,\zeta), \tag{109}$$

$$\Delta Z_i \equiv Z_i(\theta,\zeta) - Z_{i-1}(\theta,\zeta), \tag{110}$$

- The spectral constraints derived from Eqn. (106) are

$$
\begin{aligned}
I_i(\theta,\zeta) \equiv & -2\alpha_i \frac{\Theta_{i,\theta\theta}}{\Theta_{i,\theta}^2} + \beta_i \left(R_{i,\theta} X_i + Z_{i,\theta} Y_i\right) + \gamma_i \left(Z_i(0,\zeta) - Z_{i,0}\right) Z_{i,\theta}(0,\zeta) \\
& + \delta_i \frac{\Delta R_i R_{i,\theta} + \Delta Z_i Z_{i,\theta}}{L_i} - \delta_{i+1} \frac{\Delta R_{i+1} R_{i,\theta} + \Delta Z_{i+1} Z_{i,\theta}}{L_{i+1}}
\end{aligned} \tag{111}
$$

- 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, α_i, β_i, γ_i and δ_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. (111) 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. $\alpha_i = 0$.

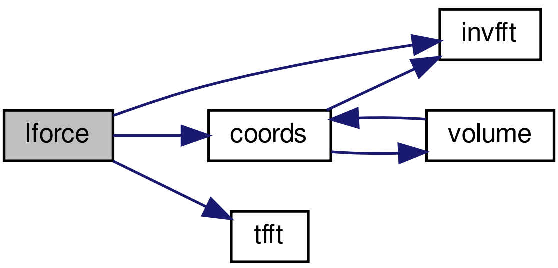
Parameters

in	*lvol*	
in	*iocons*	
in	*ideriv*	
in	*Ntz*	
	dBB	
	XX	
	YY	
	length	
	DDl	
	MMl	
in	*iflag*	

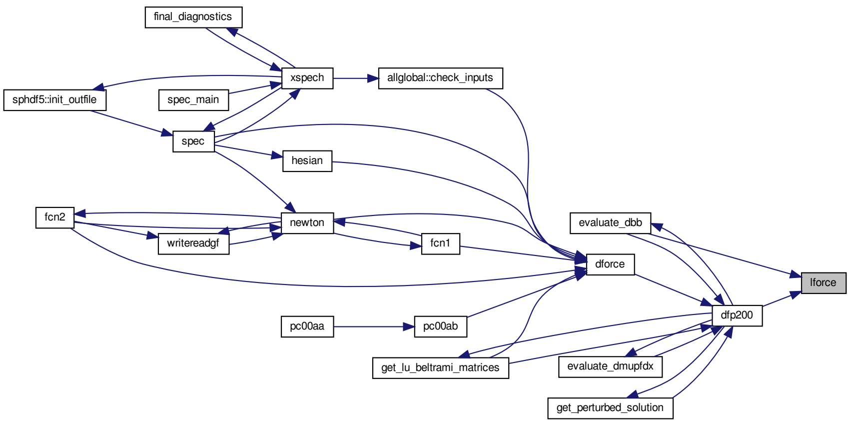
References inputlist::adiabatic, allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::bemn, allglobal::bomn, allglobal::cfmn, allglobal::comn, coords(), allglobal::cpus, allglobal::drij, allglobal::dzij, allglobal::efmn, allglobal::evmn, inputlist::gamma, allglobal::guvij, constants::half, allglobal::iemn, inputlist::igeometry, allglobal::ijimag, allglobal::ijreal, allglobal::im, allglobal::in, invfft(), allglobal::iomn, allglobal::irbc, allglobal::irbs, allglobal::irij, allglobal::izbc, allglobal::izbs, allglobal::izij, allglobal::jiimag, allglobal::jireal, inputlist::lcheck, allglobal::lcoordinatesingularity, inputlist::lrad, allglobal::mmpp, allglobal::mn, allglobal::mpi_comm_spec, allglobal::myid, allglobal::ncpu, allglobal::notstellsym, allglobal::nt, inputlist::nvol, allglobal::nz, allglobal::odmn, allglobal::ofmn, constants::one, fileunits::ounit, allglobal::pemn, allglobal::pomn, inputlist::pscale, allglobal::regumm, allglobal::rtt, allglobal::semn, allglobal::sfmn, allglobal::sg, allglobal::simn, allglobal::somn, tfft(), allglobal::trij, allglobal::tt, constants::two, allglobal::tzij, allglobal::vvolume, allglobal::yesstellsym, and constants::zero.

Referenced by dfp200(), and evaluate_dbb().

Here is the call graph for this function:



Here is the caller graph for this function:



8.9 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 (lquad, mn, lvol, lrad)

  Calculates volume integrals of Chebyshev polynomials and metric element products.
- subroutine spsint (lquad, mn, lvol, lrad)

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

8.9.1 Detailed Description

8.9.2 Function/Subroutine Documentation

8.9.2.1 df00ab()

```
subroutine df00ab (
    integer, intent(in) pNN,
    real, dimension(0:pnn-1), intent(in) xi,
    real, dimension(0:pnn-1), intent(out) Fxi,
    real, dimension(0:ldfjac-1,0:pnn-1), intent(out) DFxi,
    integer, intent(in) Ldfjac,
    integer, intent(in), value iflag )
```

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

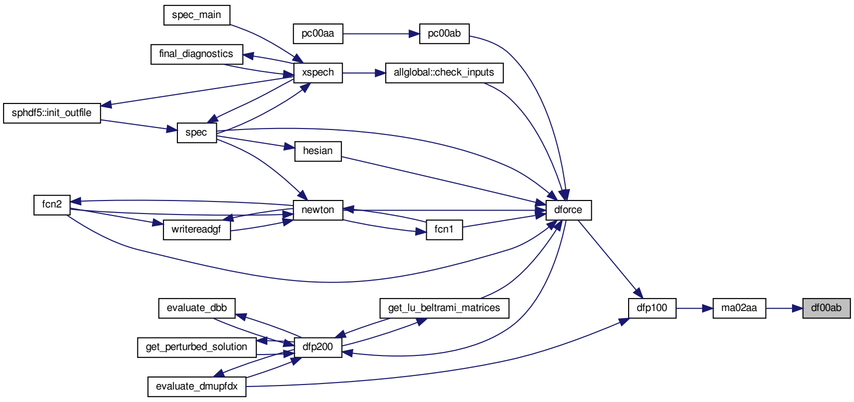
Parameters

in	*pNN*	
in	*xi*	
out	*Fxi*	
out	*DFxi*	
in	*Ldfjac*	
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:



8.9.2.2 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:

$$\texttt{DToocc(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \cos\alpha_i \cos\alpha_j \tag{112}$$

$$\texttt{DToocs(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \cos\alpha_i \sin\alpha_j \tag{113}$$

$$\texttt{DToosc(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \sin\alpha_i \cos\alpha_j \tag{114}$$

$$\texttt{DTooss(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \sin\alpha_i \sin\alpha_j \tag{115}$$

$$\texttt{TTsscc(l,p,i,j)} \equiv \int ds\, \overline{T}_{l,i}\, \overline{T}_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \cos\alpha_i \cos\alpha_j \; \bar{g}_{ss} \tag{116}$$

$$\texttt{TTsscs(l,p,i,j)} \equiv \int ds\, \overline{T}_{l,i}\, \overline{T}_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \cos\alpha_i \sin\alpha_j \; \bar{g}_{ss} \tag{117}$$

$$\texttt{TTsssc(l,p,i,j)} \equiv \int ds\, \overline{T}_{l,i}\, \overline{T}_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \sin\alpha_i \cos\alpha_j \; \bar{g}_{ss} \tag{118}$$

$$\texttt{TTssss(l,p,i,j)} \equiv \int ds\, \overline{T}_{l,i}\, \overline{T}_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \sin\alpha_i \sin\alpha_j \; \bar{g}_{ss} \tag{119}$$

$$\texttt{TDstcc(l,p,i,j)} \equiv \int ds\, \overline{T}_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \cos\alpha_i \cos\alpha_j \; \bar{g}_{s\theta} \tag{120}$$

$$\texttt{TDstcs(l,p,i,j)} \equiv \int ds\, \overline{T}_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \cos\alpha_i \sin\alpha_j \; \bar{g}_{s\theta} \tag{121}$$

$$\texttt{TDstsc(l,p,i,j)} \equiv \int ds\, \overline{T}_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \sin\alpha_i \cos\alpha_j \; \bar{g}_{s\theta} \tag{122}$$

$$\texttt{TDstss(l,p,i,j)} \equiv \int ds\, \overline{T}_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \sin\alpha_i \sin\alpha_j \; \bar{g}_{s\theta} \tag{123}$$

$$\texttt{TDstcc(l,p,i,j)} \equiv \int ds\, \overline{T}_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \cos\alpha_i \cos\alpha_j \; \bar{g}_{s\zeta} \tag{124}$$

$$\texttt{TDstcs(l,p,i,j)} \equiv \int ds\, \overline{T}_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \cos\alpha_i \sin\alpha_j \; \bar{g}_{s\zeta} \tag{125}$$

$$\texttt{TDstsc(l,p,i,j)} \equiv \int ds\, \overline{T}_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \sin\alpha_i \cos\alpha_j \; \bar{g}_{s\zeta} \tag{126}$$

$$\texttt{TDstss(l,p,i,j)} \equiv \int ds\, \overline{T}_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \sin\alpha_i \sin\alpha_j \; \bar{g}_{s\zeta} \tag{127}$$

$$\texttt{DDstcc(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \cos\alpha_i \cos\alpha_j \; \bar{g}_{\theta\theta} \tag{128}$$

$$\texttt{DDstcs(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \cos\alpha_i \sin\alpha_j \; \bar{g}_{\theta\theta} \tag{129}$$

$$\texttt{DDstsc(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \sin\alpha_i \cos\alpha_j \; \bar{g}_{\theta\theta} \tag{130}$$

$$\texttt{DDstss(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \sin\alpha_i \sin\alpha_j \; \bar{g}_{\theta\theta} \tag{131}$$

$$\texttt{DDstcc(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \cos\alpha_i \cos\alpha_j \; \bar{g}_{\theta\zeta} \tag{132}$$

$$\texttt{DDstcs(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \cos\alpha_i \sin\alpha_j \; \bar{g}_{\theta\zeta} \tag{133}$$

$$\texttt{DDstsc(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \sin\alpha_i \cos\alpha_j \; \bar{g}_{\theta\zeta} \tag{134}$$

$$\texttt{DDstss(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \sin\alpha_i \sin\alpha_j \; \bar{g}_{\theta\zeta} \tag{135}$$

$$\texttt{DDstcc(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \cos\alpha_i \cos\alpha_j \; \bar{g}_{\zeta\zeta} \tag{136}$$

$$\texttt{DDstcs(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \cos\alpha_i \sin\alpha_j \; \bar{g}_{\zeta\zeta} \tag{137}$$

$$\texttt{DDstsc(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \sin\alpha_i \cos\alpha_j \; \bar{g}_{\zeta\zeta} \tag{138}$$

$$\texttt{DDstss(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \sin\alpha_i \sin\alpha_j \; \bar{g}_{\zeta\zeta} \tag{139}$$

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

- 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 .

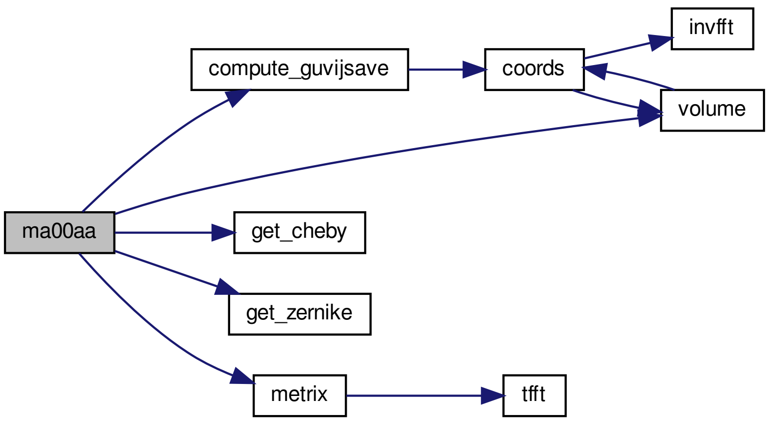
Parameters

in	*lquad*	degree of quadrature
in	*mn*	number of Fourier harmonics
in	*lvol*	index of nested volume
in	*lrad*	order of Chebychev polynomials

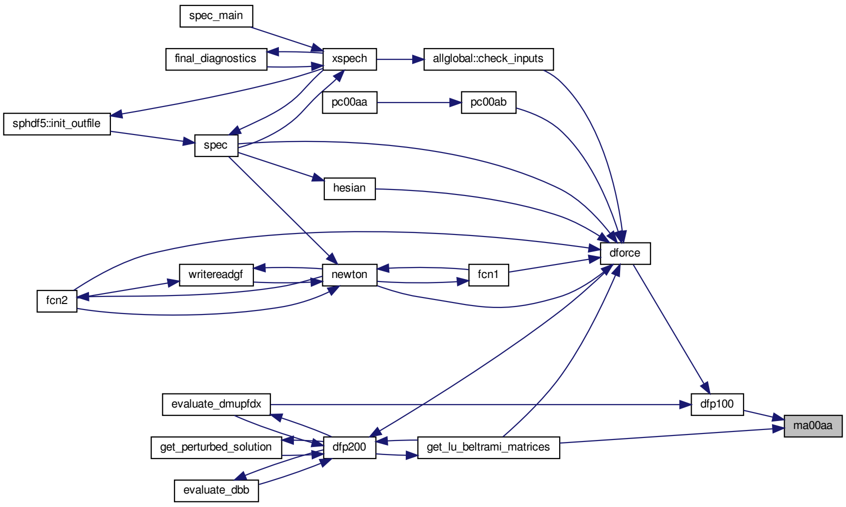
References compute_guvijsave(), allglobal::cpus, allglobal::dbdx, allglobal::ddttcc, allglobal::ddttcs, allglobal::ddttsc, allglobal::ddttss, allglobal::ddtzcc, allglobal::ddtzcs, allglobal::ddtzsc, allglobal::ddtzss, allglobal::ddzzcc, allglobal::ddzzcs, allglobal::ddzzsc, allglobal::ddzzss, allglobal::dtoocc, allglobal::dtoocs, allglobal::dtoosc, allglobal::dtooss, allglobal::gaussianabscissae, allglobal::gaussianweight, get_cheby(), get_zernike(), allglobal::goomne, allglobal::goomno, allglobal::gssmne, allglobal::gssmno, allglobal::gstmne, allglobal::gstmno, allglobal::gszmne, allglobal::gszmno, allglobal::gttmne, allglobal::gttmno, allglobal::gtzmne, allglobal::gtzmno, allglobal::gzzmne, allglobal::gzzmno, constants::half, allglobal::im, allglobal::in, allglobal::ki, allglobal::kija, allglobal::kijs, allglobal::lcoordinatesingularity, allglobal::lsavedguvij, metrix(), allglobal::mne, allglobal::mpi_comm_spec, inputlist::mpol, allglobal::myid, allglobal::ncpu, allglobal::notstellsym, constants::one, fileunits::ounit, constants::pi, constants::pi2, allglobal::regumm, allglobal::tdstcc, allglobal::tdstcs, allglobal::tdstsc, allglobal::tdstss, allglobal::tdszcc, allglobal::tdszcs, allglobal::tdszsc, allglobal::tdszss, allglobal::ttsscc, allglobal::ttsscs, allglobal::ttsssc, allglobal::ttssss, constants::two, volume(), inputlist::wmacros, allglobal::yesstellsym, and constants::zero.

Referenced by dfp100(), and get_lu_beltrami_matrices().

Here is the call graph for this function:



Here is the caller graph for this function:



8.9.2.3 spsint()

```
subroutine spsint (
    integer, intent(in) lquad,
    integer, intent(in) mn,
    integer, intent(in) lvol,
    integer, intent(in) lrad )
```

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.

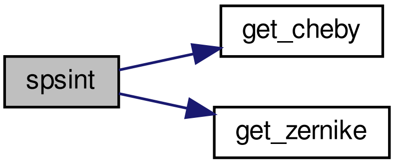
Parameters

lquad	
mn	
lvol	
lrad	

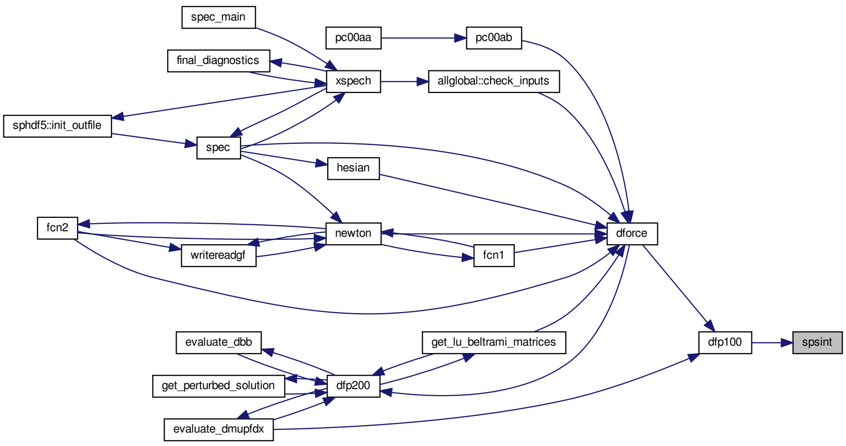
References allglobal::cpus, allglobal::ddttcc, allglobal::ddttcs, allglobal::ddttsc, allglobal::ddttss, allglobal::ddtzcc, allglobal::ddtzcs, allglobal::ddtzsc, allglobal::ddtzss, allglobal::ddzzcc, allglobal::ddzzcs, allglobal::ddzzsc, allglobal::ddzzss, allglobal::dtoocc, allglobal::dtoocs, allglobal::dtoosc, allglobal::dtooss, allglobal::gaussianabscissae, allglobal::gaussianweight, get_cheby(), get_zernike(), allglobal::guvijsave, constants::half, allglobal::im, allglobal::in, allglobal::ki, allglobal::kija, allglobal::kijs, allglobal::lcoordinatesingularity, allglobal::mne, allglobal::mpi_comm_spec, inputlist::mpol, allglobal::myid, allglobal::ncpu, allglobal::notstellsym, allglobal::ntz, constants::one, fileunits::ounit, constants::pi, constants::pi2, allglobal::regumm, numerical::small, numerical::sqrtmachprec, allglobal::tdstcc, allglobal::tdstcs, allglobal::tdstsc, allglobal::tdstss, allglobal::tdszcc, allglobal::tdszcs, allglobal::tdszsc, allglobal::tdszss, allglobal::ttsscc, allglobal::ttsscs, allglobal::ttsssc, allglobal::ttssss, constants::two, numerical::vsmall, 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:



8.10 Solver/Driver

Functions/Subroutines

- subroutine ma02aa (lvol, NN)

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

8.10.1 Detailed Description

8.10.2 Function/Subroutine Documentation

8.10.2.1 ma02aa()

```
subroutine ma02aa (
        integer, intent(in) lvol,
        integer, intent(in) NN )
```

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

Parameters

in	*lvol*	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 μ 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 μ and $\Delta\psi_p$. (Note that $\Delta\psi_p$ is not defined in a torus.)

  – These are "packed" into an array, e.g. $\boldsymbol{\mu} \equiv (\mu, \Delta\psi_p)^T$, so that standard library routines , e.g. `C05PCF`, can be used to (iteratively) find the appropriately-constrained Beltrami solution, i.e. $\mathbf{f}(\boldsymbol{\mu}) = 0$.

  – The function $\mathbf{f}(\boldsymbol{\mu})$, which is computed by mp00ac(), is defined by the input parameter `Lconstraint`:

    * If `Lconstraint` = -1, 0, then $\boldsymbol{\mu}$ is *not* varied and `Nxdof=0`.
    * If `Lconstraint` = 1, then $\boldsymbol{\mu}$ 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 $\mu = \boldsymbol{\mu}_1$ is varied in order to satisfy the transform constraint on the "outer" interface of that volume.)
    * **Todo** If `Lconstraint` = 2, then $\mu = \boldsymbol{\mu}_1$ is varied in order to satisfy the helicity constraint, and $\Delta\psi_p = \boldsymbol{\mu}_2$ 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 $\mathbf{B} \cdot \mathbf{n} \neq 0$ on the computational boundary.)

  – These are "packed" into an array, $\boldsymbol{\mu} \equiv (\Delta\psi_t, \Delta\psi_p)^T$, so that, as above, standard routines can be used to iteratively find the appropriately constrained solution, i.e. $\mathbf{f}(\boldsymbol{\mu}) = 0$.

  – The function $\mathbf{f}(\boldsymbol{\mu})$, which is computed by mp00ac(), is defined by the input parameter `Lconstraint`:

    * If `Lconstraint` = -1, then $\boldsymbol{\mu}$ is *not* varied and `Nxdof=0`.
    * If `Lconstraint` = 0,2, then $\boldsymbol{\mu}$ is varied to satisfy the enclosed current constraints, and `Nxdof=2`.

  * If `Lconstraint = 1`, then $\boldsymbol{\mu}$ 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 $\mathbf{f}(\boldsymbol{\mu})$ are calculated in mp00ac().
- This routine, mp00ac(), is called iteratively if `Nxdof>1` via `C05PCF` to determine the appropriately constrained Beltrami field, $\mathbf{B}_{\boldsymbol{\mu}}$, so that $\mathbf{f}(\boldsymbol{\mu}) = 0$.
- 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 $\boldsymbol{\mu}$.

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, μ, and the enclosed poloidal-flux, $\Delta\psi_p$, so that `C05PCF` may more efficiently find the solution.
- The required derivatives are

$$\frac{\partial \iota\!\!\!-}{\partial \mu} \tag{140}$$

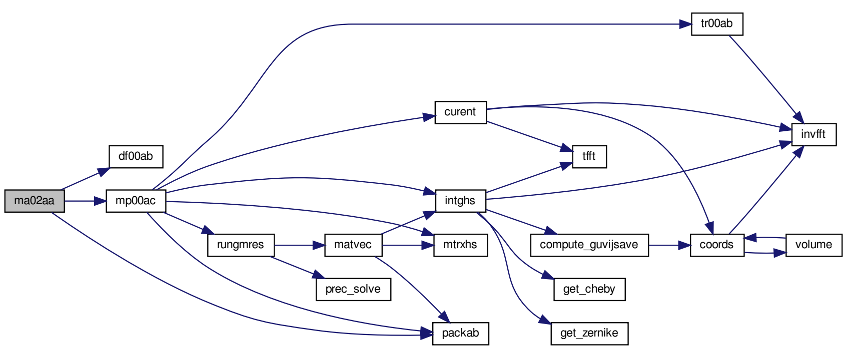
$$\frac{\partial \iota\!\!\!-}{\partial \Delta\psi_p} \tag{141}$$

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

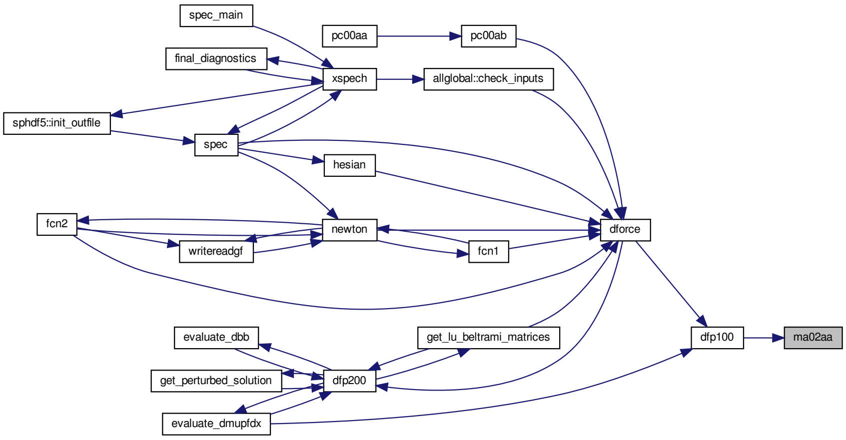
References allglobal::cpus, df00ab(), constants::half, inputlist::helicity, allglobal::im, allglobal::in, allglobal::lblinear, allglobal::lbnewton, allglobal::lbsequad, inputlist::lcheck, inputlist::lconstraint, inputlist::lrad, allglobal::mn, mp00ac(), allglobal::mpi_comm_spec, inputlist::mu, inputlist::mupfits, 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:



Here is the caller graph for this function:



8.11 Build matrices

Functions/Subroutines

- subroutine matrix (lvol, mn, lrad)

    Constructs energy and helicity matrices that represent the Beltrami linear system.
    gauge conditions
- subroutine mtrxhs (lvol, mn, lrad, resultA, resultD, idx)

    Constructs matrices that represent the Beltrami linear system, matrix-free.
- subroutine spsmat (lvol, mn, lrad)

    Constructs matrices for the precondtioner.

8.11.1 Detailed Description

8.11.2 Function/Subroutine Documentation

8.11.2.1 matrix()

```
subroutine matrix (
        integer, intent(in) lvol,
        integer, intent(in) mn,
        integer, intent(in) lrad )
```

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

$$\bar{\mathbf{A}} = \bar{A}_s \nabla s + \bar{A}_\theta \nabla \theta + \bar{A}_\zeta \nabla \zeta eta. \quad (142)$$

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

$$\begin{aligned}\partial_s g(s,\theta,\zeta) &= - \bar{A}_s(s,\theta,\zeta)\\ \partial_\theta g(-1,\theta,\zeta) &= - \bar{A}_\theta(-1,\theta,\zeta)\\ \partial_\zeta g(-1,0,\zeta) &= - \bar{A}_\zeta(-1,0,\zeta).\end{aligned} \tag{143}$$

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

$$A_\theta(-1,\theta,\zeta) = 0 \tag{144}$$
$$A_\zeta(-1,0,\zeta) = 0 \tag{145}$$

- This specifies the gauge: to see this, notice that no gauge term can be added without violating the conditions in Eqn. (144) or Eqn. (145).
- 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_θ given in Eqn. (144), this gives $\partial_\theta A_\zeta = 0$, which with Eqn. (145) gives

$$A_\zeta(-1,\theta,\zeta) = 0. \tag{146}$$

- 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

$$\int_S \mathbf{B}\cdot\mathbf{ds} = \int_{\partial S}\mathbf{A}\cdot\mathbf{dl}. \tag{147}$$

Fourier-Chebyshev representation

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

$$A_\theta(s,\theta,\zeta) = \sum_{i,l} A_{\theta,e,i,l}\,\overline{T}_{l,i}(s)\cos\alpha_i + \sum_{i,l} A_{\theta,o,i,l}\,\overline{T}_{l,i}(s)\sin\alpha_i, \tag{148}$$
$$A_\zeta(s,\theta,\zeta) = \sum_{i,l} A_{\zeta,e,i,l}\,\overline{T}_{l,i}(s)\cos\alpha_i + \sum_{i,l} A_{\zeta,o,i,l}\,\overline{T}_{l,i}(s)\sin\alpha_i, \tag{149}$$

  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

$$\begin{aligned}\sqrt{g}\,\mathbf{B} = {} & \mathbf{e}_s \sum_{i,l}[(-m_i A_{\zeta,e,i,l} - n_i A_{\theta,e,i,l})\overline{T}_{l,i}\sin\alpha_i + (+m_i A_{\zeta,o,i,l} + n_i A_{\theta,o,i,l})\overline{T}_{l,i}\cos\alpha_i]\\ + {} & \mathbf{e}_\theta \sum_{i,l}[(- A_{\zeta,e,i,l})\overline{T}'_{l,i}\cos\alpha_i + (- A_{\zeta,o,i,l})\overline{T}'_{l,i}\sin\alpha_i]\\ + {} & \mathbf{e}_\zeta \sum_{i,l}[(A_{\theta,e,i,l})\overline{T}'_{l,i}\cos\alpha_i + (A_{\theta,o,i,l})\overline{T}'_{l,i}\sin\alpha_i]\end{aligned} \tag{150}$$

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

$$v_s(s,\theta,\zeta) = \sum_{i,l} v_{s,e,i,l}\, \overline{T}_{l,i}(s) \cos\alpha_i + \sum_{i,l} v_{s,o,i,l}\, \overline{T}_{l,i}(s) \sin\alpha_i, \quad (151)$$

$$v_\theta(s,\theta,\zeta) = \sum_{i,l} v_{\theta,e,i,l}\, \overline{T}_{l,i}(s) \cos\alpha_i + \sum_{i,l} v_{\theta,o,i,l}\, \overline{T}_{l,i}(s) \sin\alpha_i, \quad (152)$$

$$v_\zeta(s,\theta,\zeta) = \sum_{i,l} v_{\zeta,e,i,l}\, \overline{T}_{l,i}(s) \cos\alpha_i + \sum_{i,l} v_{\zeta,o,i,l}\, \overline{T}_{l,i}(s) \sin\alpha_i. \quad (153)$$

constrained energy functional

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

$$\mathcal{F} \equiv \mathcal{F}[A_{\theta,e,i,l}, A_{\zeta,e,i,l}, A_{\theta,o,i,l}, A_{\zeta,o,i,l}, v_{s,e,i,l}, v_{s,o,i,l}, v_{\theta,e,i,l}, v_{\theta,o,i,l}, v_{\zeta,e,i,l}, v_{\zeta,o,i,l}, \mu, a_i, b_i, c_i, d_i, e_i, f_i, g_1, h_1], \quad (154)$$

and is given by:

$$\begin{aligned}
\mathcal{F} \equiv & \int \mathbf{B}\cdot\mathbf{B}\, dv + \int \mathbf{v}\cdot\mathbf{v}\, dv - \mu\left[\int \mathbf{A}\cdot\mathbf{B}\, dv - K\right] \\
+ & \sum_{i=1} a_i \left[\sum_l A_{\theta,e,i,l} T_l(-1) - 0\right] \\
+ & \sum_{i=1} b_i \left[\sum_l A_{\zeta,e,i,l} T_l(-1) - 0\right] \\
+ & \sum_{i=2} c_i \left[\sum_l A_{\theta,o,i,l} T_l(-1) - 0\right] \\
+ & \sum_{i=2} d_i \left[\sum_l A_{\zeta,o,i,l} T_l(-1) - 0\right] \\
+ & \sum_{i=2} e_i \left[\sum_l (-m_i A_{\zeta,e,i,l} - n_i A_{\theta,e,i,l})\, T_l(+1) - b_{s,i}\right] \\
+ & \sum_{i=2} f_i \left[\sum_l (+m_i A_{\zeta,o,i,l} + n_i A_{\theta,o,i,l})\, T_l(+1) - b_{c,i}\right] \\
+ & g_1 \left[\sum_l A_{\theta,e,1,l} T_l(+1) - \Delta\psi_t\right] \\
+ & h_1 \left[\sum_l A_{\zeta,e,1,l} T_l(+1) + \Delta\psi_p\right]
\end{aligned} \quad (1$$

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 $\sqrt{g}\,\mathbf{B}\cdot\nabla s = b$; 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

$$\frac{\partial}{\partial A_{\theta,e,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ \mathbf{B}\cdot\frac{\partial \mathbf{B}}{\partial A_{\theta,e,i,l}} = 2\int dv\ \mathbf{B}\cdot\left[-n_i\overline{T}_{l,i}\sin\alpha_i\,\mathbf{e}_s+\overline{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\zeta\right]/\sqrt{} \tag{156}$$

$$\frac{\partial}{\partial A_{\theta,o,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ \mathbf{B}\cdot\frac{\partial \mathbf{B}}{\partial A_{\theta,o,i,l}} = 2\int dv\ \mathbf{B}\cdot\left[+n_i\overline{T}_{l,i}\cos\alpha_i\,\mathbf{e}_s+\overline{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\zeta\right]/\sqrt{} \tag{157}$$

$$\frac{\partial}{\partial A_{\zeta,e,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ \mathbf{B}\cdot\frac{\partial \mathbf{B}}{\partial A_{\zeta,e,i,l}} = 2\int dv\ \mathbf{B}\cdot\left[-m_i\overline{T}_{l,i}\sin\alpha_i\,\mathbf{e}_s-\overline{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\theta\right]/\sqrt{} \tag{158}$$

$$\frac{\partial}{\partial A_{\zeta,o,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ \mathbf{B}\cdot\frac{\partial \mathbf{B}}{\partial A_{\zeta,o,i,l}} = 2\int dv\ \mathbf{B}\cdot\left[+m_i\overline{T}_{l,i}\cos\alpha_i\,\mathbf{e}_s-\overline{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\theta\right]/\sqrt{} \tag{159}$$

- 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

$$\frac{\partial}{\partial A_{\theta,e,j,p}}\frac{\partial}{\partial A_{\theta,e,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ (+n_jn_i\overline{T}_{p,j}\overline{T}_{l,i}s_js_ig_{ss}-n_j\overline{T}_{p,j}\overline{T}'_{l,i}s_jc_ig_{s\zeta}-n_i\overline{T}_{l,i}\overline{T}'_{p,j}s_ic_jg_{s\zeta}+\overline{T}'_{p,j}\overline{T}'_{l,i}c_jc_ig_{\zeta\zeta})/\sqrt{}$$

$$\frac{\partial}{\partial A_{\theta,o,j,p}}\frac{\partial}{\partial A_{\theta,e,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ (-n_jn_i\overline{T}_{p,j}\overline{T}_{l,i}c_js_ig_{ss}+n_j\overline{T}_{p,j}\overline{T}'_{l,i}c_jc_ig_{s\zeta}-n_i\overline{T}_{l,i}\overline{T}'_{p,j}s_is_jg_{s\zeta}+\overline{T}'_{p,j}\overline{T}'_{l,i}s_jc_ig_{\zeta\zeta})/\sqrt{}$$

$$\frac{\partial}{\partial A_{\zeta,e,j,p}}\frac{\partial}{\partial A_{\theta,e,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ (+m_jn_i\overline{T}_{p,j}\overline{T}_{l,i}s_js_ig_{ss}-m_j\overline{T}_{p,j}\overline{T}'_{l,i}s_jc_ig_{s\zeta}+n_i\overline{T}_{l,i}\overline{T}'_{p,j}s_ic_jg_{s\theta}-\overline{T}'_{p,j}\overline{T}'_{l,i}c_jc_ig_{\theta\zeta})/$$

$$\frac{\partial}{\partial A_{\zeta,o,j,p}}\frac{\partial}{\partial A_{\theta,e,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ (-m_jn_i\overline{T}_{p,j}\overline{T}_{l,i}c_js_ig_{ss}+m_j\overline{T}_{p,j}\overline{T}'_{l,i}c_jc_ig_{s\zeta}+n_i\overline{T}_{l,i}\overline{T}'_{p,j}s_is_jg_{s\theta}-\overline{T}'_{p,j}\overline{T}'_{l,i}s_jc_ig_{\theta\zeta})/$$

$$\frac{\partial}{\partial A_{\theta,e,j,p}}\frac{\partial}{\partial A_{\theta,o,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ (-n_jn_i\overline{T}_{p,j}\overline{T}_{l,i}s_jc_ig_{ss}-n_j\overline{T}_{p,j}\overline{T}'_{l,i}s_js_ig_{s\zeta}+n_i\overline{T}_{l,i}\overline{T}'_{p,j}c_ic_jg_{s\zeta}+\overline{T}'_{p,j}\overline{T}'_{l,i}c_js_ig_{\zeta\zeta})/\sqrt{}$$

$$\frac{\partial}{\partial A_{\theta,o,j,p}}\frac{\partial}{\partial A_{\theta,o,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ (+n_jn_i\overline{T}_{p,j}\overline{T}_{l,i}c_jc_ig_{ss}+n_j\overline{T}_{p,j}\overline{T}'_{l,i}c_js_ig_{s\zeta}+n_i\overline{T}_{l,i}\overline{T}'_{p,j}c_is_jg_{s\zeta}+\overline{T}'_{p,j}\overline{T}'_{l,i}s_js_ig_{\zeta\zeta})/\sqrt{}$$

$$\frac{\partial}{\partial A_{\zeta,e,j,p}}\frac{\partial}{\partial A_{\theta,o,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ (-m_jn_i\overline{T}_{p,j}\overline{T}_{l,i}s_jc_ig_{ss}-m_j\overline{T}_{p,j}\overline{T}'_{l,i}s_js_ig_{s\zeta}-n_i\overline{T}_{l,i}\overline{T}'_{p,j}c_ic_jg_{s\theta}-\overline{T}'_{p,j}\overline{T}'_{l,i}c_js_ig_{\theta\zeta})/$$

$$\frac{\partial}{\partial A_{\zeta,o,j,p}}\frac{\partial}{\partial A_{\theta,o,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ (+m_jn_i\overline{T}_{p,j}\overline{T}_{l,i}c_jc_ig_{ss}+m_j\overline{T}_{p,j}\overline{T}'_{l,i}c_js_ig_{s\zeta}-n_i\overline{T}_{l,i}\overline{T}'_{p,j}c_is_jg_{s\theta}-\overline{T}'_{p,j}\overline{T}'_{l,i}s_js_ig_{\theta\zeta})/$$

$$\frac{\partial}{\partial A_{\theta,e,j,p}}\frac{\partial}{\partial A_{\zeta,e,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ (+n_jm_i\overline{T}_{p,j}\overline{T}_{l,i}s_js_ig_{ss}+n_j\overline{T}_{p,j}\overline{T}'_{l,i}s_jc_ig_{s\theta}-m_i\overline{T}_{l,i}\overline{T}'_{p,j}s_ic_jg_{s\zeta}-\overline{T}'_{p,j}\overline{T}'_{l,i}c_jc_ig_{\theta\zeta})/$$

$$\frac{\partial}{\partial A_{\theta,o,j,p}}\frac{\partial}{\partial A_{\zeta,e,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ (-n_jm_i\overline{T}_{p,j}\overline{T}_{l,i}c_js_ig_{ss}-n_j\overline{T}_{p,j}\overline{T}'_{l,i}c_jc_ig_{s\theta}-m_i\overline{T}_{l,i}\overline{T}'_{p,j}s_is_jg_{s\zeta}-\overline{T}'_{p,j}\overline{T}'_{l,i}s_jc_ig_{\theta\zeta})/$$

$$\frac{\partial}{\partial A_{\zeta,e,j,p}}\frac{\partial}{\partial A_{\zeta,e,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ (+m_jm_i\overline{T}_{p,j}\overline{T}_{l,i}s_js_ig_{ss}+m_j\overline{T}_{p,j}\overline{T}'_{l,i}s_jc_ig_{s\theta}+m_i\overline{T}_{l,i}\overline{T}'_{p,j}s_ic_jg_{s\theta}+\overline{T}'_{p,j}\overline{T}'_{l,i}c_jc_ig_{\theta\theta}),$$

$$\frac{\partial}{\partial A_{\zeta,o,j,p}}\frac{\partial}{\partial A_{\zeta,e,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ (-m_jm_i\overline{T}_{p,j}\overline{T}_{l,i}c_js_ig_{ss}-m_j\overline{T}_{p,j}\overline{T}'_{l,i}c_jc_ig_{s\theta}+m_i\overline{T}_{l,i}\overline{T}'_{p,j}s_is_jg_{s\theta}+\overline{T}'_{p,j}\overline{T}'_{l,i}s_jc_ig_{\theta\theta}),$$

$$\frac{\partial}{\partial A_{\theta,e,j,p}}\frac{\partial}{\partial A_{\zeta,o,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ (-n_jm_i\overline{T}_{p,j}\overline{T}_{l,i}s_jc_ig_{ss}+n_j\overline{T}_{p,j}\overline{T}'_{l,i}s_js_ig_{s\theta}+m_i\overline{T}_{l,i}\overline{T}'_{p,j}c_ic_jg_{s\zeta}-\overline{T}'_{p,j}\overline{T}'_{l,i}c_js_ig_{\theta\zeta})/$$

$$\frac{\partial}{\partial A_{\theta,o,j,p}}\frac{\partial}{\partial A_{\zeta,o,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ (+n_jm_i\overline{T}_{p,j}\overline{T}_{l,i}c_jc_ig_{ss}-n_j\overline{T}_{p,j}\overline{T}'_{l,i}c_js_ig_{s\theta}+m_i\overline{T}_{l,i}\overline{T}'_{p,j}c_is_jg_{s\zeta}-\overline{T}'_{p,j}\overline{T}'_{l,i}s_js_ig_{\theta\zeta})/$$

$$\frac{\partial}{\partial A_{\zeta,e,j,p}}\frac{\partial}{\partial A_{\zeta,o,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ (-m_jm_i\overline{T}_{p,j}\overline{T}_{l,i}s_jc_ig_{ss}+m_j\overline{T}_{p,j}\overline{T}'_{l,i}s_js_ig_{s\theta}-m_i\overline{T}_{l,i}\overline{T}'_{p,j}c_ic_jg_{s\theta}+\overline{T}'_{p,j}\overline{T}'_{l,i}c_js_ig_{\theta\theta}),$$

$$\frac{\partial}{\partial A_{\zeta,o,j,p}}\frac{\partial}{\partial A_{\zeta,o,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ (+m_jm_i\overline{T}_{p,j}\overline{T}_{l,i}c_jc_ig_{ss}-m_j\overline{T}_{p,j}\overline{T}'_{l,i}c_js_ig_{s\theta}-m_i\overline{T}_{l,i}\overline{T}'_{p,j}c_is_jg_{s\theta}+\overline{T}'_{p,j}\overline{T}'_{l,i}s_js_ig_{\theta\theta}),$$

derivatives of helicity integrals

- 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

$$\frac{\partial}{\partial A_{\theta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv \left(\frac{\partial \mathbf{A}}{\partial A_{\theta,e,i,l}}\cdot\mathbf{B}+\mathbf{A}\cdot\frac{\partial \mathbf{B}}{\partial A_{\theta,e,i,l}}\right) = \int dv\ (\bar{T}_{l,i}\cos\alpha_i\nabla\theta\cdot\mathbf{B}+\mathbf{A}\cdot\bar{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\zeta/\sqrt{g}) \tag{160}$$

$$\frac{\partial}{\partial A_{\theta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv \left(\frac{\partial \mathbf{A}}{\partial A_{\theta,o,i,l}}\cdot\mathbf{B}+\mathbf{A}\cdot\frac{\partial \mathbf{B}}{\partial A_{\theta,o,i,l}}\right) = \int dv\ (\bar{T}_{l,i}\sin\alpha_i\nabla\theta\cdot\mathbf{B}+\mathbf{A}\cdot\bar{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\zeta/\sqrt{g}) \tag{161}$$

$$\frac{\partial}{\partial A_{\zeta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv \left(\frac{\partial \mathbf{A}}{\partial A_{\zeta,e,i,l}}\cdot\mathbf{B}+\mathbf{A}\cdot\frac{\partial \mathbf{B}}{\partial A_{\zeta,e,i,l}}\right) = \int dv\ (\bar{T}_{l,i}\cos\alpha_i\nabla\zeta\cdot\mathbf{B}-\mathbf{A}\cdot\bar{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\theta/\sqrt{g}) \tag{162}$$

$$\frac{\partial}{\partial A_{\zeta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv \left(\frac{\partial \mathbf{A}}{\partial A_{\zeta,o,i,l}}\cdot\mathbf{B}+\mathbf{A}\cdot\frac{\partial \mathbf{B}}{\partial A_{\zeta,o,i,l}}\right) = \int dv\ (\bar{T}_{l,i}\sin\alpha_i\nabla\zeta\cdot\mathbf{B}-\mathbf{A}\cdot\bar{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\theta/\sqrt{g}) \tag{163}$$

- 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

$$\frac{\partial}{\partial A_{\theta,e,j,p}}\frac{\partial}{\partial A_{\theta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[\cancel{+\bar{T}_{l,i}\cos\alpha_i\nabla\theta\cdot\bar{T}'_{p,j}\cos\alpha_j\,\mathbf{e}_\zeta}\cancel{+\bar{T}_{p,j}\cos\alpha_j\nabla\theta\cdot\bar{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\zeta}\right]/\sqrt{g} \tag{164}$$

$$\frac{\partial}{\partial A_{\theta,o,j,p}}\frac{\partial}{\partial A_{\theta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[\cancel{+\bar{T}_{l,i}\cos\alpha_i\nabla\theta\cdot\bar{T}'_{p,j}\sin\alpha_j\,\mathbf{e}_\zeta}\cancel{+\bar{T}_{p,j}\sin\alpha_j\nabla\theta\cdot\bar{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\zeta}\right]/\sqrt{g} \tag{165}$$

$$\frac{\partial}{\partial A_{\zeta,e,j,p}}\frac{\partial}{\partial A_{\theta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[-\bar{T}_{l,i}\cos\alpha_i\nabla\theta\cdot\bar{T}'_{p,j}\cos\alpha_j\,\mathbf{e}_\theta+\bar{T}_{p,j}\cos\alpha_j\nabla\zeta\cdot\bar{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\zeta\right]/\sqrt{g} \tag{166}$$

$$\frac{\partial}{\partial A_{\zeta,o,j,p}}\frac{\partial}{\partial A_{\theta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[-\bar{T}_{l,i}\cos\alpha_i\nabla\theta\cdot\bar{T}'_{p,j}\sin\alpha_j\,\mathbf{e}_\theta+\bar{T}_{p,j}\sin\alpha_j\nabla\zeta\cdot\bar{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\zeta\right]/\sqrt{g} \tag{167}$$

$$\frac{\partial}{\partial A_{\theta,e,j,p}}\frac{\partial}{\partial A_{\theta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[\cancel{+\bar{T}_{l,i}\sin\alpha_i\nabla\theta\cdot\bar{T}'_{p,j}\cos\alpha_j\,\mathbf{e}_\zeta}\cancel{+\bar{T}_{p,j}\cos\alpha_j\nabla\theta\cdot\bar{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\zeta}\right]/\sqrt{g} \tag{168}$$

$$\frac{\partial}{\partial A_{\theta,o,j,p}}\frac{\partial}{\partial A_{\theta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[\cancel{+\bar{T}_{l,i}\sin\alpha_i\nabla\theta\cdot\bar{T}'_{p,j}\sin\alpha_j\,\mathbf{e}_\zeta}\cancel{+\bar{T}_{p,j}\sin\alpha_j\nabla\theta\cdot\bar{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\zeta}\right]/\sqrt{g} \tag{169}$$

$$\frac{\partial}{\partial A_{\zeta,e,j,p}}\frac{\partial}{\partial A_{\theta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[-\bar{T}_{l,i}\sin\alpha_i\nabla\theta\cdot\bar{T}'_{p,j}\cos\alpha_j\,\mathbf{e}_\theta+\bar{T}_{p,j}\cos\alpha_j\nabla\zeta\cdot\bar{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\zeta\right]/\sqrt{g} \tag{170}$$

$$\frac{\partial}{\partial A_{\zeta,o,j,p}}\frac{\partial}{\partial A_{\theta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[-\bar{T}_{l,i}\sin\alpha_i\nabla\theta\cdot\bar{T}'_{p,j}\sin\alpha_j\,\mathbf{e}_\theta+\bar{T}_{p,j}\sin\alpha_j\nabla\zeta\cdot\bar{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\zeta\right]/\sqrt{g} \tag{171}$$

$$\frac{\partial}{\partial A_{\theta,e,j,p}}\frac{\partial}{\partial A_{\zeta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[+\bar{T}_{l,i}\cos\alpha_i\nabla\zeta\cdot\bar{T}'_{p,j}\cos\alpha_j\,\mathbf{e}_\zeta-\bar{T}_{p,j}\cos\alpha_j\nabla\theta\cdot\bar{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\theta\right]/\sqrt{g} \tag{172}$$

$$\frac{\partial}{\partial A_{\theta,o,j,p}}\frac{\partial}{\partial A_{\zeta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[+\bar{T}_{l,i}\cos\alpha_i\nabla\zeta\cdot\bar{T}'_{p,j}\sin\alpha_j\,\mathbf{e}_\zeta-\bar{T}_{p,j}\sin\alpha_j\nabla\theta\cdot\bar{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\theta\right]/\sqrt{g} \tag{173}$$

$$\frac{\partial}{\partial A_{\zeta,e,j,p}}\frac{\partial}{\partial A_{\zeta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[\cancel{-\bar{T}_{l,i}\cos\alpha_i\nabla\zeta\cdot\bar{T}'_{p,j}\cos\alpha_j\,\mathbf{e}_\theta}\cancel{-\bar{T}_{p,j}\cos\alpha_j\nabla\zeta\cdot\bar{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\theta}\right]/\sqrt{g} \tag{174}$$

$$\frac{\partial}{\partial A_{\zeta,o,j,p}}\frac{\partial}{\partial A_{\zeta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[\cancel{-\bar{T}_{l,i}\cos\alpha_i\nabla\zeta\cdot\bar{T}'_{p,j}\sin\alpha_j\,\mathbf{e}_\theta}\cancel{-\bar{T}_{p,j}\sin\alpha_j\nabla\zeta\cdot\bar{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\theta}\right]/\sqrt{g} \tag{175}$$

$$\frac{\partial}{\partial A_{\theta,e,j,p}}\frac{\partial}{\partial A_{\zeta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[+\bar{T}_{l,i}\sin\alpha_i\nabla\zeta\cdot\bar{T}'_{p,j}\cos\alpha_j\,\mathbf{e}_\zeta-\bar{T}_{p,j}\cos\alpha_j\nabla\theta\cdot\bar{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\theta\right]/\sqrt{g} \tag{176}$$

$$\frac{\partial}{\partial A_{\theta,o,j,p}}\frac{\partial}{\partial A_{\zeta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[+\bar{T}_{l,i}\sin\alpha_i\nabla\zeta\cdot\bar{T}'_{p,j}\sin\alpha_j\,\mathbf{e}_\zeta-\bar{T}_{p,j}\sin\alpha_j\nabla\theta\cdot\bar{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\theta\right]/\sqrt{g} \tag{177}$$

$$\frac{\partial}{\partial A_{\zeta,e,j,p}}\frac{\partial}{\partial A_{\zeta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[\cancel{-\bar{T}_{l,i}\sin\alpha_i\nabla\zeta\cdot\bar{T}'_{p,j}\cos\alpha_j\,\mathbf{e}_\theta}\cancel{-\bar{T}_{p,j}\cos\alpha_j\nabla\zeta\cdot\bar{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\theta}\right]/\sqrt{g} \tag{178}$$

$$\frac{\partial}{\partial A_{\zeta,o,j,p}}\frac{\partial}{\partial A_{\zeta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[\cancel{-\bar{T}_{l,i}\sin\alpha_i\nabla\zeta\cdot\bar{T}'_{p,j}\sin\alpha_j\,\mathbf{e}_\theta}\cancel{-\bar{T}_{p,j}\sin\alpha_j\nabla\zeta\cdot\bar{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\theta}\right]/\sqrt{g} \tag{179}$$

- In these expressions the terms $\nabla\theta\cdot\mathbf{e}_\theta=\nabla\zeta\cdot\mathbf{e}_\zeta=1$, and $\cancel{\nabla\theta\cdot\mathbf{e}_\zeta}=\cancel{\nabla\zeta\cdot\mathbf{e}_\theta}=0$ 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

$$\frac{\partial}{\partial v_{s,e,i,l}} \int dv \; \mathbf{v} \cdot \mathbf{v} \;\; = \;\; 2 \int dv \; \mathbf{v} \cdot \overline{T}_{l,i} \cos \alpha_i \nabla s \tag{180}$$

$$\frac{\partial}{\partial v_{s,o,i,l}} \int dv \; \mathbf{v} \cdot \mathbf{v} \;\; = \;\; 2 \int dv \; \mathbf{v} \cdot \overline{T}_{l,i} \sin \alpha_i \nabla s \tag{181}$$

$$\frac{\partial}{\partial v_{\theta,e,i,l}} \int dv \; \mathbf{v} \cdot \mathbf{v} \;\; = \;\; 2 \int dv \; \mathbf{v} \cdot \overline{T}_{l,i} \cos \alpha_i \nabla \theta \tag{182}$$

$$\frac{\partial}{\partial v_{\theta,o,i,l}} \int dv \; \mathbf{v} \cdot \mathbf{v} \;\; = \;\; 2 \int dv \; \mathbf{v} \cdot \overline{T}_{l,i} \sin \alpha_i \nabla \theta \tag{183}$$

$$\frac{\partial}{\partial v_{\zeta,e,i,l}} \int dv \; \mathbf{v} \cdot \mathbf{v} \;\; = \;\; 2 \int dv \; \mathbf{v} \cdot \overline{T}_{l,i} \cos \alpha_i \nabla \zeta \tag{184}$$

$$\frac{\partial}{\partial v_{\zeta,o,i,l}} \int dv \; \mathbf{v} \cdot \mathbf{v} \;\; = \;\; 2 \int dv \; \mathbf{v} \cdot \overline{T}_{l,i} \sin \alpha_i \nabla \zeta \tag{185}$$

$$\tag{186}$$

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

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

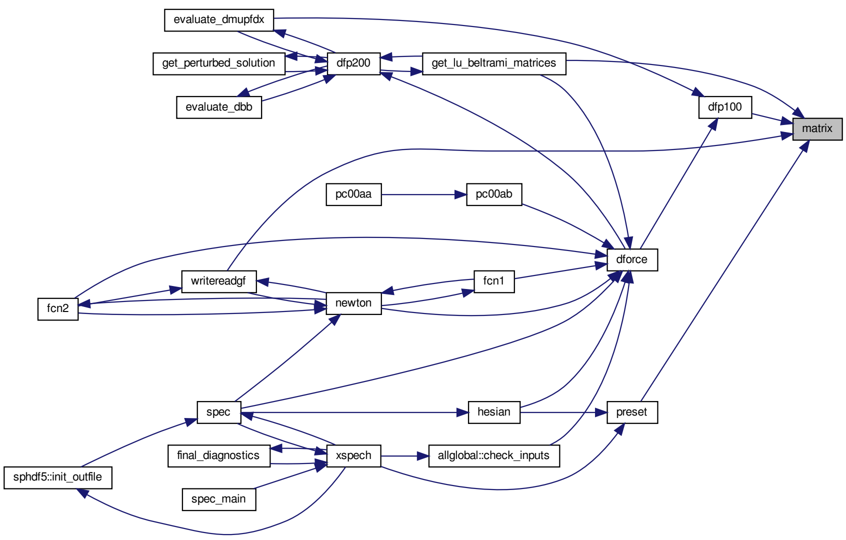
Parameters

in	*lvol*	
in	*mn*	
in	*lrad*	

References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::cpus, allglobal::dbdx, allglobal::ddttcc, allglobal::ddttcs, allglobal::ddttsc, allglobal::ddttss, allglobal::ddtzcc, allglobal::ddtzcs, allglobal::ddtzsc, allglobal::ddtzss, allglobal::ddzzcc, allglobal::ddzzcs, allglobal::ddzzsc, allglobal::ddzzss, allglobal::dma, allglobal::dmb, allglobal::dmd, allglobal::dmg, allglobal::dtoocc, allglobal::dtoocs, allglobal::dtoosc, allglobal::dtooss, allglobal::ibnc, allglobal::ibns, allglobal::im, allglobal::in, allglobal::ivnc, allglobal::ivns, allglobal::lcoordinatesingularity, allglobal::lma, allglobal::lmb, allglobal::lmc, allglobal::lmd, allglobal::lme, allglobal::lmf, allglobal::lmg, allglobal::lmh, allglobal::mpi_comm_spec, inputlist::mpol, allglobal::myid, allglobal::nadof, allglobal::ncpu, allglobal::notstellsym, constants::one, fileunits::ounit, allglobal::rtm, allglobal::rtt, numerical::small, allglobal::tdstcc, allglobal::tdstcs, allglobal::tdstsc, allglobal::tdstss, allglobal::tdszcc, allglobal::tdszcs, allglobal::tdszsc, allglobal::tdszss, allglobal::tt, allglobal::ttsscc, allglobal::ttsscs, allglobal::ttsssc, allglobal::ttssss, constants::two, inputlist::wmacros, allglobal::yesstellsym, and constants::zero.

Referenced by dfp100(), get_lu_beltrami_matrices(), preset(), and writereadgf().

Here is the caller graph for this function:



8.11.2.2 mtrxhs()

```
subroutine mtrxhs (
    integer, intent(in) lvol,
    integer, intent(in) mn,
    integer, intent(in) lrad,
    real, dimension(0:nadof(lvol)), intent(out) resultA,
    real, dimension(0:nadof(lvol)), intent(out) resultD,
    integer, intent(in) idx )
```

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

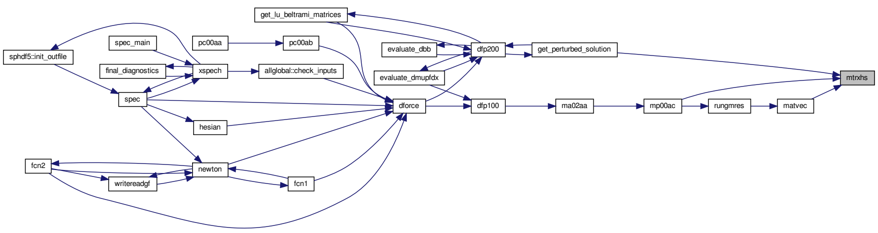
Parameters

lvol	
mn	
lrad	
resultA	
resultD	
idx	

References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::cpus, allglobal::dbdx, allglobal::dtc, allglobal::dts, allglobal::dzc, allglobal::dzs, constants::half, allglobal::im, allglobal::in, allglobal::lcoordinatesingularity, allglobal::lma, 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::mpi_comm_spec, inputlist::mpol, allglobal::myid, allglobal::nadof, allglobal::ncpu, allglobal::notstellsym, constants::one, fileunits::ounit, allglobal::rtm, allglobal::rtt, numerical::small, allglobal::tsc, allglobal::tss, allglobal::tt, allglobal::ttc, allglobal::tts, constants::two, 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:



8.11.2.3 spsmat()

```
subroutine spsmat (
    integer, intent(in) lvol,
    integer, intent(in) mn,
    integer, intent(in) lrad )
```

Constructs matrices for the precondtioner.

Preconditioner

GMRES iteratively looks for $\mathbf{a}_n$ that minimises the residual $\epsilon_{\text{GMRES}} = \|\hat{\mathcal{A}} \cdot \mathbf{a}_n - \mathbf{b}\|$, 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 $\mathbf{a}$ correspond to A_{θ,m_i,n_i,l_i} and A_{θ,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_{θ,m_i,n_i,l_i} and A_{θ,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

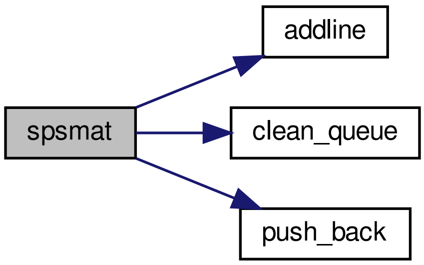
lvol	
mn	
lrad	

References addline(), clean_queue(), allglobal::cpus, allglobal::dma, allglobal::dmas, allglobal::dmb, allglobal::dmd, allglobal::dmds, allglobal::dmg, allglobal::idmas, allglobal::im, allglobal::in, allglobal::jdmas, allglobal

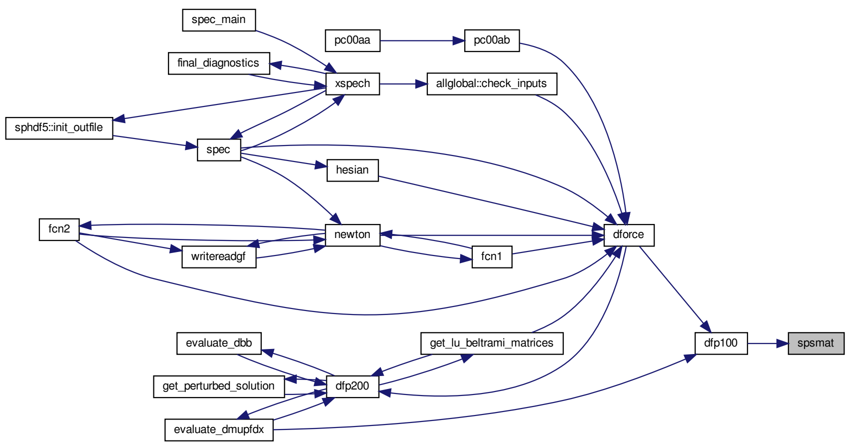
::liluprecond, allglobal::mpi_comm_spec, inputlist::mpol, allglobal::myid, allglobal::nadof, allglobal::ncpu, allglobal::ndmas, allglobal::ndmasmax, allglobal::notstellsym, constants::one, fileunits::ounit, push_back(), numerical::small, constants::two, inputlist::wmacros, allglobal::yesstellsym, and constants::zero.

Referenced by dfp100().

Here is the call graph for this function:



Here is the caller graph for this function:



8.12 Metric quantities

Functions/Subroutines

- subroutine metrix (lquad, lvol)

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

8.12.1 Detailed Description

8.12.2 Function/Subroutine Documentation

8.12.2.1 metrix()

```
subroutine metrix (
    integer, intent(in) lquad,
    integer, intent(in) lvol )
```

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. (θ, ζ), at a given radial location, i.e. where s is input.

plasma region

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

$$\begin{array}{lcl}
\sqrt{g}\; g^{ss} & = & \left(g_{\theta\theta} g_{\zeta\zeta} - g_{\theta\zeta} g_{\theta\zeta}\right) / \sqrt{g} \\
\sqrt{g}\; g^{s\theta} & = & \left(g_{\theta\zeta} g_{s\zeta} - g_{s\theta} g_{\zeta\zeta}\right) / \sqrt{g} \\
\sqrt{g}\; g^{s\zeta} & = & \left(g_{s\theta} g_{\theta\zeta} - g_{\theta\theta} g_{s\zeta}\right) / \sqrt{g} \\
\sqrt{g}\; g^{\theta\theta} & = & \left(g_{\zeta\zeta} g_{ss} - g_{s\zeta} g_{s\zeta}\right) / \sqrt{g} \\
\sqrt{g}\; g^{\theta\zeta} & = & \left(g_{s\zeta} g_{s\theta} - g_{\theta\zeta} g_{ss}\right) / \sqrt{g} \\
\sqrt{g}\; g^{\zeta\zeta} & = & \left(g_{ss} g_{\theta\theta} - g_{s\theta} g_{s\theta}\right) / \sqrt{g}
\end{array} \tag{187}$$

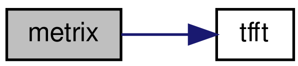
FFTs

- 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.)

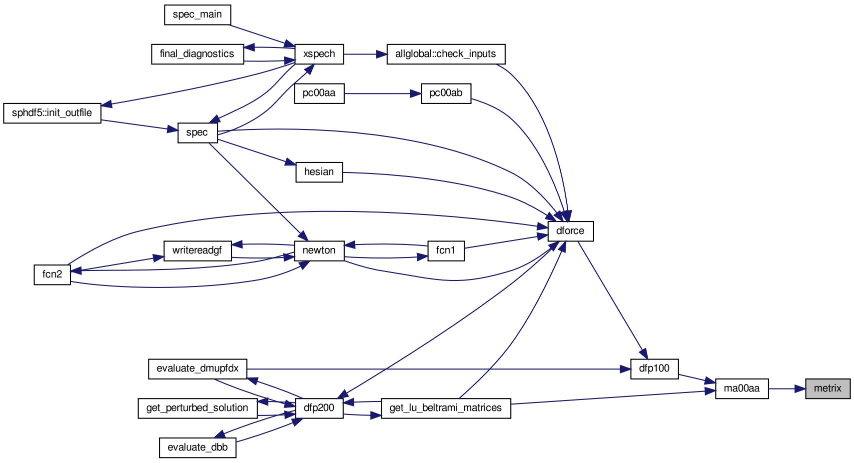
References allglobal::cfmn, allglobal::cpus, allglobal::dbdx, allglobal::efmn, allglobal::im, allglobal::ime, allglobal::in, allglobal::ine, allglobal::mn, allglobal::mne, allglobal::myid, allglobal::ncpu, allglobal::nt, allglobal::ntz, allglobal::nz, allglobal::ofmn, constants::one, fileunits::ounit, allglobal::sfmn, numerical::small, tfft(), and constants::zero.

Referenced by ma00aa().

Here is the call graph for this function:



Here is the caller graph for this function:



8.13 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

8.13.1 Detailed Description

8.13.2 Function/Subroutine Documentation

8.13.2.1 mp00ac()

```
subroutine mp00ac (
        integer, intent(in) Ndof,
        real, dimension(1:ndof), intent(in) Xdof,
        real, dimension(1:ndof) Fdof,
        real, dimension(1:ldfjac,1:ndof) Ddof,
        integer, intent(in) Ldfjac,
        integer iflag )
```

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

unpacking fluxes, helicity multiplier

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

construction of linear system

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

$$\mathcal{M} \cdot \mathbf{a} = \mathcal{R}, \tag{188}$$

where $\mathbf{a}$ 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 $\mathcal{A} \equiv \texttt{dMA}$ and $\mathcal{D} \equiv \texttt{dMD}$, which were constructed in matrix() , according to

$$\mathcal{M} \equiv \mathcal{A} - \mu \mathcal{D}. \tag{189}$$

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

$$\mathcal{R} \equiv -\left(\mathcal{B} - \mu \mathcal{E}\right) \cdot \boldsymbol{\psi} \tag{190}$$

  - if `Lcoordinatesingularity=F` and `Lplasmaregion=T` , then

$$\mathcal{R} \equiv -\mathcal{B} \cdot \boldsymbol{\psi} \tag{191}$$

  - if `Lcoordinatesingularity=F` and `Lvacuumregion=T` , then

$$\mathcal{R} \equiv -\mathcal{G} - \mathcal{B} \cdot \boldsymbol{\psi} \tag{192}$$

The quantities $\mathcal{B} \equiv \texttt{dMB}$, $\mathcal{E} \equiv \texttt{dME}$ and $\mathcal{G} \equiv \texttt{dMG}$ 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 $\mathbf{f}(\boldsymbol{\mu})$ 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:

$$\mathbf{f}(\mu, \Delta\psi_p) \equiv \left\{ \begin{array}{cccccccc} (& 0 & , & 0 &)^T, & \text{if } \texttt{Lconstraint} & = & -1 \\ (& 0 & , & 0 &)^T, & \text{if } \texttt{Lconstraint} & = & 0 \\ (& \cancel{\iota}(+1) - \texttt{iota (lvol)} & , & 0 &)^T, & \text{if } \texttt{Lconstraint} & = & 1 \\ (& ? & , & ? &)^T, & \text{if } \texttt{Lconstraint} & = & 2 \end{array} \right. \tag{193}$$

- For `Lcoordinatesingularity=F` , the returned function is:

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

vacuum region

- For the vacuum region, the returned function is:

$$\mathbf{f}(\Delta\psi_t,\Delta\psi_p) \equiv \left\{ \begin{array}{cccccccc} (& 0 & , & 0 &)^T, & \text{if } \texttt{Lconstraint} & = & -1 \\ (& I - \texttt{curtor} & , & G - \texttt{curpol} &)^T, & \text{if } \texttt{Lconstraint} & = & 0 \\ (& \iota\!\!\!-(-1) - \texttt{oita(lvol-1)} & , & G - \texttt{curpol} &)^T, & \text{if } \texttt{Lconstraint} & = & 1 \\ (& ? & , & ? &)^T, & \text{if } \texttt{Lconstraint} & = & 2 \end{array} \right. \quad (195)$$

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

early termination

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

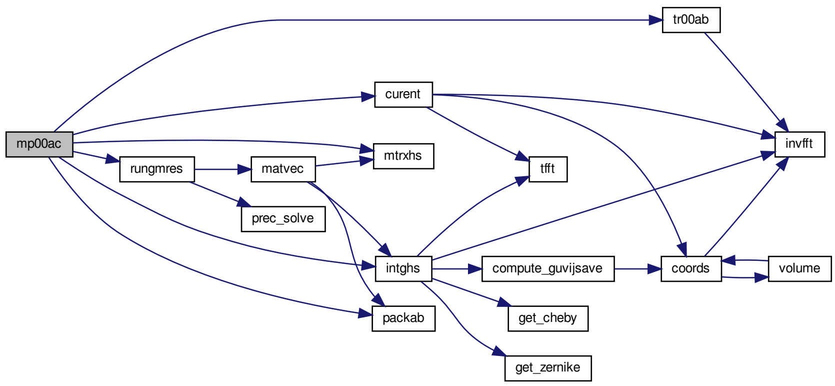
Parameters

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

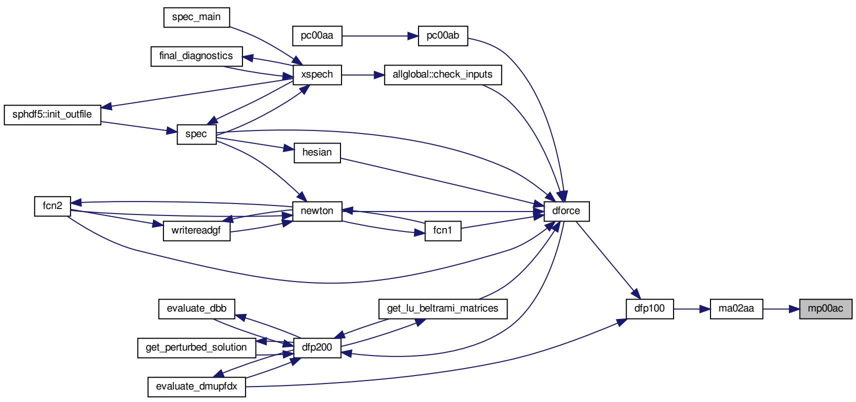
References allglobal::cpus, curent(), inputlist::curpol, inputlist::curtor, constants::half, inputlist::helicity, allglobal::im, allglobal::in, intghs(), inputlist::iota, allglobal::ivol, allglobal::lcoordinatesingularity, allglobal::lplasmaregion, inputlist::lrad, allglobal::lvacuumregion, numerical::machprec, allglobal::mn, allglobal::mns, allglobal::mpi_comm_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:



8.14 Force-driver

Functions/Subroutines

- subroutine newton (NGdof, position, ihybrd)

  Employs Newton method to find $\mathbf{F}(\mathbf{x}) = 0$, *where* $\mathbf{x} \equiv \{\mathrm{geometry}\}$ *and* $\mathbf{F}$ *is defined in dforce() .*
- subroutine writereadgf (readorwrite, NGdof, ireadhessian)

  read or write force-derivative matrix
- subroutine fcn1 (NGdof, xx, fvec, irevcm)

  fcn1
- subroutine fcn2 (NGdof, xx, fvec, fjac, Ldfjac, irevcm)

  fcn2

8.14.1 Detailed Description

8.14.2 Function/Subroutine Documentation

8.14.2.1 newton()

```
subroutine newton (
        integer, intent(in) NGdof,
        real, dimension(0:ngdof), intent(inout) position,
        integer, intent(out) ihybrd )
```

Employs Newton method to find $\mathbf{F}(\mathbf{x}) = 0$, where $\mathbf{x} \equiv \{\mathrm{geometry}\}$ and $\mathbf{F}$ is defined in dforce() .

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 $\mathbf{x} \equiv \{\mathrm{geometry}\} \equiv \{R_{i,l}, Z_{i,l}\}$ 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 .

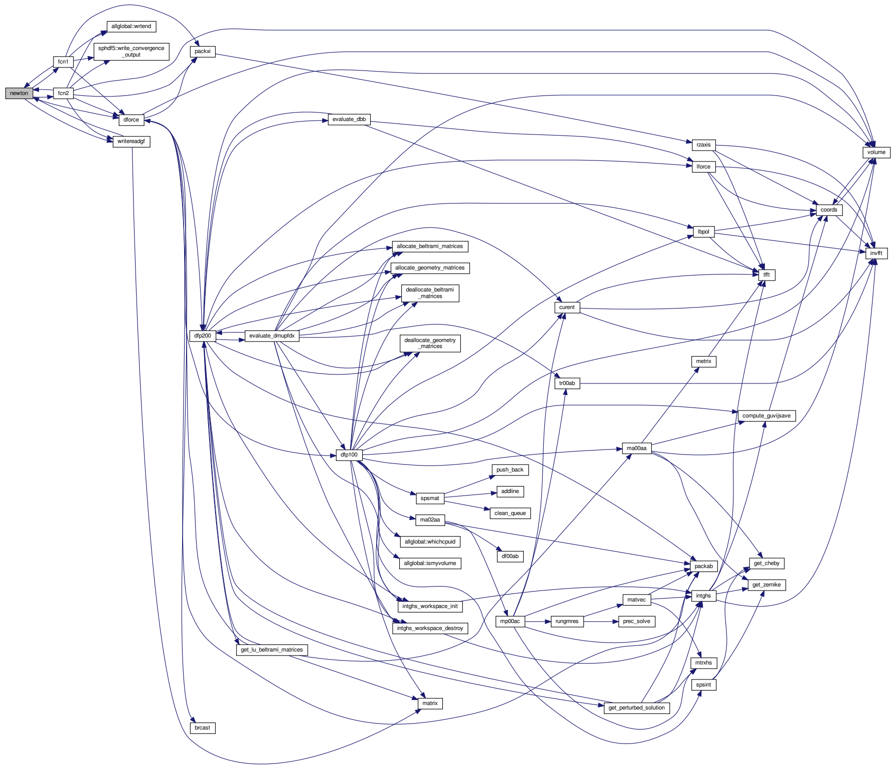
Parameters

`in`	*NGdof*	
`in,out`	*position*	
`out`	*ihybrd*	

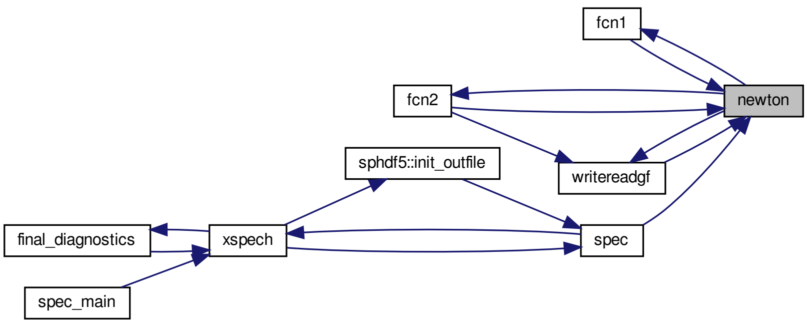
References allglobal::bbe, allglobal::bbo, allglobal::cpus, allglobal::dbbdmp, allglobal::dessian, allglobal::dffdrz, dforce(), allglobal::dmupfdx, allglobal::energy, fcn1(), fcn2(), allglobal::forceerr, allglobal::hessian, inputlist::igeometry, allglobal::iie, allglobal::iio, allglobal::im, allglobal::in, allglobal::irbc, allglobal::irbs, allglobal::izbc, allglobal::izbs, newtontime::lastcpu, allglobal::lgdof, allglobal::lhessianallocated, 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:



8.14.2.2 writereadgf()

```
subroutine writereadgf (
        character, intent(in) readorwrite,
        integer, intent(in) NGdof,
        integer, intent(out) ireadhessian )
```

read or write force-derivative matrix

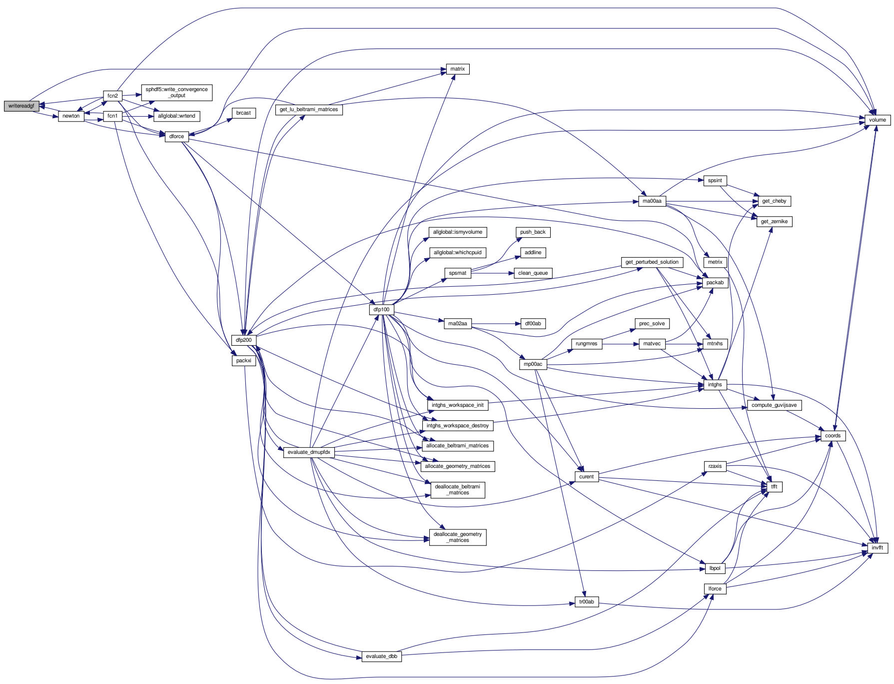
Parameters

`in`	*readorwrite*	
`in`	*NGdof*	
`out`	*ireadhessian*	

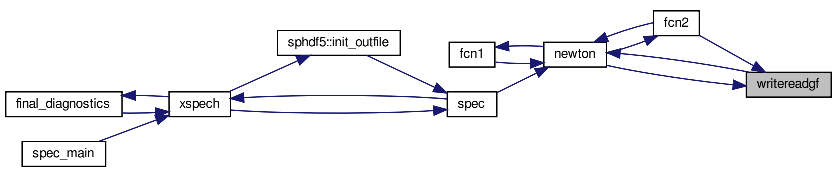
References allglobal::cpus, fileunits::dunit, allglobal::hessian, inputlist::igeometry, allglobal::im, allglobal::in, inputlist::istellsym, inputlist::lfreebound, allglobal::lhessianallocated, matrix(), allglobal::mn, allglobal::mpi_comm↩_spec, inputlist::mpol, allglobal::myid, newton(), inputlist::ntor, inputlist::nvol, fileunits::ounit, and constants::zero.

Referenced by fcn2(), and newton().

Here is the call graph for this function:



Here is the caller graph for this function:



8.14.2.3 fcn1()

```
subroutine fcn1 (
        integer, intent(in) NGdof,
        real, dimension(1:ngdof), intent(in) xx,
        real, dimension(1:ngdof), intent(out) fvec,
        integer, intent(in) irevcm )
```

fcn1

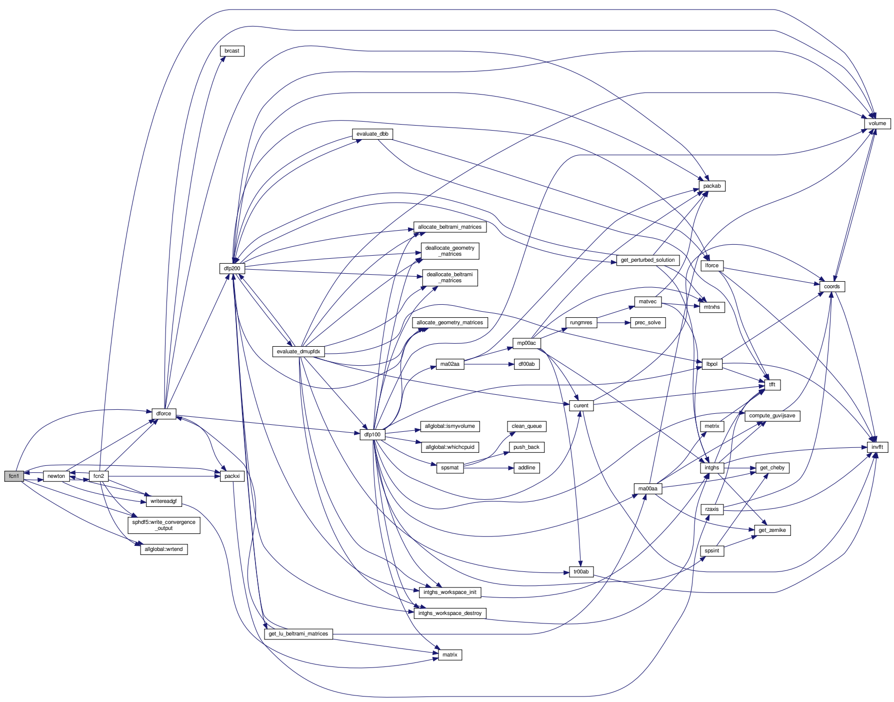
Parameters

in	*NGdof*	
in	*xx*	
out	*fvec*	
in	*irevcm*	

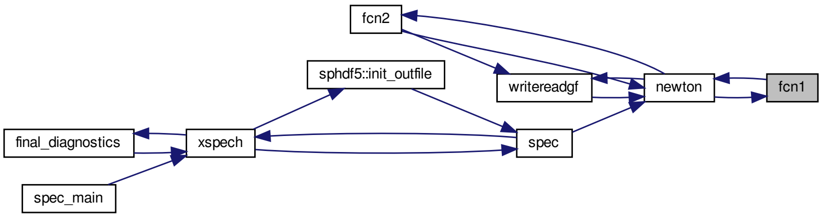
References allglobal::bbe, allglobal::bbo, allglobal::cpus, allglobal::dbbdmp, allglobal::dessian, allglobal::dffdrz, dforce(), allglobal::dmupfdx, allglobal::energy, allglobal::forceerr, allglobal::hessian, inputlist::igeometry, allglobal::iie, allglobal::iio, allglobal::im, allglobal::in, allglobal::irbc, allglobal::irbs, allglobal::izbc, allglobal::izbs, newtontime::lastcpu, allglobal::lgdof, allglobal::lhessianallocated, 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:



8.14.2.4 fcn2() `subroutine fcn2 (`

```
integer, intent(in) NGdof,
real, dimension(1:ngdof), intent(in) xx,
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

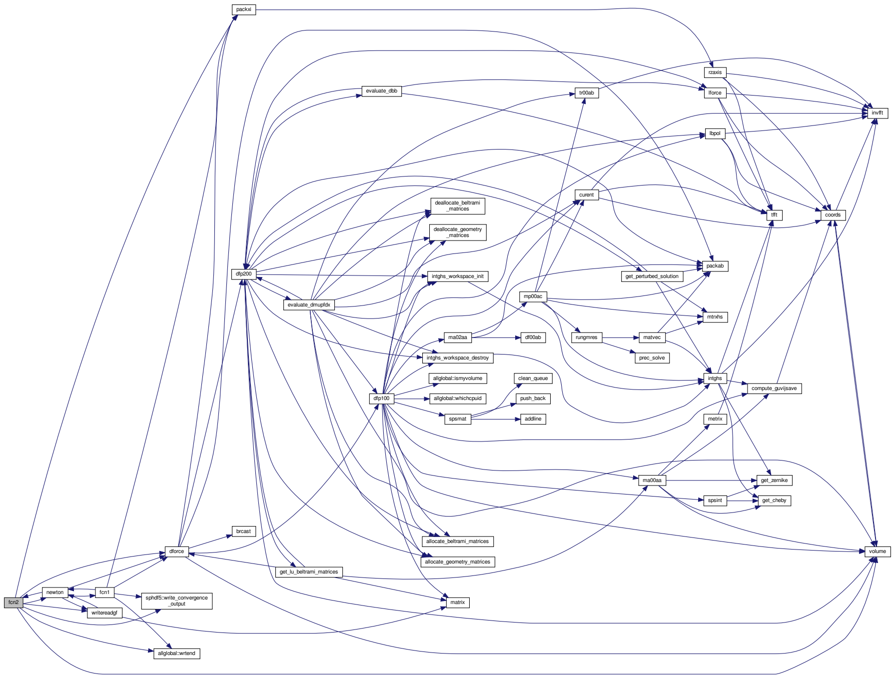
Parameters

in	*NGdof*	
in	*xx*	
out	*fvec*	
out	*fjac*	
in	*Ldfjac*	
in	*irevcm*	

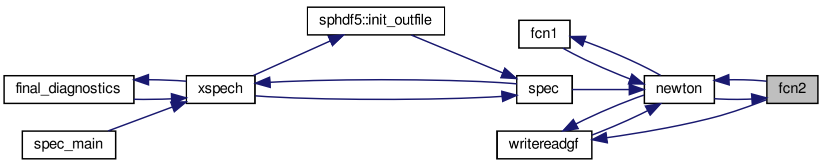
References allglobal::bbe, allglobal::bbo, allglobal::cpus, allglobal::dbbdmp, allglobal::dessian, allglobal::dffdrz, dforce(), allglobal::dmupfdx, allglobal::energy, allglobal::forceerr, allglobal::hessian, inputlist::igeometry, allglobal::iie, allglobal::iio, allglobal::im, allglobal::in, allglobal::irbc, allglobal::irbs, allglobal::izbc, allglobal::izbs, newtontime::lastcpu, allglobal::lgdof, allglobal::lhessianallocated, 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, 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:



8.15 Some miscellaneous numerical routines

Functions/Subroutines

- subroutine gi00ab (Mpol, Ntor, Nfp, mn, im, in)

    Assign Fourier mode labels.
- subroutine tfft (Nt, Nz, ijreal, ijimag, mn, im, in, efmn, ofmn, cfmn, sfmn, ifail)

    Forward Fourier transform (fftw wrapper)
- subroutine invfft (mn, im, in, efmn, ofmn, cfmn, sfmn, Nt, Nz, ijreal, ijimag)

    Inverse Fourier transform (fftw wrapper)
- subroutine gauleg (n, weight, abscis, ifail)

    Gauss-Legendre weights and abscissae.

8.15.1 Detailed Description

8.15.2 Function/Subroutine Documentation

8.15.2.1 gi00ab()

```
subroutine gi00ab (
    integer, intent(in) Mpol,
    integer, intent(in) Ntor,
    integer, intent(in) Nfp,
    integer, intent(in) mn,
    integer, dimension(mn), intent(out) im,
    integer, dimension(mn), intent(out) in )
```

Assign Fourier mode labels.

- This routine assigns the Fourier mode labels that converts a double-sum into a single sum; i.e., the m_j and n_j are assigned where

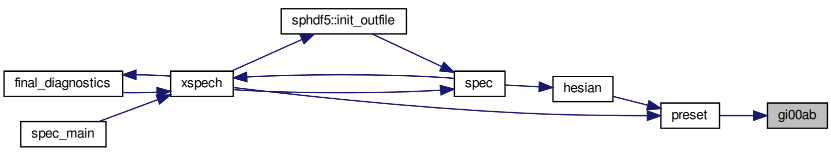
$$f(\theta,\zeta) = \sum_{n=0}^{N} f_{0,n} \cos(-n\,N_P\,\zeta) + \sum_{m=1}^{M} \sum_{n=-N}^{N} f_{m,n} \cos(m\theta - n\,N_P\,\zeta) \tag{196}$$

$$= \sum_{j} f_j \cos(m_j\theta - n_j\zeta), \tag{197}$$

where $N \equiv \texttt{Ntor}$ and $M \equiv \texttt{Mpol}$ are given on input, and $N_P \equiv \texttt{Nfp}$ is the field periodicity.

Referenced by preset().

Here is the caller graph for this function:



8.15.2.2 tfft()

```
subroutine tfft (
    integer Nt,
    integer Nz,
    real, dimension(1:nt*nz) ijreal,
    real, dimension(1:nt*nz) ijimag,
    integer mn,
    integer, dimension(1:mn) im,
    integer, dimension(1:mn) in,
    real, dimension(1:mn) efmn,
    real, dimension(1:mn) ofmn,
    real, dimension(1:mn) cfmn,
    real, dimension(1:mn) sfmn,
    integer ifail )
```

Forward Fourier transform (fftw wrapper)

- This constructs the "forward" Fourier transform.
- Given a set of data, (f_i, g_i) for $i = 1, \ldots N_\theta N_\zeta$, on a regular two-dimensional angle grid, where $\theta_j = 2\pi j/N_\theta$ for $j = 0, N_\theta - 1$, and $\zeta_k = 2\pi k/N_\zeta$ for $k = 0, N_\zeta - 1$. The "packing" is governed by $i = 1 + j + kN_\theta$. The "discrete" resolution is $N_\theta \equiv \texttt{Nt}$, $N_\zeta \equiv \texttt{Nz}$ and $\texttt{Ntz} = \texttt{Nt} \times \texttt{Nz}$, which are set in preset() .
- The Fourier harmonics consistent with Eqn. (197) are constructed. The mode identification labels appearing in Eqn. (197) are $m_j \equiv \texttt{im(j)}$ and $n_j \equiv \texttt{in(j)}$, which are set in readin() via a call to gi00ab() .

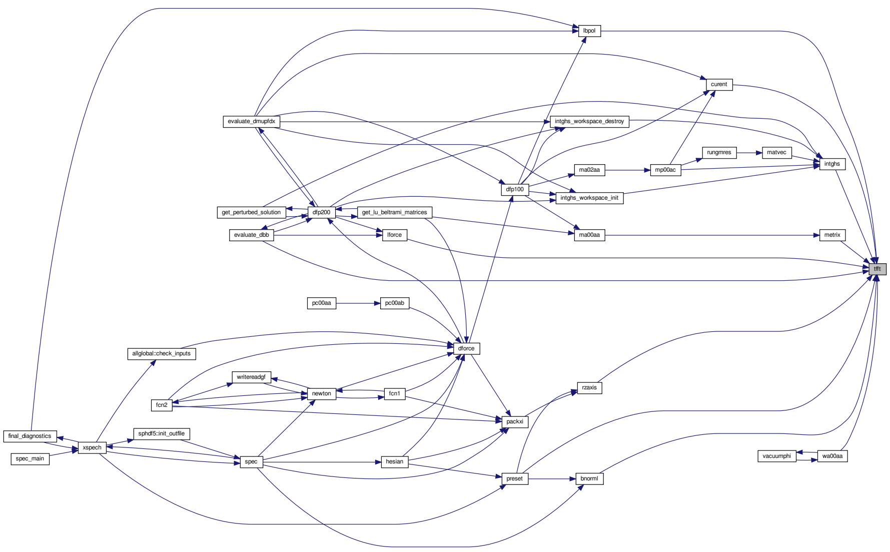
Parameters

Nt	
Nz	
ijreal	
ijimag	
mn	
im	
in	
efmn	
ofmn	
cfmn	
sfmn	
ifail	

References fftw_interface::cplxin, fftw_interface::cplxout, constants::half, inputlist::nfp, fileunits::ounit, constants::pi2, fftw_interface::planf, and constants::zero.

Referenced by bnorml(), curent(), evaluate_dbb(), intghs(), lbpol(), lforce(), metrix(), preset(), rzaxis(), and wa00aa().

Here is the caller graph for this function:



8.15.2.3 invfft()

```
subroutine invfft (
    integer, intent(in) mn,
    integer, dimension(mn), intent(in) im,
    integer, dimension(mn), intent(in) in,
    real, dimension(mn), intent(in) efmn,
    real, dimension(mn), intent(in) ofmn,
    real, dimension(mn), intent(in) cfmn,
    real, dimension(mn), intent(in) sfmn,
    integer, intent(in) Nt,
    integer, intent(in) Nz,
    real, dimension(nt*nz), intent(out) ijreal,
    real, dimension(nt*nz), intent(out) ijimag )
```

Inverse Fourier transform (fftw wrapper)

- Given the Fourier harmonics, the data on a regular angular grid are constructed.
- This is the inverse routine to tfft() .

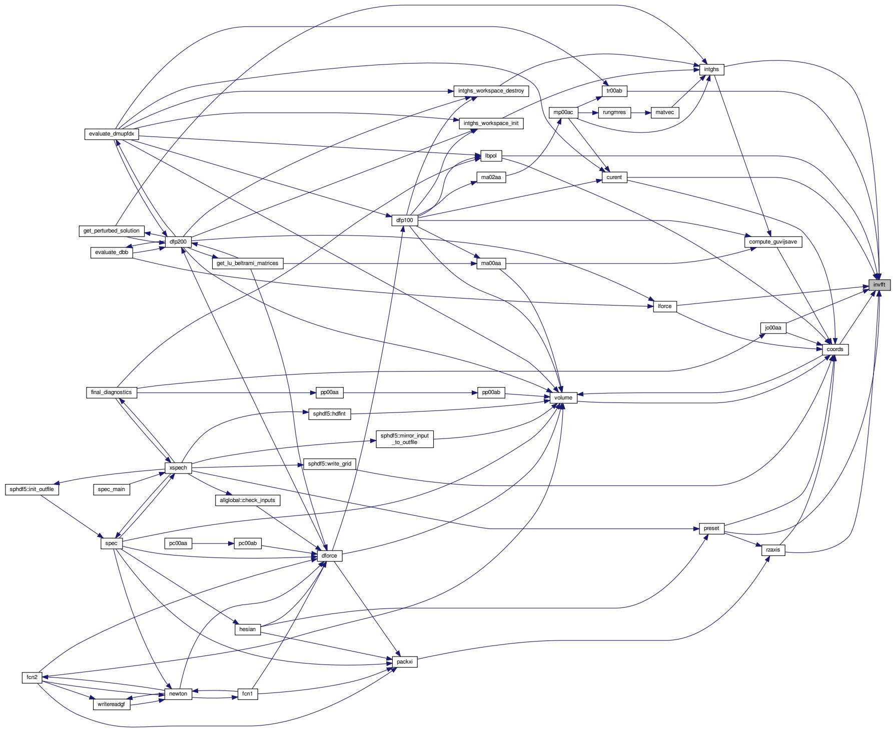
Parameters

in	*mn*	
in	*im*	
in	*in*	
in	*efmn*	
in	*ofmn*	
in	*cfmn*	
in	*sfmn*	
in	*Nt*	
in	*Nz*	
out	*ijreal*	
out	*ijimag*	

References fftw_interface::cplxin, fftw_interface::cplxout, constants::half, inputlist::nfp, fftw_interface::planb, constants::two, and constants::zero.

Referenced by coords(), curent(), intghs(), jo00aa(), lbpol(), lforce(), preset(), rzaxis(), and tr00ab().

Here is the caller graph for this function:



8.15.2.4 gauleg()

```
subroutine gauleg (
    integer, intent(in) n,
    real, dimension(n), intent(out) weight,
    real, dimension(n), intent(out) abscis,
    integer, intent(out) ifail )
```

Gauss-Legendre weights and abscissae.

- Compute Gaussian integration weights and abscissae.
- From Numerical Recipes.

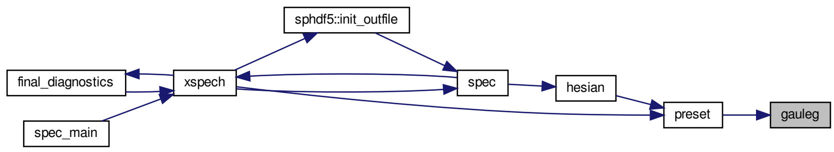
Parameters

in	*n*	
out	*weight*	
out	*abscis*	
out	*ifail*	

References constants::one, constants::pi, constants::two, and constants::zero.

Referenced by preset().

Here is the caller graph for this function:



8.16 "packing" of Beltrami field solution vector

Functions/Subroutines

- subroutine packab (packorunpack, lvol, 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.

8.16.1 Detailed Description

8.16.2 Function/Subroutine Documentation

8.16.2.1 packab()

```
subroutine packab (
        character, intent(in) packorunpack,
        integer, intent(in) lvol,
        integer, intent(in) NN,
        real, dimension(1:nn) solution,
        integer, intent(in) ideriv )
```

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:

$$\mathbf{x} \equiv \{A_{\theta,e,i,l}, A_{\zeta,e,i,l}, A_{\theta,o,i,l}, A_{\zeta,o,i,l}, a_i, b_i, c_i, d_i, e_i, f_i, g_1, h_1\}. \quad (198)$$

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

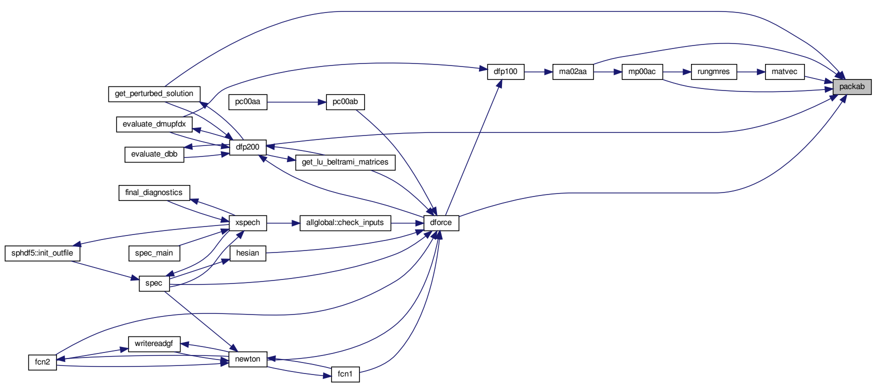
Parameters

packorunpack	
lvol	
NN	
solution	
ideriv	

References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::cpus, allglobal::im, allglobal::in, allglobal::lma, 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, inputlist::lrad, 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:



8.16.2.2 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) iZbs,
        real, dimension(1:mn,0:mvol) iRbs,
        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, $\boldsymbol{\xi}$, so that standard numerical routines can be called to find solutions to force-balance, i.e. $\mathbf{F}[\boldsymbol{\xi}] = 0$.
- A coordinate "pre-conditioning" factor is included:

$$\boldsymbol{\xi}_k \equiv \frac{R_{j,v}}{\Psi_{j,v}}, \tag{199}$$

where $\Psi_{j,v} \equiv$ `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,

$$R_0(\zeta) \equiv \frac{\int_0^{2\pi} R_1(\theta,\zeta) dl}{L(\zeta)}, \qquad Z_0(\zeta) \equiv \frac{\int_0^{2\pi} Z_1(\theta,\zeta) dl}{L(\zeta)}, \tag{200}$$

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 θ, i.e. if θ 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 θ to construct $L \equiv \int dl$ is now trivial: just multiply the $m = 0$ harmonics of dl by 2π. 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.

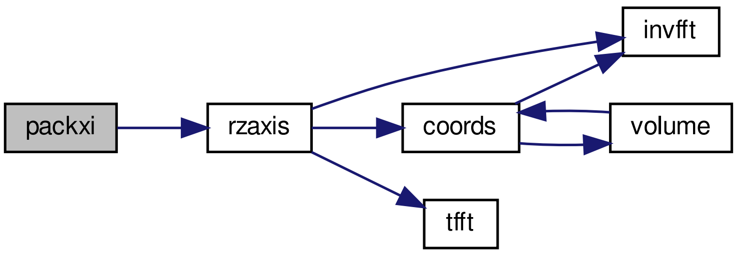
Parameters

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

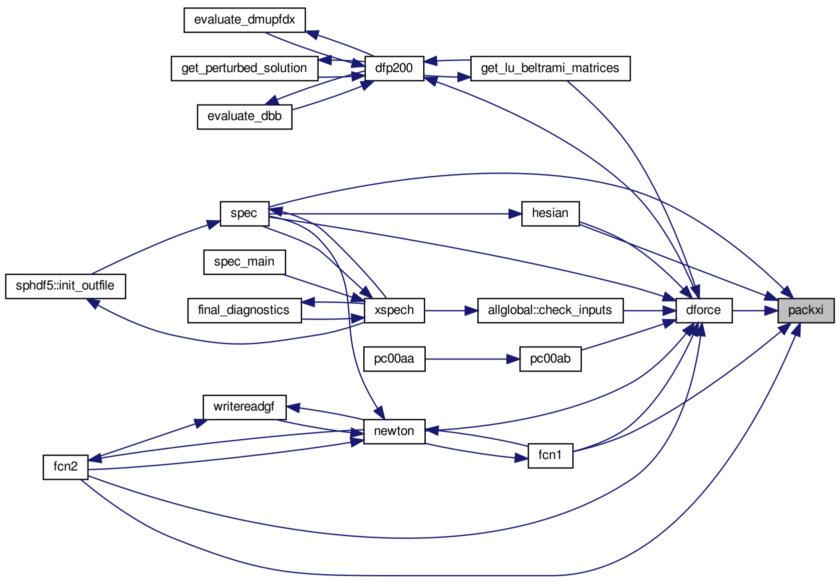
References allglobal::ajk, allglobal::cfmn, allglobal::comn, allglobal::cpus, allglobal::efmn, allglobal::evmn, inputlist::igeometry, allglobal::ijimag, allglobal::ijreal, allglobal::im, allglobal::in, allglobal::irij, allglobal::izij, allglobal↩ ::jiimag, allglobal::jireal, inputlist::lfindzero, allglobal::mpi_comm_spec, allglobal::myid, allglobal::ncpu, allglobal↩ ::notstellsym, allglobal::nt, inputlist::ntor, allglobal::ntz, inputlist::nvol, allglobal::nz, allglobal::odmn, allglobal::ofmn, fileunits::ounit, allglobal::psifactor, allglobal::rscale, rzaxis(), allglobal::sfmn, allglobal::simn, allglobal::trij, allglobal↩ ::tzij, 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:



8.17 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.

8.17.1 Detailed Description

8.17.2 Function/Subroutine Documentation

8.17.2.1 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

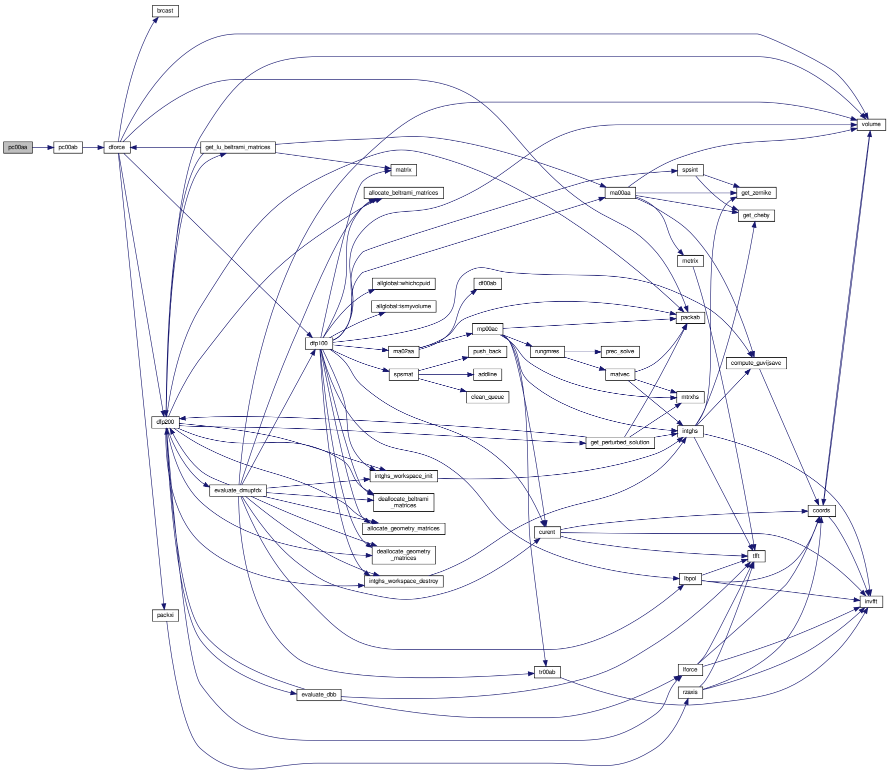
- The following input variables control the operation of `E04DGF` :
  - `epsilon` : weighting of "spectral energy"; see pc00ab()
  - `maxstep` : this is given to `E04DGF` for the `Maximum Step Length`
  - `maxiter` : upper limit on derivative calculations used in the conjugate gradient iterations
  - `verify` : if `verify=1`, then `E04DGF` will confirm user supplied gradients (provided by pc00ab()) are correct;
- **Todo** Unfortunately, `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:



8.17.2.2 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

$$F \equiv \sum_{l=1}^{N} \int_{\mathcal{V}} \left(\frac{p}{\gamma - 1} + \frac{B^2}{2} \right) dv, \tag{201}$$

  where $N \equiv$ `Nvol` is the number of interfaces.

- Assuming that the toroidal and poloidal fluxes, ψ_t and ψ_p, the helicity, $\mathcal{K}$, the helicity multiplier, μ, and/or the interface rotational-transforms, $\iota\!\!\!-$, 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

$$\begin{aligned}\frac{\partial R_j}{\partial t} &\equiv -\frac{\partial}{\partial R_j}\sum_{l=1}^{N}\int\left(\frac{p}{\gamma-1}+\frac{B^2}{2}\right)dv,\\ \frac{\partial Z_j}{\partial t} &\equiv -\frac{\partial}{\partial Z_j}\sum_{l=1}^{N}\int\left(\frac{p}{\gamma-1}+\frac{B^2}{2}\right)dv.\end{aligned} \tag{202}$$

- 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,

$$\delta R = R_\theta\, u, \tag{203}$$

$$\delta Z = Z_\theta\, u, \tag{204}$$

where u is a angle variation.

- The corresponding variation in each of the Fourier harmonics is

$$\delta R_j \equiv \oint\!\!\oint d\theta d\zeta\;\; R_\theta\; u\; \cos\alpha_j, \tag{205}$$

$$\delta Z_j \equiv \oint\!\!\oint d\theta d\zeta\;\; Z_\theta\; u\; \sin\alpha_j, \tag{206}$$

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

$$M \equiv \frac{\sum_j (m_j^p + n_j^q)(R_{l,j}^2 + Z_{l,j}^2)}{\sum_j (R_{l,j}^2 + Z_{l,j}^2)}, \tag{207}$$

- Using the notation

$$N \equiv \sum_j \lambda_j (R_{l,j}^2 + Z_{l,j}^2), \tag{208}$$

$$D \equiv \sum_j (R_{l,j}^2 + Z_{l,j}^2), \tag{209}$$

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

$$\delta M = (\delta N - M\delta D)/D. \tag{210}$$

- For tangential variations,

$$\delta N = 2\oint\!\!\oint d\theta d\zeta\;\; u\left(R_\theta \sum_j \lambda_j R_j \cos\alpha_j + Z_\theta \sum_j \lambda_j Z_j \sin\alpha_j\right), \tag{211}$$

$$\delta D = 2\oint\!\!\oint d\theta d\zeta\;\; u\left(R_\theta \sum_j R_j \cos\alpha_j + Z_\theta \sum_j Z_j \sin\alpha_j\right). \tag{212}$$

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

$$\frac{\partial u}{\partial t} = -\left[R_\theta \sum_j (\lambda_j - M) R_j \cos\alpha_j / D + Z_\theta \sum_j (\lambda_j - M) Z_j \sin\alpha_j / D\right]. \tag{213}$$

- This suggests that position should be advanced according to

$$\frac{\partial R_j}{\partial t} \equiv -\frac{\partial}{\partial R_j}\sum_{l=1}^{N}\int\left(\frac{p}{\gamma-1}+\frac{B^2}{2}\right)dv - [R_\theta(R_\theta X + Z_\theta Y)]_j, \qquad (214)$$

$$\frac{\partial Z_j}{\partial t} \equiv -\frac{\partial}{\partial Z_j}\sum_{l=1}^{N}\int\left(\frac{p}{\gamma-1}+\frac{B^2}{2}\right)dv - [Z_\theta(R_\theta X + Z_\theta Y)]_j, \qquad (215)$$

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,

$$R_\theta(R_\theta X + Z_\theta Y) = \sum_{j,k,l} m_j m_k(\lambda_l - M)R_j(+R_k R_l \sin\alpha_j \sin\alpha_k \cos\alpha_l - Z_k Z_l \sin\alpha_j \cos\alpha_k \sin\alpha_l)(216)$$

$$Z_\theta(R_\theta X + Z_\theta Y) = \sum_{j,k,l} m_j m_k(\lambda_l - M)Z_j(-R_k R_l \cos\alpha_j \sin\alpha_k \cos\alpha_l + Z_k Z_l \cos\alpha_j \cos\alpha_k \sin\alpha_l)(217)$$

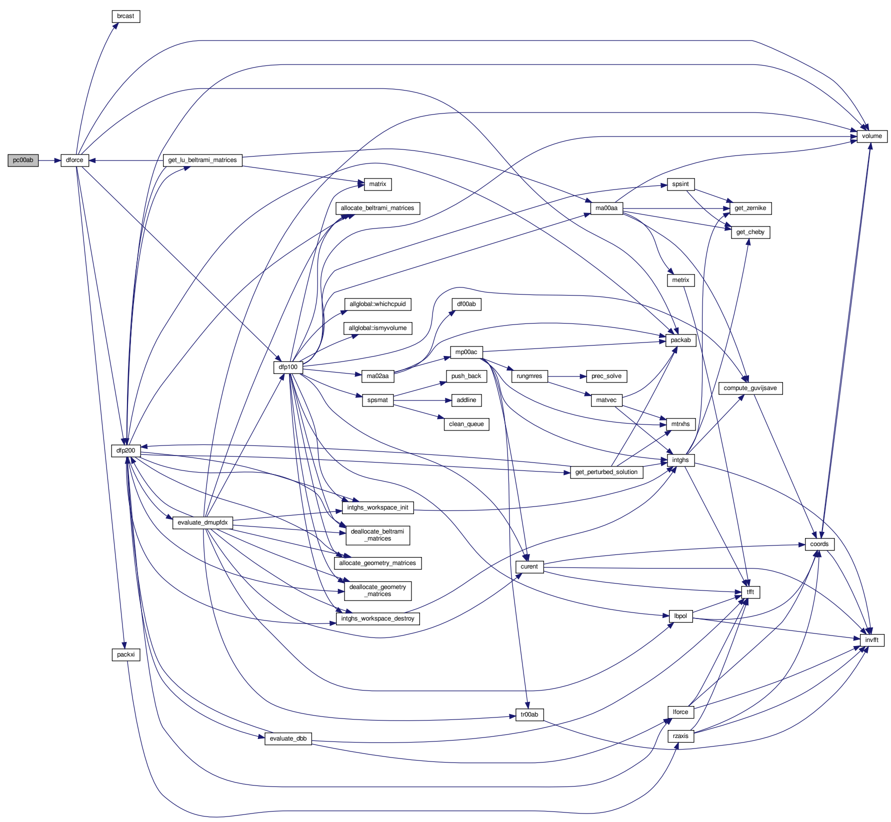
are calculated using triple angle expressions...

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

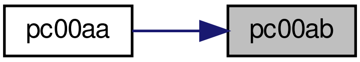
References allglobal::cpus, allglobal::dbbdrz, dforce(), allglobal::diidrz, inputlist::epsilon, allglobal::forceerr, inputlist::forcetol, constants::half, inputlist::igeometry, allglobal::lbbintegral, allglobal::mn, allglobal::myid, inputlist::nvol, constants::one, fileunits::ounit, allglobal::yesstellsym,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

Referenced by pc00aa().

Here is the call graph for this function:



Here is the caller graph for this function:



8.18 Initialization of the code

Functions/Subroutines

- subroutine preset

  Allocates and initializes internal arrays.

8.18.1 Detailed Description

8.18.2 Function/Subroutine Documentation

8.18.2.1 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

$$\iota\!\!\!- \equiv \frac{p_l + \gamma p_r}{q_l + \gamma q_r}, \tag{218}$$

  where $p_l \equiv$ `pl`, $q_l \equiv$ `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 $\Phi_{edge} \equiv$ phiedge .
- $\psi_{tor} \equiv$ tflux and $\psi_{pol} \equiv$ pflux are immediately normalized (in readin()) according to $\psi_{tor,i} \rightarrow \psi_{tor,i}/\psi_0$ and $\psi_{pol,i} \rightarrow \psi_{pol,i}/\psi_0$, 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

$$\texttt{sweight}_v \equiv \texttt{upsilon} \times (l_v/N_{vol})^w, \tag{219}$$

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 $s = -1$ and $s = +1$.
- Precisely, TT(l,i,d) $\equiv T_l^{(d)}(s_i)$ 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

$$T_l(-1) = \begin{cases} +1, & \text{if } l \text{ is even,} \\ -1, & \text{if } l \text{ is odd;} \end{cases} \qquad T_l(+1) = \begin{cases} +1, & \text{if } l \text{ is even,} \\ +1, & \text{if } l \text{ is odd;} \end{cases} \tag{220}$$

$$T_l'(-1) = \begin{cases} -l^2, & \text{if } l \text{ is even,} \\ +l^2, & \text{if } l \text{ is odd;} \end{cases} \qquad T_l'(+1) = \begin{cases} +l^2, & \text{if } l \text{ is even,} \\ +l^2, & \text{if } l \text{ is odd.} \end{cases} \tag{221}$$

- TT(0:Mrad,0:1,0:1) is used in routines that explicity require interface information, such as
  - the interface force-balance routine, lforce()
  - 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 second-partial 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,

$$\sum_i f_i \cos(m_i\theta - n_i\zeta) \equiv \sum_{n=0}^{N_0} f_{0,n} \cos(-n\zeta) + \sum_{m=1}^{M_0} \sum_{n=-N_0}^{N_0} f_{m,n} \cos(m\theta - n\zeta), \tag{222}$$

and the same representation but with enhanced resolution,

$$\sum_k \bar{f}_k \cos(\bar{m}_k\theta - \bar{n}_k\zeta) \equiv \sum_{n=0}^{N_1} f_{0,n} \cos(-n\zeta) + \sum_{m=1}^{M_1} \sum_{n=-N_1}^{N_1} f_{m,n} \cos(m\theta - n\zeta), \tag{223}$$

with $M_1 \geq M_0$ and $N_1 \geq N_0$; then $k_i \equiv$ `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 $\alpha_k \equiv m_k\theta - n_k\zeta$,

$$\oint\!\!\oint d\theta d\zeta \;\; \bar{g}^{\mu\nu} \cos\alpha_i \;\; \cos\alpha_j \;\; = \;\; \frac{1}{2}\oint\!\!\oint d\theta d\zeta \;\; \bar{g}^{\mu\nu}(+\cos\alpha_{k_{ij+}} + \cos\alpha_{k_{ij-}}), \tag{224}$$

$$\oint\!\!\oint d\theta d\zeta \;\; \bar{g}^{\mu\nu} \cos\alpha_i \;\; \sin\alpha_j \;\; = \;\; \frac{1}{2}\oint\!\!\oint d\theta d\zeta \;\; \bar{g}^{\mu\nu}(+\sin\alpha_{k_{ij+}} - \sin\alpha_{k_{ij-}}), \tag{225}$$

$$\oint\!\!\oint d\theta d\zeta \;\; \bar{g}^{\mu\nu} \sin\alpha_i \;\; \cos\alpha_j \;\; = \;\; \frac{1}{2}\oint\!\!\oint d\theta d\zeta \;\; \bar{g}^{\mu\nu}(+\sin\alpha_{k_{ij+}} + \sin\alpha_{k_{ij-}}), \tag{226}$$

$$\oint\!\!\oint d\theta d\zeta \;\; \bar{g}^{\mu\nu} \sin\alpha_i \;\; \sin\alpha_j \;\; = \;\; \frac{1}{2}\oint\!\!\oint d\theta d\zeta \;\; \bar{g}^{\mu\nu}(-\cos\alpha_{k_{ij+}} + \cos\alpha_{k_{ij-}}), \tag{227}$$

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. (223) 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 $T_l(s) = 2\,s\,T_{l-1}(s) - T_{l-2}(s)$.
- 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. $\displaystyle\int f(s)ds = \sum_k \omega_k f(s_k)$.
- 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;

$$\texttt{BBweight}_i \equiv \texttt{opsilon} \times \exp\left[-\texttt{escale} \times (m_i^2 + n_i^2)\right] \tag{228}$$

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

mmpp(1:mn): spectral condensation weight factors

- spectral condensation weight factors;

$$\texttt{mmpp(i)} \equiv m_i^p, \tag{229}$$

where $p \equiv$ `pcondense` .

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

- `NAdof(1:Mvol)` $\equiv$ 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

$$A_\theta(s,\theta,\zeta) = \sum_{i,l} A_{\theta,e,i,l}\, \overline{T}_{l,i}(s) \cos\alpha_i + \sum_{i,l} A_{\theta,o,i,l}\, \overline{T}_{l,i}(s) \sin\alpha_i, \tag{230}$$

$$A_\zeta(s,\theta,\zeta) = \sum_{i,l} A_{\zeta,e,i,l}\, \overline{T}_{l,i}(s) \cos\alpha_i + \sum_{i,l} A_{\zeta,o,i,l}\, \overline{T}_{l,i}(s) \sin\alpha_i, \tag{231}$$

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

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

$$A_{\theta,e,i,l} \equiv \texttt{Ate(v,0,j)\%s(l)}, \tag{232}$$
$$A_{\zeta,e,i,l} \equiv \texttt{Aze(v,0,j)\%s(l)}, \tag{233}$$
$$A_{\theta,o,i,l} \equiv \texttt{Ato(v,0,j)\%s(l)}, \text{and} \tag{234}$$
$$A_{\zeta,o,i,l} \equiv \texttt{Azo(v,0,j)\%s(l)}; \tag{235}$$

  where $v = 1, \texttt{Mvol}$ labels volume, $j = 1, \texttt{mn}$ labels Fourier harmonic, and $l = 0, \texttt{Lrad}\,(v)$ 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

$$\texttt{cosi}_{j,i} = \cos(m_i\theta_j - n_i\zeta_j), \tag{236}$$
$$\texttt{sini}_{j,i} = \sin(m_i\theta_j - n_i\zeta_j). \tag{237}$$

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

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

$$f_{j,v} \equiv \begin{cases} \psi^0_{t,v} & , \text{ for } m_j = 0, \\ \psi^{m_j/2}_{t,v} & , \text{ otherwise.} \end{cases} \tag{238}$$

  where $\psi_{t,v} \equiv$`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

$$f_{j,v} \equiv \begin{cases} \psi^{1/2}_{t,v} & , \text{ for } m_j = 0, \\ \psi^{m_j/2}_{t,v} & , \text{ otherwise.} \end{cases} \tag{239}$$

  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. $\iota\!\!\!-_\pm = \iota\!\!\!-(\mathbf{B}_\pm)$, so that

$$\delta \iota\!\!\!-_\pm = \frac{\partial \iota\!\!\!-_\pm}{\partial \mathbf{B}_\pm} \cdot \delta \mathbf{B}_\pm. \tag{240}$$

- 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

$$\delta \mathbf{B}_\pm = \frac{\partial \mathbf{B}_\pm}{\partial x_j}\delta x_j + \frac{\partial \mathbf{B}_\pm}{\partial \mu}\delta \mu + \frac{\partial \mathbf{B}_\pm}{\partial \Delta\psi_p}\delta \Delta\psi_p. \tag{241}$$

- The rotational-transforms, thus, can be considered to be functions of the geometry, the helicity-multiplier and the enclosed poloidal flux, $\iota\!\!\!-_\pm = \iota\!\!\!-_\pm(x_j, \mu, \Delta\psi_p)$.
- 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
    * `-1` : indicating the derivative with respect to the interface geometry, i.e. $\dfrac{\partial \iota\!\!\!-_\pm}{\partial x_j}$,
    * `0` : the rotational-transform itself,
    * `1`,2 : the derivatives with respec to μ and $\Delta\psi_p$, i.e. $\dfrac{\partial \iota\!\!\!-_\pm}{\partial \mu}$ and $\dfrac{\partial \iota\!\!\!-_\pm}{\partial \Delta\psi_p}$;
  - The third index labels volume.
- The values of `diotadxup` are assigned in mp00aa() after calling tr00ab().

vvolume, lBBintegral and lABintegral

- volume integrals

$$\texttt{vvolume(i)} = \int_{\mathcal{V}_i} dv \tag{242}$$

$$\texttt{lBBintegral(i)} = \int_{\mathcal{V}_i} \mathbf{B}\cdot\mathbf{B}\, dv \tag{243}$$

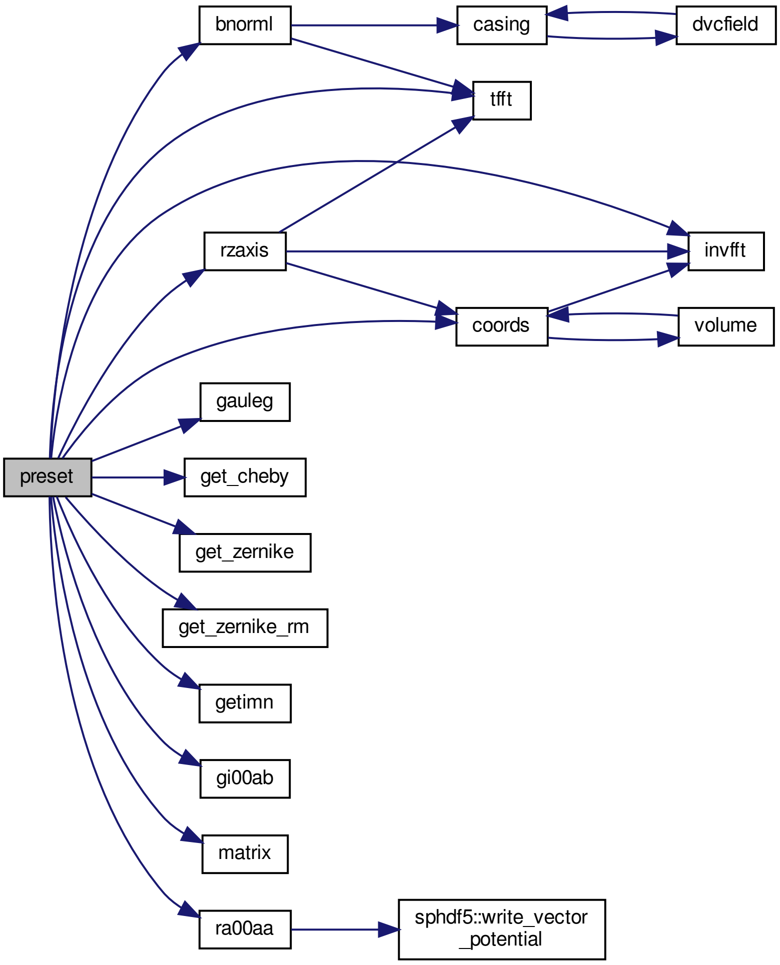
$$\texttt{lABintegral(i)} = \int_{\mathcal{V}_i} \mathbf{A}\cdot\mathbf{B}\, dv \tag{244}$$

References allglobal::ajk, allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::bbe, allglobal↩::bbo, allglobal::bbweight, allglobal::beltramierror, allglobal::bemn, allglobal::bloweremn, allglobal::bloweromn, inputlist::bnc, bnorml(), inputlist::bns, allglobal::bomn, allglobal::bsupumn, allglobal::bsupvmn, allglobal::btemn, allglobal::btomn, allglobal::bzemn, allglobal::bzomn, allglobal::cfmn, allglobal::cheby, allglobal::comn, coords(), allglobal::cosi, fftw_interface::cplxin, fftw_interface::cplxout, allglobal::cpus, allglobal::diotadxup, allglobal::ditgpdxtp, allglobal::djkm, allglobal::djkp, allglobal::dpflux, allglobal::dradr, allglobal::dradz, allglobal::drbc, allglobal::drbs, allglobal::drij, allglobal::drodr, allglobal::drodz, allglobal::dtflux, allglobal::dxyz, allglobal::dzadr, allglobal::dzadz, allglobal::dzbc, allglobal::dzbs, allglobal::dzij, allglobal::dzodr, allglobal::dzodz, allglobal::efmn, inputlist::escale,

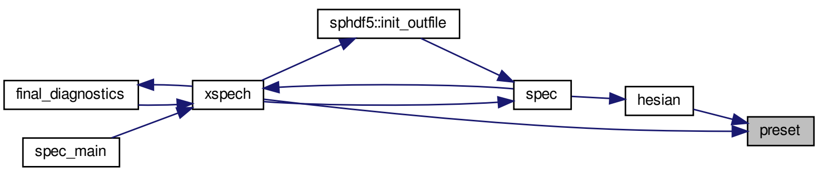
allglobal::evmn, inputlist::forcetol, allglobal::fse, allglobal::fso, gauleg(), allglobal::gaussianabscissae, allglobal↩
::gaussianweight, get_cheby(), get_zernike(), get_zernike_rm(), getimn(), gi00ab(), allglobal::glambda, allglobal↩
::gmreslastsolution, allglobal::goomne, allglobal::goomno, allglobal::gssmne, allglobal::gssmno, allglobal::gstmne, allglobal::gstmno, allglobal::gszmne, allglobal::gszmno, allglobal::gteta, allglobal::gttmne, allglobal::gttmno, allglobal::gtzmne, 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, invfft(), allglobal::iomn, inputlist::iota, allglobal::iotakadd, allglobal::iotakkii, allglobal::iotaksgn, allglobal::iotaksub, 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↩
::lntor, 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::sqrtmachprec, allglobal::sweight, tfft(), inputlist::tflux, allglobal::trij, allglobal::tt, allglobal::tzij, inputlist::upsilon, inputlist::vnc, inputlist::vns, numerical::vsmall, allglobal::vvolume, inputlist::wpoloidal, allglobal↩
::yesstellsym, inputlist::zac, inputlist::zas, inputlist::zbc, inputlist::zbs, allglobal::zernike, constants::zero, allglobal↩
::zij, inputlist::zwc, and inputlist::zws.

Referenced by hesian(), and xspech().

Here is the call graph for this function:



Here is the caller graph for this function:



8.19 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.

8.19.1 Detailed Description

8.19.2 Function/Subroutine Documentation

8.19.2.1 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

$$A_\theta(s,\theta,\zeta) = \sum_{i,l} A_{\theta,e,i,l}\, \overline{T}_{l,i}(s)\cos\alpha_i + \sum_{i,l} A_{\theta,o,i,l}\, \overline{T}_{l,i}(s)\sin\alpha_i, \quad (245)$$

$$A_\zeta(s,\theta,\zeta) = \sum_{i,l} A_{\zeta,e,i,l}\, \overline{T}_{l,i}(s)\cos\alpha_i + \sum_{i,l} A_{\zeta,o,i,l}\, \overline{T}_{l,i}(s)\sin\alpha_i, \quad (246)$$

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

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)
```

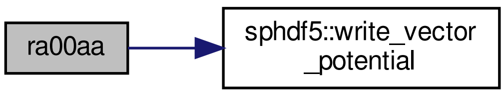
Parameters

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

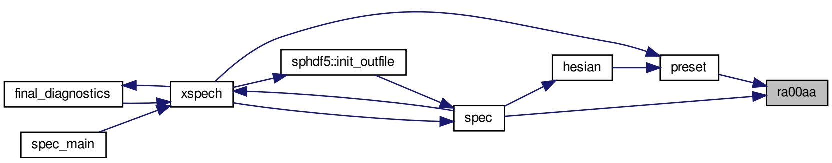
References allglobal::ate, allglobal::ato, fileunits::aunit, allglobal::aze, allglobal::azo, allglobal::cpus, allglobal::im, allglobal::in, inputlist::lrad, allglobal::mn, allglobal::mpi_comm_spec, inputlist::mpol, allglobal::myid, allglobal::ncpu, inputlist::nfp, inputlist::ntor, fileunits::ounit, inputlist::wmacros, 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:



8.19.2.2 mirror_input_to_outfile() `subroutine sphdf5::mirror_input_to_outfile`

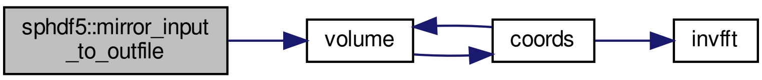
Mirror input variables into output file.

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.

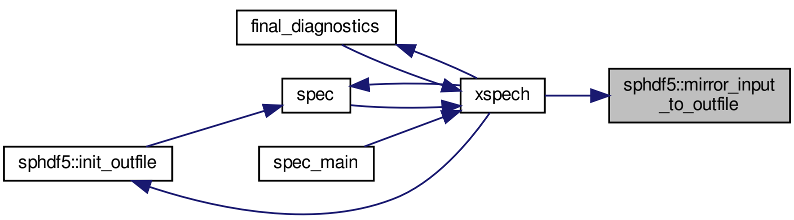
References inputlist::absacc, inputlist::absreq, inputlist::adiabatic, inputlist::bnc, inputlist::bns, inputlist::bnsblend, inputlist::bnstol, inputlist::c05factor, inputlist::c05xmax, inputlist::c05xtol, inputlist::curpol, inputlist::curtor, inputlist::dpp, inputlist::dqq, inputlist::epsgmres, inputlist::epsilon, inputlist::epsilu, inputlist::epsr, inputlist::escale, sphdf5::file_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::iotatol, inputlist::iprecon, inputlist::istellsym, inputlist::isurf, inputlist::ivolume, inputlist::ladiabatic, inputlist::lbeltrami, inputlist::lcheck, inputlist::lconstraint, inputlist::lerrortype, inputlist::lextrap, inputlist::lfindzero, inputlist::lfreebound, inputlist::lgmresprec, inputlist::lhevalues, inputlist::lhevectors, inputlist::lhmatrix, inputlist::linitgues, inputlist::linitialize, inputlist::lmatsolver, inputlist::lp, inputlist::lperturbed, inputlist::lposdef, inputlist::lq, inputlist::lrad, inputlist::lreadgf, inputlist::lreflect, inputlist::lrzaxis, inputlist::lsparse, inputlist::lsvdiota, inputlist::ltiming, inputlist::lzerovac, inputlist::maxrndgues, inputlist::mcasingcal, inputlist::mfreeits, inputlist::mpol, inputlist::mregular, inputlist::mu, inputlist::mupfits, inputlist::mupftol, inputlist::ndiscrete, inputlist::nfp, inputlist::ngrid, inputlist::nppts, inputlist::nptrj, inputlist::nquad, inputlist::ntor, inputlist::ntoraxis, inputlist::nvol, inputlist::odetol, inputlist::oita, inputlist::opsilon, inputlist::pcondense, inputlist::pflux, inputlist::phiedge, inputlist::pl, inputlist::ppts, inputlist::pr, inputlist::pressure, inputlist::pscale, inputlist::ql, inputlist::qr, inputlist::rac, inputlist::ras, inputlist::rbc, inputlist::rbs, inputlist::relreq, inputlist::rp, inputlist::rpol, inputlist::rq, inputlist::rtor, inputlist::rwc, inputlist::rws, inputlist::scaling, inputlist::tflux, inputlist::upsilon, inputlist::vcasingeps, inputlist::vcasingits, inputlist::vcasingper, inputlist::vcasingtol, inputlist::vnc, inputlist::vns, volume(), inputlist::wpoloidal, inputlist::zac, inputlist::zas, inputlist::zbc, inputlist::zbs, inputlist::zwc, and inputlist::zws.

Referenced by xspech().

Here is the call graph for this function:



Here is the caller graph for this function:



8.19.2.3 init_convergence_output() `subroutine sphdf5::init_convergence_output`

Prepare convergence evolution output.

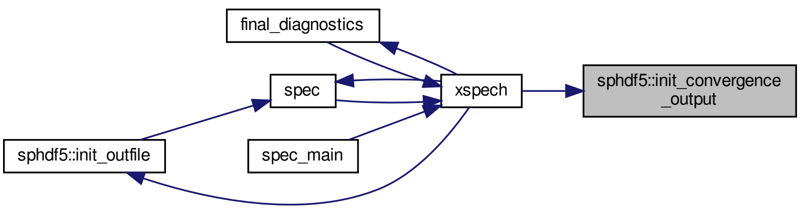
- The group `iterations` is created in the output file. This group contains the interface geometry at each iteration, which is useful for constructing movies illustrating the convergence. The data structure in use is an unlimited array of the following compound datatype:

```
DATATYPE  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";
}
```

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:



8.19.2.4 write_grid() `subroutine sphdf5::write_grid`

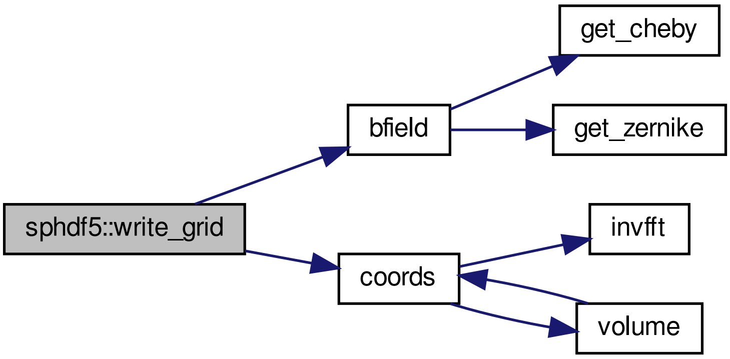
Write the magnetic field on a grid.

The magnetic field is evaluated on a regular grid in (s, θ, ζ) and the corresponding cylindrical coordinates (R, Z) as well as the cylindrical components of the magnetic field (B^R, B^φ, B^Z) are written out.

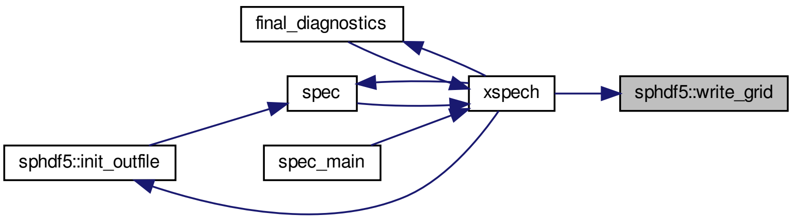
References bfield(), coords(), sphdf5::file_id, allglobal::gbzeta, inputlist::igeometry, allglobal::ijimag, allglobal↩ ::ijreal, allglobal::ivol, allglobal::jireal, allglobal::lcoordinatesingularity, allglobal::lplasmaregion, inputlist::lrad, allglobal::lvacuumregion, allglobal::mn, allglobal::myid, 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:



8.19.2.5 init_flt_output()

```
subroutine sphdf5::init_flt_output (
    integer, intent(in) numTrajTotal )
```

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

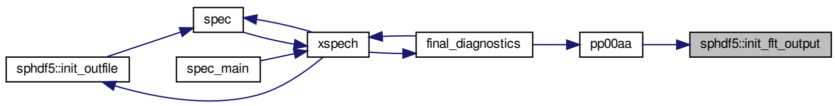
in	*numTrajTotal*	total number of Poincare trajectories

References sphdf5::dset_id_diotadxup, sphdf5::dset_id_fiota, sphdf5::dset_id_r, sphdf5::dset_id_s, sphdf5::dset↩
_id_success, sphdf5::dset_id_t, sphdf5::dset_id_z, sphdf5::file_id, sphdf5::filespace_diotadxup, sphdf5::filespace↩

_fiota, sphdf5::filespace_r, sphdf5::filespace_s, sphdf5::filespace_success, sphdf5::filespace_t, sphdf5::filespace↩
_z, sphdf5::grppoincare, sphdf5::grptransform, sphdf5::hdfier, sphdf5::memspace_diotadxup, sphdf5::memspace↩
_r, sphdf5::memspace_s, sphdf5::memspace_success, 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:



8.19.2.6 write_poincare() `subroutine sphdf5::write_poincare (`

```
integer, intent(in) offset,
real, dimension(:,:,:), intent(in) data,
integer, dimension(:), intent(in) success )
```

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

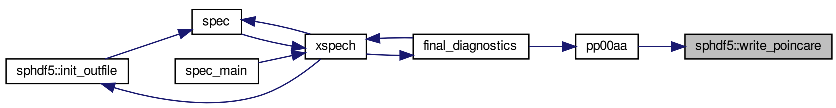
Parameters

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_↩
z, sphdf5::hdfier, sphdf5::memspace_r, sphdf5::memspace_s, sphdf5::memspace_success, sphdf5::memspace_t,
sphdf5::memspace_z, inputlist::nppts, and allglobal::nz.

Referenced by pp00aa().

Here is the caller graph for this function:



8.19.2.7 write_transform() `subroutine sphdf5::write_transform (`

```
integer, intent(in) offset,
integer, intent(in) length,
integer, intent(in) lvol,
real, dimension(:), intent(in) diotadxup,
real, dimension(:,:), intent(in) fiota )
```

Write the rotational transform output from field line following.

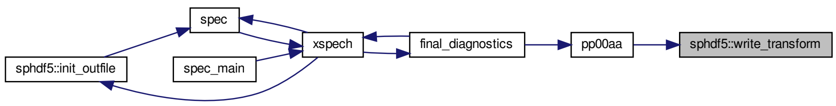
Parameters

offset	radial offset at which the data belongs
length	length of dataset to write
lvol	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:



8.19.2.8 finalize_flt_output() `subroutine sphdf5::finalize_flt_output`

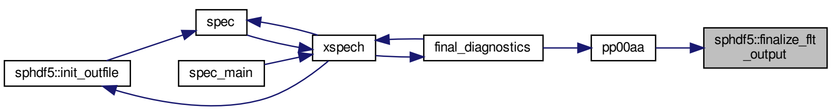
Finalize Poincare output.

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_success, sphdf5::dset_id_t, sphdf5::dset_id_z, sphdf5::filespace_diotadxup, sphdf5::filespace_fiota, sphdf5::filespace_r, sphdf5::filespace_s, sphdf5::filespace_success, sphdf5::filespace_t, sphdf5::filespace_z, sphdf5::grppoincare, sphdf5::grptransform, sphdf5::hdfier, sphdf5::memspace_diotadxup, sphdf5::memspace_r, sphdf5::memspace_s, sphdf5::memspace_success, sphdf5::memspace_t, and sphdf5::memspace_z.

Referenced by pp00aa().

Here is the caller graph for this function:



8.19.2.9 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.

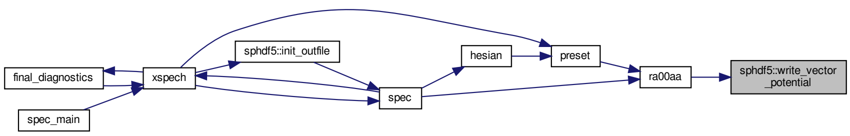
Parameters

sumLrad	total sum over `Lrad` in all nested volumes
allAte	$A^{\theta}_{\rm even}$ for all nested volumes
allAze	$A^{\zeta}_{\rm even}$ for all nested volumes
allAto	$A^{\theta}_{\rm odd}$ for all nested volumes
allAzo	$A^{\zeta}_{\rm odd}$ for all nested volumes

References sphdf5::file_id, and allglobal::mn.

Referenced by ra00aa().

Here is the caller graph for this function:



8.19.2.10 hdfint() `subroutine sphdf5::hdfint`

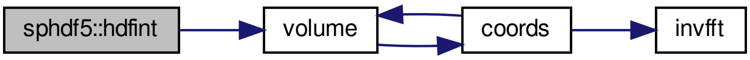
Write the final state of the equilibrium to the output file.

- 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.

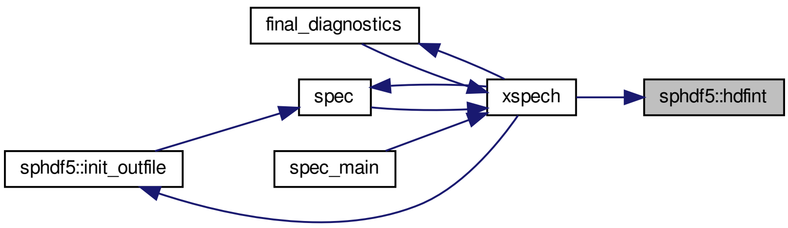
References inputlist::adiabatic, allglobal::beltramierror, inputlist::bnc, inputlist::bns, allglobal::bsupumn, allglobal::bsupvmn, allglobal::btemn, allglobal::btomn, allglobal::bzemn, allglobal::bzomn, allglobal::cpus, allglobal::drbc, allglobal::drbs, allglobal::dvolume, allglobal::dzbc, allglobal::dzbs, sphdf5::file_id, allglobal::forceerr, inputlist::helicity, allglobal::ibnc, allglobal::ibns, allglobal::im, allglobal::in, allglobal::irbc, allglobal::irbs, allglobal::ivnc, allglobal::ivns, inputlist::ivolume, allglobal::izbc, allglobal::izbs, 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:



8.20 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.

8.20.1 Detailed Description

8.20.2 Function/Subroutine Documentation

8.20.2.1 rzaxis()

```
subroutine rzaxis (
    integer, intent(in) Mvol,
    integer, intent(in) mn,
    real, dimension(1:mn,0:mvol) inRbc,
    real, dimension(1:mn,0:mvol) inZbs,
    real, dimension(1:mn,0:mvol) inRbs,
    real, dimension(1:mn,0:mvol) inZbc,
    integer, intent(in) ivol,
    logical, intent(in) LcomputeDerivatives )
```

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 $i \equiv$ `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.
- Define the arc-length-weighted averages,

$$R_0(\zeta) \equiv \frac{\displaystyle\int_0^{2\pi} R_i(\theta,\zeta)\, dl}{\displaystyle\int_0^{2\pi} dl}, \qquad Z_0(\zeta) \equiv \frac{\displaystyle\int_0^{2\pi} Z_i(\theta,\zeta)\, dl}{\displaystyle\int_0^{2\pi} dl}, \tag{247}$$

  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 $\dot{l}$ does not depend on θ, i.e. if θ 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

$$\begin{aligned}
\frac{\partial R_0}{\partial R^c_{i,j}} &= \int \left(\cos\alpha_j \, \dot{l} - \Delta R_i R_{i,\theta}\, m_j \sin\alpha_j / \, \dot{l}\right) d\theta/L & (248)\\
\frac{\partial R_0}{\partial R^s_{i,j}} &= \int \left(\sin\alpha_j \, \dot{l} + \Delta R_i R_{i,\theta}\, m_j \cos\alpha_j / \, \dot{l}\right) d\theta/L & (249)\\
\frac{\partial R_0}{\partial Z^c_{i,j}} &= \int \left(\qquad -\Delta R_i Z_{i,\theta}\, m_j \sin\alpha_j / \, \dot{l}\right) d\theta/L & (250)\\
\frac{\partial R_0}{\partial Z^s_{i,j}} &= \int \left(\qquad +\Delta R_i Z_{i,\theta}\, m_j \cos\alpha_j / \, \dot{l}\right) d\theta/L & (251)\\
\frac{\partial Z_0}{\partial R^c_{i,j}} &= \int \left(\qquad -\Delta Z_i R_{i,\theta}\, m_j \sin\alpha_j / \, \dot{l}\right) d\theta/L & (252)\\
\frac{\partial Z_0}{\partial R^s_{i,j}} &= \int \left(\qquad +\Delta Z_i R_{i,\theta}\, m_j \cos\alpha_j / \, \dot{l}\right) d\theta/L & (253)\\
\frac{\partial Z_0}{\partial Z^c_{i,j}} &= \int \left(\cos\alpha_j \, \dot{l} - \Delta Z_i Z_{i,\theta}\, m_j \sin\alpha_j / \, \dot{l}\right) d\theta/L & (254)\\
\frac{\partial Z_0}{\partial Z^s_{i,j}} &= \int \left(\sin\alpha_j \, \dot{l} + \Delta Z_i Z_{i,\theta}\, m_j \cos\alpha_j / \, \dot{l}\right) d\theta/L & (255)
\end{aligned}$$

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 θ to construct $L \equiv \int dl$ is now trivial: just multiply the $m = 0$ harmonics of dl by 2π. 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.

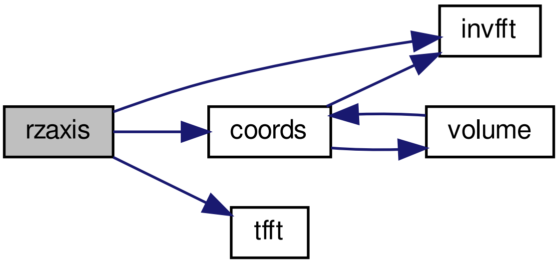
Parameters

in	*Mvol*	
in	*mn*	
	iRbc	
	iZbs	
	iRbs	
	iZbc	
in	*ivol*	
	LcomputeDerivatives	

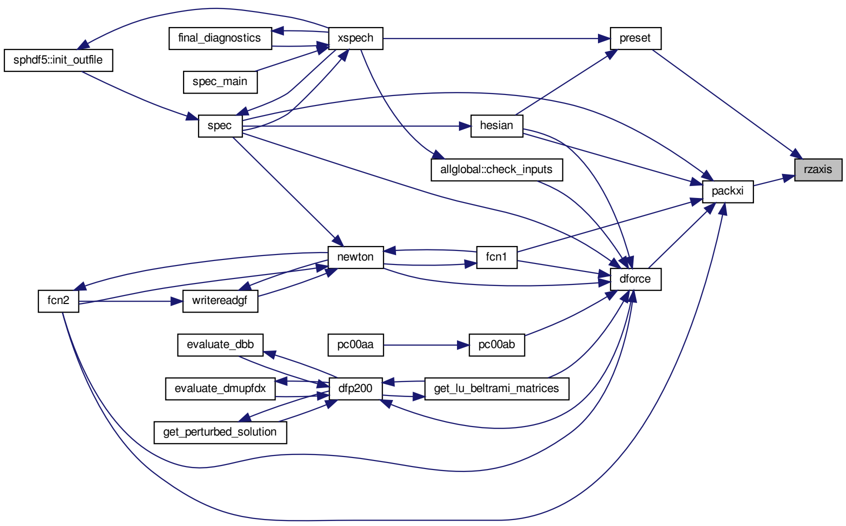
References allglobal::ajk, allglobal::cfmn, allglobal::comn, coords(), allglobal::cosi, allglobal::cpus, allglobal::dbdx, allglobal::dradr, allglobal::dradz, allglobal::drodr, allglobal::drodz, allglobal::dzadr, allglobal::dzadz, allglobal::dzodr, allglobal::dzodz, allglobal::efmn, allglobal::evmn, constants::half, inputlist::igeometry, allglobal::ijimag, allglobal::ijreal, allglobal::im, allglobal::in, invfft(), allglobal::irbc, allglobal::irbs, allglobal::izbc, allglobal::izbs, allglobal::jiimag, allglobal::jireal, allglobal::jkimag, allglobal::jkreal, allglobal::kjimag, allglobal::kjreal, inputlist::lcheck, allglobal::lcoordinatesingularity, inputlist::lreflect, inputlist::lrzaxis, allglobal::mpi_comm_spec, allglobal::myid, allglobal::ncpu, allglobal::notstellsym, allglobal::nt, inputlist::ntor, inputlist::ntoraxis, allglobal::ntz, allglobal::nz, allglobal::odmn, allglobal::ofmn, constants::one, fileunits::ounit, allglobal::rij, allglobal::sfmn, allglobal::sg, allglobal::simn, allglobal::sini, tfft(), constants::two, numerical::vsmall, inputlist::wmacros, 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:



8.21 Rotational Transform

Functions/Subroutines

- subroutine tr00ab (lvol, mn, NN, Nt, Nz, iflag, ldiota)

  Calculates rotational transform given an arbitrary tangential field.

8.21.1 Detailed Description

8.21.2 Function/Subroutine Documentation

8.21.2.1 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

$$\lambda = \sum_j \lambda_{o,j}\sin(m_j\theta - n_j\zeta) + \sum_j \lambda_{e,j}\cos(m_j\theta - n_j\zeta) \tag{256}$$

  and insisting that

$$\frac{\mathbf{B}\cdot\nabla\theta_s}{\mathbf{B}\cdot\nabla\zeta} = \dot{\theta}(1+\lambda_\theta)+\lambda_\zeta = {\iota\!\!\!{-}}, \tag{257}$$

  where ${\iota\!\!\!{-}}$ is a constant that is to be determined.

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

$$\partial_s A_\theta \, {\iota\!\!\!{-}} + \partial_s A_\zeta \,\lambda_\theta - \partial_s A_\theta\,\lambda_\zeta = -\partial_s A_\zeta \tag{258}$$

- Expanding this equation we obtain

$$\begin{aligned} & \left(A'_{\theta,e,k}\cos\alpha_k + A'_{\theta,o,k}\sin\alpha_k\right)\ {\iota\!\!\!{-}} \\ + & \left(A'_{\zeta,e,k}\cos\alpha_k + A'_{\zeta,o,k}\sin\alpha_k\right)\ (+m_j\lambda_{o,j}\cos\alpha_j - m_j\lambda_{e,j}\sin\alpha_j) \\ - & \left(A'_{\theta,e,k}\cos\alpha_k + A'_{\theta,o,k}\sin\alpha_k\right)\ (-n_j\lambda_{o,j}\cos\alpha_j + n_j\lambda_{e,j}\sin\alpha_j) \\ = \ - & \left(A'_{\zeta,e,k}\cos\alpha_k + A'_{\zeta,o,k}\sin\alpha_k\right), \end{aligned} \tag{259}$$

  where summation over $k=1,\texttt{mn}$ and $j=2,\texttt{mns}$ is implied

- After applying double angle formulae,

$$\begin{aligned} & \left(A'_{\theta,e,k}\cos\alpha_k + A'_{\theta,o,k}\sin\alpha_k\right)\ {\iota\!\!\!{-}} \\ + & \ \lambda_{o,j}\left(+m_jA'_{\zeta,e,k}+n_jA'_{\theta,e,k}\right)\left[+\cos(\alpha_k+\alpha_j)+\cos(\alpha_k-\alpha_j)\right]/2 \\ + & \ \lambda_{e,j}\left(-m_jA'_{\zeta,e,k}-n_jA'_{\theta,e,k}\right)\left[+\sin(\alpha_k+\alpha_j)-\sin(\alpha_k-\alpha_j)\right]/2 \\ + & \ \lambda_{o,j}\left(+m_jA'_{\zeta,o,k}+n_jA'_{\theta,o,k}\right)\left[+\sin(\alpha_k+\alpha_j)+\sin(\alpha_k-\alpha_j)\right]/2 \\ + & \ \lambda_{e,j}\left(-m_jA'_{\zeta,o,k}-n_jA'_{\theta,o,k}\right)\left[-\cos(\alpha_k+\alpha_j)+\cos(\alpha_k-\alpha_j)\right]/2 \\ = \ - & \left(A'_{\zeta,e,k}\cos\alpha_k + A'_{\zeta,o,k}\sin\alpha_k\right), \end{aligned} \tag{260}$$

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

$$\mathbf{x} = (\underbrace{\ {\iota\!\!\!{-}}\ }_{\texttt{x[1]}},\ \underbrace{\lambda_{o,2},\lambda_{o,3},\dots}_{\texttt{x[2: N]}},\ \underbrace{\lambda_{e,2},\lambda_{e,3},\dots}_{\texttt{x[N+1:2N-1]}}\ )^T. \tag{261}$$

alternative iterative method

- Consider the equation $\dot{\theta}(1+\lambda_\theta)+\lambda_\zeta = {\iota\!\!\!{-}}$, where $\lambda=\sum_j \lambda_j\sin\alpha_j$, given on a grid

$$\dot{\theta}_i + \dot{\theta}_i\sum_j m_j\cos\alpha_{i,j}\lambda_j - \sum_j n_j\cos\alpha_{i,j}\lambda_j = {\iota\!\!\!{-}}, \tag{262}$$

  where i labels the grid point.

- This is a matrix equation...

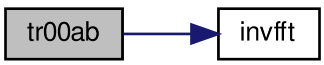
Parameters

lvol	
mn	
NN	
Nt	
Nz	
iflag	
ldiota	

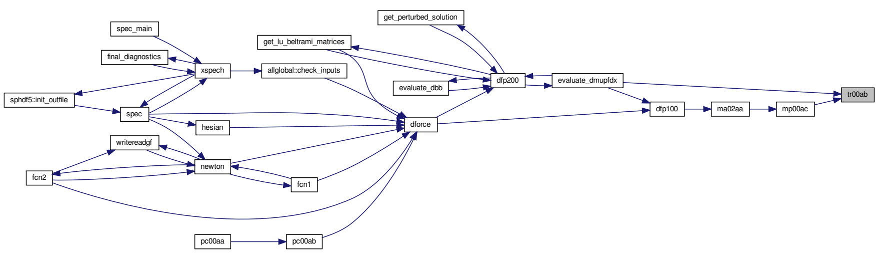
References allglobal::cpus, allglobal::glambda, constants::goldenmean, constants::half, allglobal::im, inputlist::imethod, allglobal::ims, allglobal::in, allglobal::ins, invfft(), inputlist::iorder, inputlist::iotatol, inputlist::iprecon, inputlist::lrad, inputlist::lsparse, inputlist::lsvdiota, numerical::machprec, 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().

Here is the call graph for this function:



Here is the caller graph for this function:



8.22 Plasma volume

Functions/Subroutines

- subroutine volume (lvol, vflag)

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

8.22.1 Detailed Description

8.22.2 Function/Subroutine Documentation

8.22.2.1 volume()

```
subroutine volume (
    integer, intent(in) lvol,
    integer vflag )
```

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

Calculates volume of each region; $\mathcal{V}_i \equiv \int dv$.

volume integral

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

$$V = \int_{\mathcal{V}} dv = \frac{1}{3}\int_{\mathcal{V}} \nabla\cdot\mathbf{x}\, dv = \frac{1}{3}\int_{\mathcal{S}} \mathbf{x}\cdot d\mathbf{s} = \frac{1}{3}\int_0^{2\pi} d\theta \int_0^{2\pi/N} d\zeta \quad \mathbf{x}\cdot\mathbf{x}_\theta\times\mathbf{x}_\zeta|^s \tag{263}$$

  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

$$\begin{aligned} R(\theta,\zeta) &= \sum_i R_{e,i}\ \cos\alpha_i + \sum_i R_{o,i}\ \sin\alpha_i & (264)\\ Z(\theta,\zeta) &= \sum_i Z_{e,i}\ \cos\alpha_i + \sum_i Z_{o,i}\ \sin\alpha_i, & (265)\end{aligned}$$

  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 : $\sqrt{g} = R_s$

$$\begin{aligned} V &= \int_0^{2\pi} d\theta \int_0^{2\pi/N} d\zeta\ R \\ &= 2\pi\ \frac{2\pi}{N}\ R_{e,1} & (266)\end{aligned}$$

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

$$\begin{aligned} V &= \frac{1}{2}\int_0^{2\pi} d\theta \int_0^{2\pi/N} d\zeta\ R^2 \\ &= \frac{1}{2}\,2\pi\ \frac{2\pi}{N}\ \frac{1}{2}\ \sum_i\sum_j R_{e,i}R_{e,j}\left[\cos(\alpha_i-\alpha_j)+\cos(\alpha_i+\alpha_j)\right] \\ &+ \frac{1}{2}\,2\pi\ \frac{2\pi}{N}\ \frac{1}{2}\ \sum_i\sum_j R_{o,i}R_{o,j}\left[\cos(\alpha_i-\alpha_j)-\cos(\alpha_i+\alpha_j)\right] & (267)\end{aligned}$$

- `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:

$$
\begin{aligned}
V &= \frac{1}{3}\int_0^{2\pi} d\theta \int_0^{2\pi/N} d\zeta \; R\left(ZR_\theta - RZ_\theta\right) \\
&= \frac{1}{3}\sum_i\sum_j\sum_k R_{e,i}\left(Z_{e,j}R_{o,k} - R_{e,j}Z_{o,k}\right)(+m_k)\iint d\theta d\zeta \;\; \cos\alpha_i\cos\alpha_j\cos\alpha_k \\
&+ \frac{1}{3}\sum_i\sum_j\sum_k R_{e,i}\left(Z_{o,j}R_{e,k} - R_{o,j}Z_{e,k}\right)(-m_k)\iint d\theta d\zeta \;\; \cos\alpha_i\sin\alpha_j\sin\alpha_k \\
&+ \frac{1}{3}\sum_i\sum_j\sum_k R_{o,i}\left(Z_{e,j}R_{e,k} - R_{e,j}Z_{e,k}\right)(-m_k)\iint d\theta d\zeta \;\; \sin\alpha_i\cos\alpha_j\sin\alpha_k \\
&+ \frac{1}{3}\sum_i\sum_j\sum_k R_{o,i}\left(Z_{o,j}R_{o,k} - R_{o,j}Z_{o,k}\right)(+m_k)\iint d\theta d\zeta \;\; \sin\alpha_i\sin\alpha_j\cos\alpha_k
\end{aligned} \tag{268}
$$

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

$$
\begin{array}{rcl}
4\;\cos\alpha_i\cos\alpha_j\cos\alpha_k &=& +\;\;\cos(\alpha_i+\alpha_j+\alpha_k) \;+\; \cos(\alpha_i+\alpha_j-\alpha_k) \;+\; \cos(\alpha_i-\alpha_j+\alpha_k) \;+\; \cos(\alpha_i-\alpha_j-\alpha_k) \\
4\;\cos\alpha_i\sin\alpha_j\sin\alpha_k &=& -\;\;\cos(\alpha_i+\alpha_j+\alpha_k) \;+\; \cos(\alpha_i+\alpha_j-\alpha_k) \;+\; \cos(\alpha_i-\alpha_j+\alpha_k) \;-\; \cos(\alpha_i-\alpha_j-\alpha_k) \\
4\;\sin\alpha_i\cos\alpha_j\sin\alpha_k &=& -\;\;\cos(\alpha_i+\alpha_j+\alpha_k) \;+\; \cos(\alpha_i+\alpha_j-\alpha_k) \;-\; \cos(\alpha_i-\alpha_j+\alpha_k) \;+\; \cos(\alpha_i-\alpha_j-\alpha_k) \\
4\;\sin\alpha_i\sin\alpha_j\cos\alpha_k &=& -\;\;\cos(\alpha_i+\alpha_j+\alpha_k) \;-\; \cos(\alpha_i+\alpha_j-\alpha_k) \;+\; \cos(\alpha_i-\alpha_j+\alpha_k) \;+\; \cos(\alpha_i-\alpha_j-\alpha_k)
\end{array}
$$

- The required derivatives are

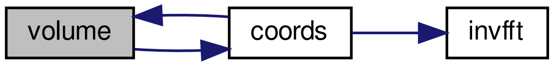
$$
\begin{aligned}
3\frac{\partial V}{\partial R_{e,i}} &= \left(+Z_{e,j}R_{o,k}m_k - R_{e,j}Z_{o,k}m_k - R_{e,j}Z_{o.k}m_k\right) & \iint d\theta d\zeta \;\; \cos\alpha_i\cos\alpha_j\cos\alpha_k \\
&+ \left(-Z_{o,j}R_{e,k}m_k + R_{o,j}Z_{e,k}m_k + R_{o,j}Z_{e,k}m_k\right) & \iint d\theta d\zeta \;\; \cos\alpha_i\sin\alpha_j\sin\alpha_k \\
&+ \left(-R_{o,k}Z_{e,j}m_i\right) & \iint d\theta d\zeta \;\; \sin\alpha_i\cos\alpha_j\sin\alpha_k \\
&+ \left(-R_{e,k}Z_{o,j}m_i\right) & \iint d\theta d\zeta \;\; \sin\alpha_i\sin\alpha_j\cos\alpha_k
\end{aligned} \tag{270}
$$

$$
\begin{aligned}
3\frac{\partial V}{\partial Z_{o,i}} &= \left(-R_{e,k}R_{e,j}m_i\right) & \iint d\theta d\zeta \;\; \cos\alpha_i\cos\alpha_j\cos\alpha_k \\
&+ \left(-R_{o,k}R_{o,j}m_i\right) & \iint d\theta d\zeta \;\; \cos\alpha_i\sin\alpha_j\sin\alpha_k \\
&+ \left(-R_{e,j}R_{e,k}m_k\right) & \iint d\theta d\zeta \;\; \sin\alpha_i\cos\alpha_j\sin\alpha_k \\
&+ \left(+R_{o,j}R_{o,k}m_k\right) & \iint d\theta d\zeta \;\; \sin\alpha_i\sin\alpha_j\cos\alpha_k
\end{aligned} \tag{271}
$$

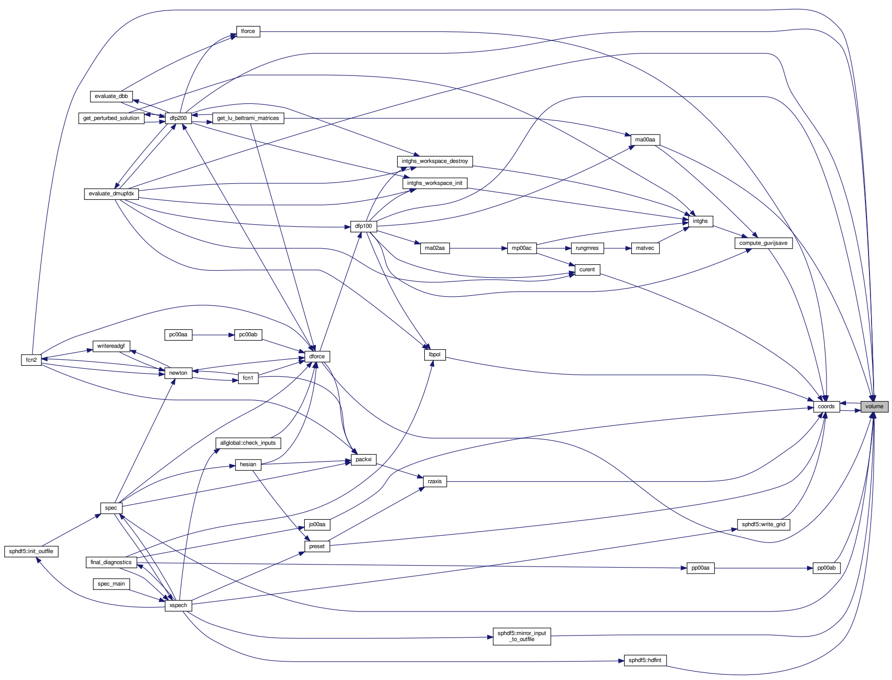
References coords(), allglobal::cosi, allglobal::cpus, allglobal::dbdx, allglobal::djkm, allglobal::djkp, allglobal::dvolume, constants::four, constants::half, inputlist::igeometry, allglobal::im, allglobal::in, allglobal::irbc, allglobal::irbs, allglobal::izbc, allglobal::izbs, allglobal::mn, allglobal::mpi_comm_spec, 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::yesstellsym, 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:



8.23 Smooth boundary

Functions/Subroutines

- subroutine wa00aa (iwa00aa)

  Constructs smooth approximation to wall.
- subroutine vacuumphi (Nconstraints, rho, fvec, iflag)

  Compute vacuum magnetic scalar potential (?)

8.23.1 Detailed Description

8.23.2 Function/Subroutine Documentation

8.23.2.1 wa00aa() `subroutine wa00aa (`
`integer` *`iwa00aa`* `)`

Constructs smooth approximation to wall.

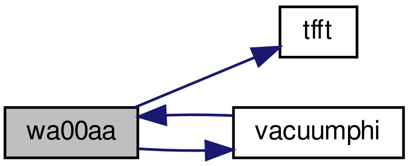
solution of Laplace's equation in two-dimensions

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

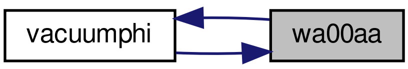
References laplaces::alpha, laplaces::cc, allglobal::cpus, laplaces::dorm, laplaces::exterior, fileunits::gunit, constants::half, laplaces::iangle, laplaces::ic, laplaces::icint, allglobal::im, allglobal::in, allglobal::irbc, allglobal↔::irbs, allglobal::izbc, allglobal::izbs, allglobal::lcoordinatesingularity, 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↔::originalalpha, fileunits::ounit, laplaces::phi, laplaces::phid, constants::pi2, allglobal::rij, laplaces::rmid, laplaces↔::stage1, constants::ten, tfft(), 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:



8.23.2.2 vacuumphi() `subroutine vacuumphi (`
`integer` *`Nconstraints,`*
`real, dimension(1:nconstraints)` *`rho,`*
`real, dimension(1:nconstraints)` *`fvec,`*
`integer` *`iflag`* `)`

Compute vacuum magnetic scalar potential (?)

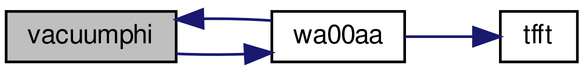
Parameters

Nconstraints	
rho	
fvec	
iflag	

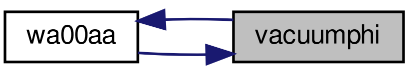
References laplaces::alpha, laplaces::cc, allglobal::cpus, laplaces::dorm, laplaces::exterior, constants::half, laplaces::iangle, laplaces::ic, laplaces::icint, allglobal::myid, allglobal::ncpu, laplaces::nintervals, laplaces::niterations, laplaces::np1, laplaces::np4, laplaces::nsegments, allglobal::ntz, 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:



8.24 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 `lMpol=2*Mpol` and `lNtor=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

8.24.1 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 `lMpol=2*Mpol` and `lNtor=2*Ntor`.

8.25 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

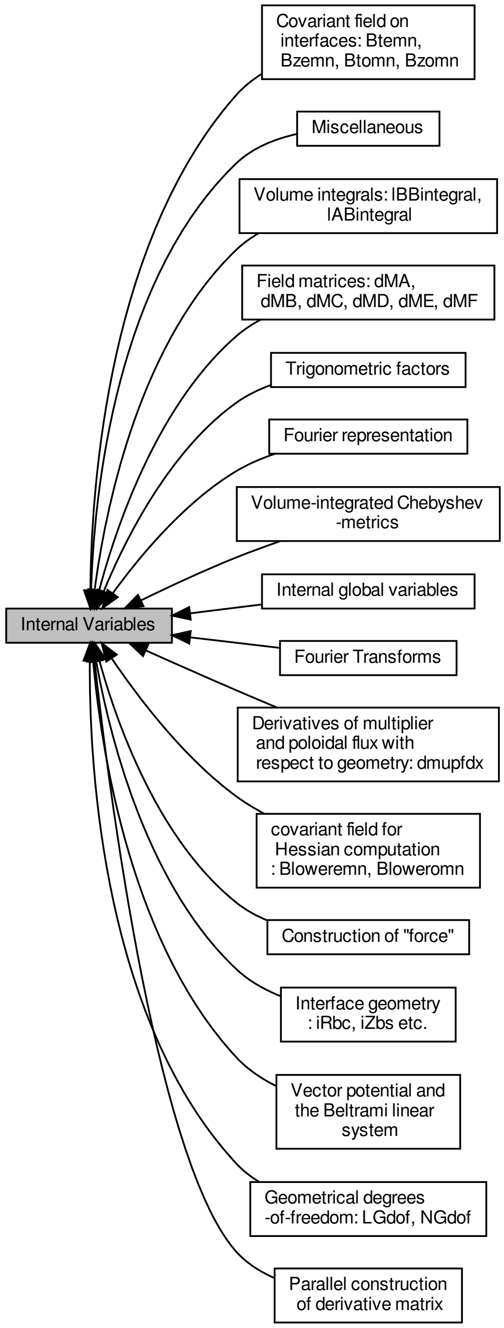
  enhanced toroidal mode numbers for straight field line transformation

8.25.1 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`.

8.26 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(l,j)`, `iZbs(l,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

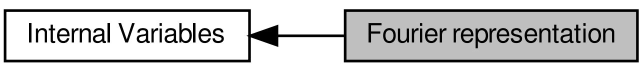
- type(derivative) allglobal::dbdx

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

8.26.1 Detailed Description

8.27 Fourier representation

Collaboration diagram for Fourier representation:



Variables

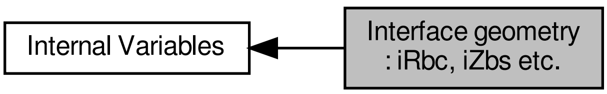
- integer allglobal::mn
  total number of Fourier harmonics for coordinates/fields; calculated from Mpol, Ntor in readin()
- integer, dimension(:), allocatable allglobal::im
  poloidal mode numbers for Fourier representation
- integer, dimension(:), allocatable allglobal::in
  toroidal mode numbers for 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

8.27.1 Detailed Description

8.28 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(l,j)`, `iZbs(l,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**

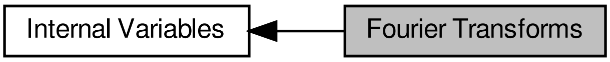
8.28.1 Detailed Description

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

8.29 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 θ of grid in real space
- integer allglobal::nz

  discrete resolution along ζ 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
- real, dimension(:,:,:), allocatable allglobal::bsupvmn

  tangential field on interfaces; ζ -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()

8.29.1 Detailed Description

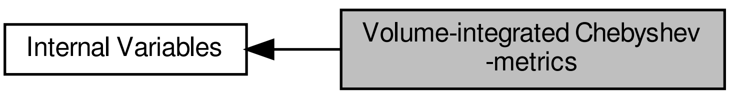
The coordinate geometry and fields are mapped to/from Fourier space and real space using FFTW3. The resolution of the real space grid is given by `Nt=Ndiscrete*4*Mpol` and `Nz=Ndiscrete*4*Ntor`.

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.

8.30 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:



Variables

- 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

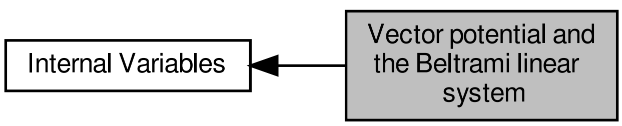
  minimum poloidal length constraint weight

8.30.1 Detailed Description

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

8.31 Vector potential and the Beltrami linear system

Collaboration diagram for Vector potential and the Beltrami linear system:



Variables

- 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::lmd

  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::lmbvalue

  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::lmfvalue

  what is this?
- real, dimension(:,:), allocatable allglobal::lmgvalue

  what is this?
- real, dimension(:,:), allocatable allglobal::lmhvalue

  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?

8.31.1 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

$$A_\theta = \sum_i \sum_{l=0}^{L} A_{\theta,e,i,l}\, T_l(s) \cos\alpha_i + \sum_i \sum_{l=0}^{L} A_{\theta,o,i,l}\, T_l(s) \sin\alpha_i \tag{272}$$

$$A_\zeta = \sum_i \sum_{l=0}^{L} A_{\zeta,e,i,l}\, T_l(s) \cos\alpha_i + \sum_i \sum_{l=0}^{L} A_{\zeta,o,i,l}\, T_l(s) \sin\alpha_i, \tag{273}$$

  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`(l) $\equiv A_{\theta,e,i,l}$

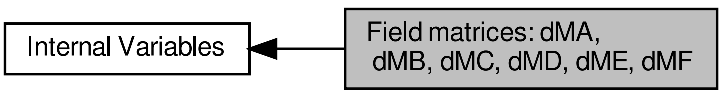
  `dAze(0,i)%s`(l) $\equiv A_{\zeta,e,i,l}$

  `dAto(0,i)%s`(l) $\equiv A_{\theta,o,i,l}$

  `dAzo(0,i)%s`(l) $\equiv A_{\zeta,o,i,l}$

8.32 Field matrices: dMA, dMB, dMC, dMD, dME, dMF

Collaboration diagram for Field matrices: dMA, dMB, dMC, dMD, dME, dMF:



Variables

- 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(Itor,Gpol)/dx; (see dforce)
- real, dimension(:,:,:,:), allocatable allglobal::glambda

  save initial guesses for iterative calculation of rotational-transform
- integer allglobal::lmns

  what is this?

8.32.1 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

$$W = \frac{1}{2}\, a_i\, A_{i,j}\, a_j + a_i\, B_{i,j}\, \psi_j + \frac{1}{2}\, \psi_i\, C_{i,j}\, \psi_j \quad (274)$$

$$K = \frac{1}{2}\, a_i\, D_{i,j}\, a_j + a_i\, E_{i,j}\, \psi_j + \frac{1}{2}\, \psi_i\, F_{i,j}\, \psi_j \quad (275)$$

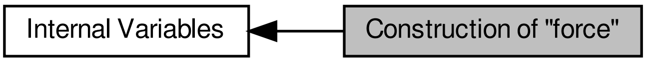
  where $\mathbf{a} \equiv \{A_{\theta,e,i,l}, A_{\zeta,e,i,l}, A_{\theta,o,i,l}, A_{\zeta,o,i,l}, f_{e,i}, f_{o,i}\}$ contains the independent degrees of freedom and $\boldsymbol{\psi} \equiv \{\Delta\psi_t, \Delta\psi_p\}$.

- These are allocated and deallocated in dforce(), assigned in matrix(), and used in mp00ac() and (?) df00aa().

8.33 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 (?)

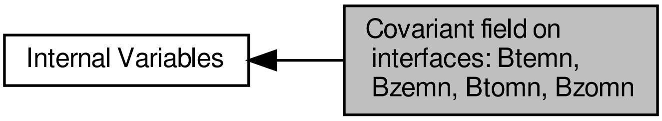
8.33.1 Detailed Description

The force vector is comprised of `Bomn` and `Iomn`.

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

The covariant field.

Collaboration diagram for Covariant field on interfaces: Btemn, Bzemn, Btomn, Bzomn:



Variables

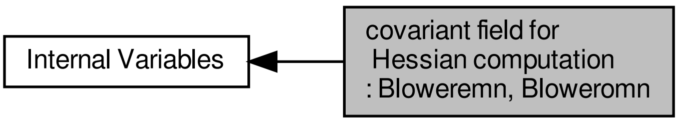
- real, dimension(:,:,:), allocatable allglobal::btemn
  covariant θ cosine component of the tangential field on interfaces; stellarator-symmetric
- real, dimension(:,:,:), allocatable allglobal::bzemn
  covariant ζ cosine component of the tangential field on interfaces; stellarator-symmetric
- real, 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

8.34.1 Detailed Description

The covariant field.

8.35 covariant field for Hessian computation: Bloweremn, Bloweromn

Collaboration diagram for covariant field for Hessian computation: Bloweremn, Bloweromn:



Variables

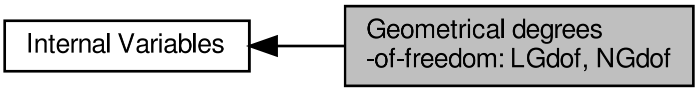
- real, dimension(:,:), allocatable allglobal::bloweremn
  covariant field for Hessian computation
- real, dimension(:,:), allocatable allglobal::bloweromn
  covariant field for Hessian computation

8.35.1 Detailed Description

8.36 Geometrical degrees-of-freedom: LGdof, NGdof

The geometrical degrees-of-freedom.

Collaboration diagram for Geometrical degrees-of-freedom: LGdof, NGdof:



Variables

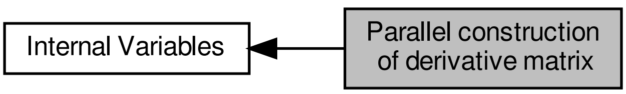
- integer allglobal::lgdof
  geometrical degrees of freedom associated with each interface
- integer allglobal::ngdof
  total geometrical degrees of freedom

8.36.1 Detailed Description

The geometrical degrees-of-freedom.

8.37 Parallel construction of derivative matrix

Collaboration diagram for Parallel construction of derivative matrix:



Variables

- 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, dimension(:,:,:,:), allocatable allglobal::dbbdmp

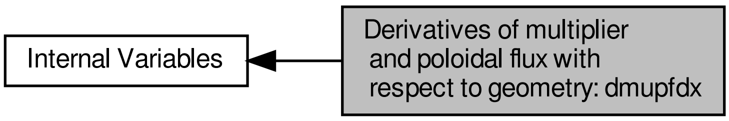
  derivatives of B^2 at the interfaces wrt mu and dpflux

8.37.1 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.

8.38 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 (?)

8.38.1 Detailed Description

- The information in `dmupfdx` describes how the helicity multiplier, μ, 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

$$\delta\mathbf{B}_\pm = \frac{\partial \mathbf{B}_\pm}{\partial x_j}\delta x_j + \frac{\partial \mathbf{B}_\pm}{\partial \mu}\delta\mu + \frac{\partial \mathbf{B}_\pm}{\partial \Delta\psi_p}\delta\Delta\psi_p. \tag{276}$$

- 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

$$B_\pm^2 = B_\pm^2(x_j, \mu, \Delta\psi_p), \tag{277}$$

  we may derive

$$\frac{\partial B_\pm^2}{\partial x_j} = \frac{\partial B_\pm^2}{\partial x_j} + \frac{\partial B_\pm^2}{\partial \mu}\frac{\partial \mu}{\partial x_j} + \frac{\partial B_\pm^2}{\partial \Delta\psi_p}\frac{\partial \Delta\psi_p}{\partial x_j} \tag{278}$$

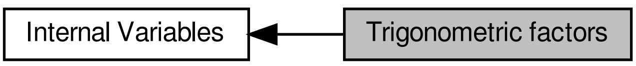
- The constraint to be enforced is that μ and $\Delta\psi_p$ must generally vary as the geometry is varied if the value of the rotational-transform constraint on the inner/outer interface is to be preserved, i.e.

$$\left(\begin{array}{ccc} \dfrac{\partial \iota\!\!\!-_-}{\partial \mathbf{B}_-}\cdot\dfrac{\partial \mathbf{B}_-}{\partial \mu} & , & \dfrac{\partial \iota\!\!\!-_-}{\partial \mathbf{B}_-}\cdot\dfrac{\partial \mathbf{B}_-}{\partial \Delta\psi_p} \\ \dfrac{\partial \iota\!\!\!-_+}{\partial \mathbf{B}_+}\cdot\dfrac{\partial \mathbf{B}_+}{\partial \mu} & , & \dfrac{\partial \iota\!\!\!-_+}{\partial \mathbf{B}_+}\cdot\dfrac{\partial \mathbf{B}_+}{\partial \Delta\psi_p} \end{array}\right)\left(\begin{array}{c} \dfrac{\partial \mu}{\partial x_j} \\ \dfrac{\partial \Delta\psi_p}{\partial x_j} \end{array}\right) = -\left(\begin{array}{c} \dfrac{\partial \iota\!\!\!-_-}{\partial \mathbf{B}_-}\cdot\dfrac{\partial \mathbf{B}_-}{\partial x_j} \\ \dfrac{\partial \iota\!\!\!-_+}{\partial \mathbf{B}_+}\cdot\dfrac{\partial \mathbf{B}_+}{\partial x_j} \end{array}\right). \tag{279}$$

- This 2×2 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`.

8.39 Trigonometric factors

Collaboration diagram for Trigonometric factors:



Variables

- 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 θ ?
- real, dimension(:), allocatable allglobal::gzeta

  something related to $\sqrt{g}$ and ζ ?
- 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

8.39.1 Detailed Description

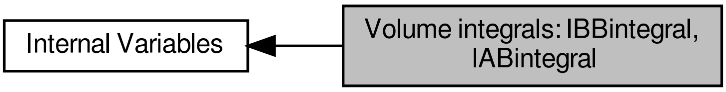
- To facilitate construction of the metric integrals, various trigonometric identities are exploited.
- The following are used for volume integrals (see volume()):

$$a_{i,j,k} \;=\; 4\, m_k \oint\!\!\oint d\theta d\zeta \;\; \cos(\alpha_i)\cos(\alpha_j)\cos(\alpha_k)/(2\pi)^2, \tag{280}$$

$$b_{i,j,k} \;=\; 4\, m_j \oint\!\!\oint d\theta d\zeta \;\; \cos(\alpha_i)\sin(\alpha_j)\sin(\alpha_k)/(2\pi)^2, \tag{281}$$

8.40 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

8.40.1 Detailed Description

- The energy functional, $F \equiv \sum_l F_l$, where

$$F_l \equiv \left(\int_{\mathcal{V}_l} \frac{p_l}{\gamma - 1} + \frac{B_l^2}{2} dv \right) = \frac{P_l}{\gamma - 1} V_l^{1-\gamma} + \int_{\mathcal{V}_l} \frac{B_l^2}{2} dv, \tag{282}$$

  where the second expression is derived using $p_l V_l^\gamma = P_l$, where P_l is the adiabatic-constant. In Eqn. (282), it is implicit that $\mathbf{B}$ satisfies (i) the toroidal and poloidal flux constraints; (ii) the interface constraint, $\mathbf{B} \cdot \nabla s = 0$; 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`↩
  :Nvol,0:1,0:mn+mn-1), where

  $F_l \equiv$ `dFF(l,0, 0)`

  $\partial F_l / \partial R_{l-1,j} \equiv$ `dFF(ll,0, j)`

  $\partial F_l / \partial Z_{l-1,j} \equiv$ `dFF(ll,0,mn j)`

  $\partial F_l / \partial R_{l,j} \equiv$ `dFF(ll,1, j)`

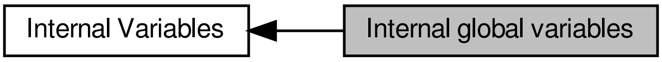
  $\partial F_l / \partial Z_{l,j} \equiv$ `dFF(ll,1,mn j)`

- 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`↩
  `:2,1:Nvol)`.

8.41 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^θ, $\dot{s}$ *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, θ, ζ) *given* (R, Z, φ)

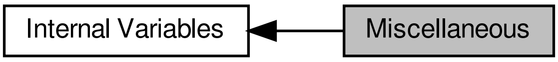
8.41.1 Detailed Description

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

8.42 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

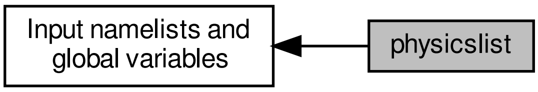
8.42.1 Detailed Description

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

8.43 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::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, ψ_t*, enclosed by each interface*
- real, dimension(1:mnvol+1) inputlist::pflux = 0.0

  poloidal flux, ψ_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, μ, in each volume
- real, dimension(1:mnvol+1) inputlist::ivolume = 0.0

  Toroidal current constraint normalized by μ_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 μ_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 γ 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 γ 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 γ 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 γ is the golden mean, $\gamma = (1 + \sqrt{5})/2$.
- real, dimension(0:mnvol) inputlist::iota = 0.0

  rotational-transform, $\iota\!\!\!-$, 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 γ 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 γ 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 γ 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 γ is the golden mean, $\gamma = (1 + \sqrt{5})/2$.
- real, dimension(0:mnvol) inputlist::oita = 0.0

  rotational-transform, $\iota\!\!\!-$, on outer side of each interface
- real inputlist::mupftol = 1.0e-14

  accuracy to which μ 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;

8.43.1 Detailed Description

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

8.43.2 Variable Documentation

8.43.2.1 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(), dforce(), dfp100(), dfp200(), dvcfield(), evaluate_dbb(), evaluate_dmupfdx(), fcn1(), fcn2(), final_diagnostics(), hesian(), jo00aa(), lbpol(), lforce(), sphdf5::mirror_input_to_outfile(), newton(), packxi(), pc00ab(), pp00aa(), preset(), rzaxis(), spec(), stzxyz(), volume(), sphdf5::write_grid(), writereadgf(), and allglobal::wrtend().

8.43.2.2 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 $N \equiv$`Nfp`
- constraint: `Nfp` $>$= 1

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), invfft(), jo00aa(), sphdf5::mirror_input_to_outfile(), preset(), ra00aa(), spec(), tfft(), and allglobal::wrtend().

8.43.2.3 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().

8.43.2.4 mpol `integer inputlist::mpol = 0`

number of poloidal Fourier harmonics

- all Fourier representations of doubly-periodic functions are of the form

$$f(\theta,\zeta) = \sum_{n=0}^{\texttt{Ntor}} f_{0,n}\cos(-n\,\texttt{Nfp}\,\zeta) + \sum_{m=1}^{\texttt{Mpol}}\sum_{n=\texttt{-Ntor}}^{\texttt{Ntor}} f_{m,n}\cos(m\theta - n\,\texttt{Nfp}\,\zeta), \tag{283}$$

  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().

8.43.2.5 ntor `integer inputlist::ntor = 0`

number of toroidal Fourier harmonics

- all Fourier representations of doubly-periodic functions are of the form

$$f(\theta,\zeta) = \sum_{n=0}^{\texttt{Ntor}} f_{0,n}\cos(-n\,\texttt{Nfp}\,\zeta) + \sum_{m=1}^{\texttt{Mpol}} \sum_{n=-\texttt{Ntor}}^{\texttt{Ntor}} f_{m,n}\cos(m\theta - n\,\texttt{Nfp}\,\zeta), \tag{284}$$

  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().

8.43.2.6 lrad `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(), lbpol(), lforce(), ma02aa(), matvec(), sphdf5::mirror_input_to_outfile(), mp00ac(), packab(), pp00aa(), preset(), ra00aa(), spec(), tr00ab(), sphdf5::write_grid(), and allglobal::wrtend().

8.43.2.7 lconstraint `integer inputlist::lconstraint = -1`

selects constraints; primarily used in ma02aa() and mp00ac().

- if `Lconstraint==-1`, then in the plasma regions $\Delta\psi_t$, μ 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 $\Delta\psi_t$, μ 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, `curtor`, and the "linking" current, `curpol`, and $\mu = 0$
- if `Lconstraint==1`, then in the plasma regions μ 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 μ 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 μ and ψ_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(), sphdf5::mirror_input_to_outfile(), pp00aa(), preset(), spec(), and allglobal::wrtend().

8.43.2.8 tflux `real, dimension(1:mnvol+1) inputlist::tflux = 0.0`

toroidal flux, ψ_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().

8.43.2.9 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().

8.43.2.10 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().

8.43.2.11 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().

8.43.2.12 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().

8.43.2.13 adiabatic `real, dimension(1:mnvol+1) inputlist::adiabatic = 0.0`

adiabatic constants in each volume

- The pressure is *not* held constant, but $p_l V_l^\gamma = P_l \equiv$`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().

8.43.2.14 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 γ 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 `iota` .

Referenced by allglobal::broadcast_inputs(), sphdf5::mirror_input_to_outfile(), preset(), and allglobal::wrtend().

8.43.2.15 ql `integer, dimension(0:mnvol) inputlist::ql = 0`

"inside" interface rotational-transform is $\iota = (p_l + \gamma p_r)/(q_l + \gamma q_r)$, where γ 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 `iota` .

Referenced by allglobal::broadcast_inputs(), sphdf5::mirror_input_to_outfile(), preset(), and allglobal::wrtend().

8.43.2.16 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 γ 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 `iota` .

Referenced by allglobal::broadcast_inputs(), sphdf5::mirror_input_to_outfile(), preset(), and allglobal::wrtend().

8.43.2.17 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 γ 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 `iota` .

Referenced by allglobal::broadcast_inputs(), sphdf5::mirror_input_to_outfile(), preset(), and allglobal::wrtend().

8.43.2.18 iota `real, dimension(0:mnvol) inputlist::iota = 0.0`

rotational-transform, $\iota\!\!\!-$, 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().

8.43.2.19 lp `integer, dimension(0:mnvol) inputlist::lp = 0`

"outer" interface rotational-transform is $\iota\!\!\!- = (p_l + \gamma p_r)/(q_l + \gamma q_r)$, where γ 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().

8.43.2.20 lq `integer, dimension(0:mnvol) inputlist::lq = 0`

"outer" interface rotational-transform is $\iota\!\!\!- = (p_l + \gamma p_r)/(q_l + \gamma q_r)$, where γ 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().

8.43.2.21 rp `integer, dimension(0:mnvol) inputlist::rp = 0`

"outer" interface rotational-transform is $\iota = (p_l + \gamma p_r)/(q_l + \gamma q_r)$, where γ 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().

8.43.2.22 rq `integer, dimension(0:mnvol) inputlist::rq = 0`

"outer" interface rotational-transform is $\iota = (p_l + \gamma p_r)/(q_l + \gamma q_r)$, where γ 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().

8.43.2.23 oita `real, dimension(0:mnvol) inputlist::oita = 0.0`

rotational-transform, ι, on outer 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().

8.43.2.24 mupftol `real inputlist::mupftol = 1.0e-14`

accuracy to which μ 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().

8.43.2.25 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().

8.43.2.26 rpol `real inputlist::rpol = 1.0`

poloidal extent of slab (effective radius)

- only relevant if `Igeometry==1`
- poloidal size is $L = 2\pi *$`rpol`

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), coords(), sphdf5::mirror_input_to_outfile(), sphdf5::write_grid(), and allglobal::wrtend().

8.43.2.27 rtor `real inputlist::rtor = 1.0`

toroidal extent of slab (effective radius)

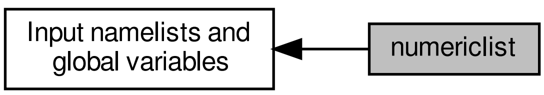
- only relevant if `Igeometry==1`
- toroidal size is $L = 2\pi *$`rtor`

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), coords(), sphdf5::mirror_input_to_outfile(), sphdf5::write_grid(), and allglobal::wrtend().

8.44 numericlist

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

Collaboration diagram for numericlist:



Variables

- 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.↩ge.1`*.*

8.44.1 Detailed Description

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

8.44.2 Variable Documentation

8.44.2.1 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().

8.44.2.2 lautoinitbn `integer inputlist::lautoinitbn = 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().

8.44.2.3 lzerovac `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().

8.44.2.4 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().

8.44.2.5 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().

8.44.2.6 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().

8.44.2.7 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 `lNtor` = 0

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), sphdf5::mirror_input_to_outfile(), preset(), and allglobal::wrtend().

8.44.2.8 lsparse `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().

8.44.2.9 lsvdiota `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().

8.44.2.10 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().

8.44.2.11 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().

8.44.2.12 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().

8.44.2.13 mregular `integer inputlist::mregular = -1`

maximum regularization factor

- if `Mregular.ge.2`, then $\mathtt{regumm}_i$ = $\mathtt{Mregular}/2$ where $\mathtt{m}_i > \mathtt{Mregular}$

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), sphdf5::mirror_input_to_outfile(), preset(), and allglobal::wrtend().

8.44.2.14 lrzaxis `integer inputlist::lrzaxis = 1`

controls the guess of geometry axis in the innermost volume or initialization of interfaces

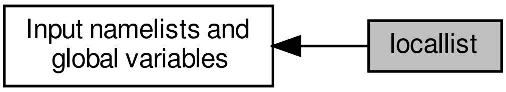
- if `iprecon` = 1, the centroid is used
- if `iprecon` = 2, the Jacobian $m = 1$ harmonic elimination method is used

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), sphdf5::mirror_input_to_outfile(), rzaxis(), and allglobal::wrtend().

8.45 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

8.45.1 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.

8.45.2 Variable Documentation

8.45.2.1 lbeltrami `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 μ 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 μ; in this case, it is only required to solve $\nabla\times\mathbf{B} = \mu\mathbf{B}$ which reduces to a system of linear equations; μ 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().

8.45.2.2 linitgues `integer inputlist::linitgues = 1`

controls how initial guess for Beltrami field is constructed

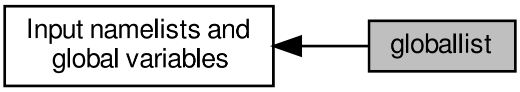
- only relevant for routines that require an initial guess for the Beltrami fields, such as the SQP and Newton methods, or the sparse linear solver;
- if `Linitgues` = 0, the initial guess for the Beltrami field is trivial
- if `Linitgues` = 1, the initial guess for the Beltrami field is an integrable approximation
- if `Linitgues` = 2, the initial guess for the Beltrami field is read from file
- if `Linitgues` = 3, the initial guess for the Beltrami field will be randomized with the maximum `maxrndgues`

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), sphdf5::mirror_input_to_outfile(), preset(), and allglobal::wrtend().

8.46 globallist

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

Collaboration diagram for 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 `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 casing()
- integer inputlist::mcasingcal = 8

  minimum number of calls to adaptive virtual casing routine; see casing(); redundant;

8.46.1 Detailed Description

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

Comments:

- The "force" vector, $\mathbf{F}$, which is constructed in dforce(), is a combination of pressure-imbalance Fourier harmonics,

  $$F_{i,v} \equiv [[p + B^2/2]]_{i,v} \times \exp\left[-\texttt{escale}(m_i^2 + n_i^2)\right] \times \texttt{opsilon}, \tag{285}$$

  and spectral-condensation constraints, $I_{i,v}$, and the "star-like" angle constraints, $S_{i,v,}$, (see lforce() for details)

  $$F_{i,v} \equiv \texttt{epsilon} \times I_{i,v} + \texttt{upsilon} \times \left(\psi_v^\omega S_{i,v,1} - \psi_{v+1}^\omega S_{i,v+1,0}\right), \tag{286}$$

  where $\psi_v \equiv$ normalized toroidal flux, `tflux`, and $\omega \equiv$ `wpoloidal`.

8.46.2 Variable Documentation

8.46.2.1 Lfindzero `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 `C05PDF` (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().

8.46.2.2 escale `real inputlist::escale = 0.0`

controls the weight factor, `BBweight`, in the force-imbalance harmonics

- $\texttt{BBweight(i)} \equiv \texttt{opsilon} \times \exp\left[-\texttt{escale} \times (m_i^2+n_i^2)\right]$
- defined in preset() ; used in dforce()
- also see Eqn. (285)

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), sphdf5::mirror_input_to_outfile(), preset(), and allglobal::wrtend().

8.46.2.3 opsilon `real inputlist::opsilon = 1.0`

weighting of force-imbalance

- used in dforce(); also see Eqn. (285)

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), sphdf5::mirror_input_to_outfile(), preset(), and allglobal::wrtend().

8.46.2.4 pcondense `real inputlist::pcondense = 2.0`

spectral condensation parameter

- used in preset() to define $\texttt{mmpp(i)} \equiv m_i^p$, where $p \equiv \texttt{pcondense}$
- the angle freedom is exploited to minimize $\texttt{epsilon} \sum_i m_i^p (R_i^2+Z_i^2)$ with respect to tangential variations in the interface geometry
- also see Eqn. (286)

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), sphdf5::mirror_input_to_outfile(), preset(), and allglobal::wrtend().

8.46.2.5 epsilon `real inputlist::epsilon = 0.0`

weighting of spectral-width constraint

- used in dforce(); also see Eqn. (286)

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), dforce(), dfp200(), evaluate_dbb(), sphdf5↩
::mirror_input_to_outfile(), pc00ab(), and allglobal::wrtend().

8.46.2.6 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` $<$ 0

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), sphdf5::mirror_input_to_outfile(), pc00aa(), pc00ab(), preset(), and allglobal::wrtend().

8.46.2.7 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().

8.46.2.8 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().

8.46.2.9 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().

8.46.2.10 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().

8.46.2.11 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().

8.46.2.12 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:

$$(\mathbf{B}\cdot\mathbf{n})^{j+1} = \texttt{gBnbld} \times (\mathbf{B}\cdot\mathbf{n})^{j} + (1-\texttt{gBnbld}) \times (\mathbf{B}\cdot\mathbf{n})^{*}, \tag{287}$$

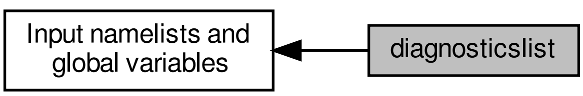
  where j labels free-boundary iterations, and $(\mathbf{B}\cdot\mathbf{n})^{*}$ is computed by virtual casing.
- only used if `Lfreebound` = 1
- only used in xspech()

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), sphdf5::mirror_input_to_outfile(), spec(), and allglobal::wrtend().

8.47 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 π) 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 $\nabla \mathbf{F}$
- 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

8.47.1 Detailed Description

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

8.47.2 Variable Documentation

8.47.2.1 nptrj `integer, dimension(1:mnvol+1) inputlist::nptrj = -1`

number of trajectories in each annulus to be followed in constructing Poincaré plot

- if `nPtrj(l)`$<$`0`, then `nPtrj(l)` = Ni(l), where `Ni(l)` 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().

8.47.2.2 lcheck `integer inputlist::lcheck = 0`

implement various checks

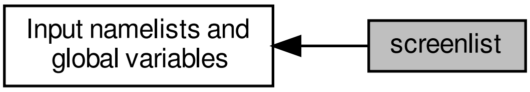
- if `Lcheck` = 0, no additional check on the calculation is performed
- if `Lcheck` = 1, the error in the current, i.e. $\nabla \times \mathbf{B} - \mu \mathbf{B}$ is computed as a post-diagnostic
- if `Lcheck` = 2, the analytic derivatives of the interface transform w.r.t. the helicity multiplier, μ, 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
  - must set `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 [7])
  - 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(), lbpol(), lforce(), ma02aa(), sphdf5::mirror_input_to_outfile(), preset(), rzaxis(), spec(), and allglobal::wrtend().

8.48 screenlist

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

Collaboration diagram for screenlist:



Variables

- 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

8.48.1 Detailed Description

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

8.48.2 Variable Documentation

8.48.2.1 wbuild_vector_potential `logical inputlist::wbuild_vector_potential = .false.`

Todo : what is this?

9 Module Documentation

9.1 allglobal Module Reference

global variable storage used as "workspace" throughout the code

Functions/Subroutines

- subroutine **build_vector_potential** (lvol, 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 lmpol

  what is this?
- integer lntor

  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

  no idea
- real, dimension(:,:), allocatable inifactor

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 lrbs

  local workspace
- real, dimension(:), allocatable lzbc

  local workspace
- integer **num_modes**
- integer, dimension(:), allocatable **mmrzrz**

- integer, dimension(:), allocatable **nnrzrz**
- real, dimension(:,:,:), allocatable **allrzrz**
- integer nt

  discrete resolution along θ of grid in real space
- integer nz

  discrete resolution along ζ 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

  Fourier harmonics; dummy workspace.
- real, dimension(:), allocatable sfmn

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 kjreal

  what is this ?
- real, dimension(:), allocatable kjimag

  what is this ?
- real, dimension(:,:,:), allocatable bsupumn

  tangential field on interfaces; θ-component; required for virtual casing construction of field; 11 Oct 12
- real, dimension(:,:,:), allocatable bsupvmn

  tangential field on interfaces; ζ -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 lma

  Lagrange multipliers (?)

- integer, dimension(:,:), allocatable lmb
  Lagrange multipliers (?)
- integer, dimension(:,:), allocatable lmc
  Lagrange multipliers (?)
- integer, dimension(:,:), allocatable lmd
  Lagrange multipliers (?)
- integer, dimension(:,:), allocatable lme
  Lagrange multipliers (?)
- integer, dimension(:,:), allocatable lmf
  Lagrange multipliers (?)
- integer, dimension(:,:), allocatable lmg
  Lagrange multipliers (?)
- integer, dimension(:,:), allocatable lmh
  Lagrange multipliers (?)
- real, dimension(:,:), allocatable lmavalue
  what is this?
- real, dimension(:,:), allocatable lmbvalue
  what is this?
- real, dimension(:,:), allocatable lmcvalue
  what is this?
- real, dimension(:,:), allocatable lmdvalue
  what is this?
- real, dimension(:,:), allocatable lmevalue
  what is this?
- real, dimension(:,:), allocatable lmfvalue
  what is this?
- real, dimension(:,:), allocatable lmgvalue
  what is this?
- real, dimension(:,:), allocatable lmhvalue
  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 lsavedguvij
  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(Itor,Gpol)/dx; (see dforce)
- real, dimension(:,:,:,:), allocatable glambda

  save initial guesses for iterative calculation of rotational-transform
- integer lmns

  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 θ cosine component of the tangential field on interfaces; stellarator-symmetric
- real, dimension(:,:,:), allocatable bzemn

  covariant ζ cosine component of the tangential field on interfaces; stellarator-symmetric
- real, dimension(:,:,:), allocatable btomn

  covariant θ 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^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 lhessianallocated

  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 θ ?
- real, dimension(:), allocatable gzeta

  something related to $\sqrt{g}$ and ζ ?
- real, dimension(:), allocatable ajk

  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^θ, $\dot{s}$ 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 lblinear

  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,θ,ζ) given (R,Z,φ)
- type(derivative) dbdx

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

9.1.1 Detailed Description

global variable storage used as "workspace" throughout the code

9.1.2 Function/Subroutine Documentation

9.1.2.1 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 $\Phi_{edge} \equiv$ `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,

$$Isurf_i \quad \rightarrow Isurf_i \cdot \frac{curtor}{\sum_{i=1}^{Mvol-1} Isurf_i + Ivol_i} Ivol_i \quad \rightarrow Ivol_i \cdot \frac{curtor}{\sum_{i=1}^{Mvol-1} Isurf_i + Ivol_i} \tag{288}$$

Finally, the volume current in the vacuum region is set to 0.

reading of numericlist

reading of locallist

reading of globallist

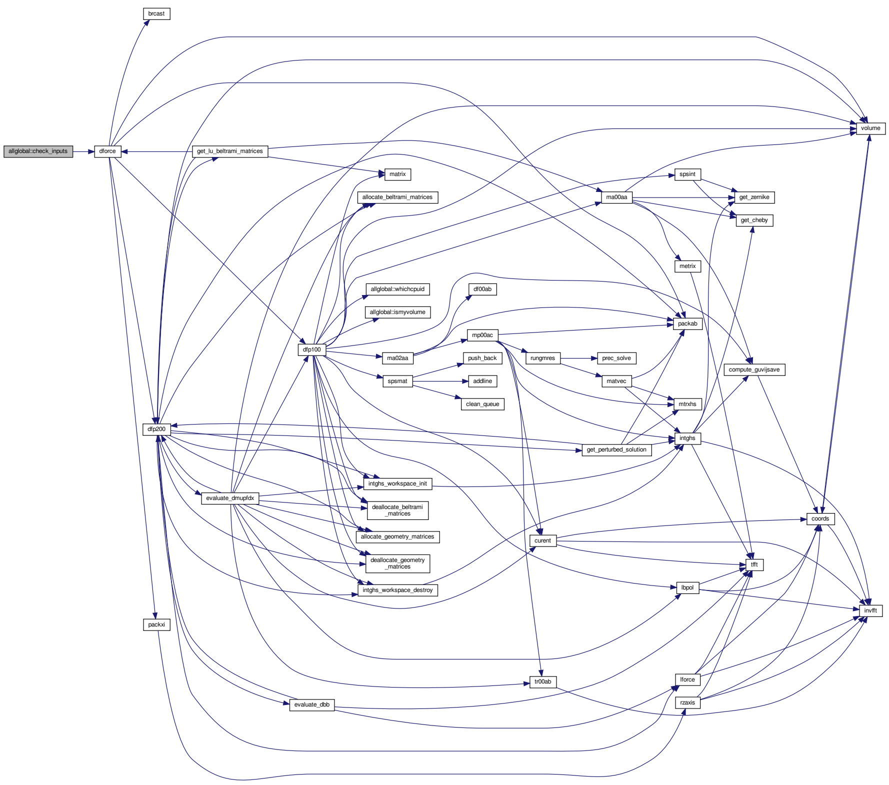
reading of diagnosticslist

reading of screenlist

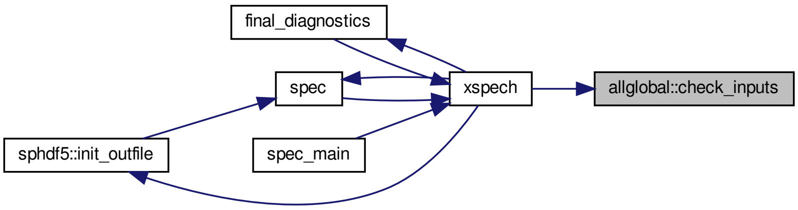
References inputlist::bnc, inputlist::c05factor, inputlist::c05xmax, inputlist::c05xtol, cpus, inputlist::curpol, inputlist::curtor, dforce(), inputlist::dpp, inputlist::dqq, inputlist::drz, inputlist::epsgmres, inputlist::epsilon, inputlist::epsilu, inputlist::escale, inputlist::forcetol, inputlist::gamma, 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::lconstraint, inputlist::lextrap, inputlist::lfindzero, 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::lsvdiota, inputlist::ltiming, inputlist::lzerovac, 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, cputiming::treadin, 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:



9.1.2.2 broadcast_inputs() `subroutine allglobal::broadcast_inputs`

broadcast physicslist

broadcast numericlist

broadcast globallist

broadcast locallist

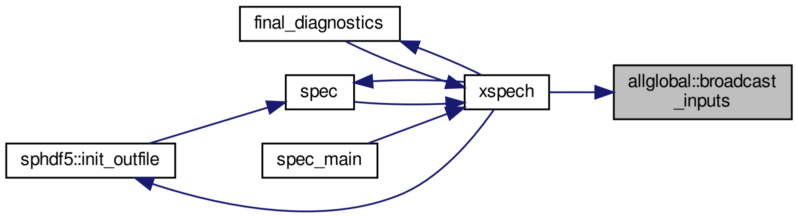
broadcast diagnosticslist

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::epsilu, 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::lconstraint, inputlist::lerrortype, inputlist::lextrap, inputlist::lfindzero, inputlist::lfreebound, inputlist::lgmresprec, inputlist::lhevalues, inputlist::lhevectors, inputlist::lhmatrix, 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::ngrid, inputlist::nitergmres, 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::ppts, 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::vcasingper, inputlist::vcasingtol, inputlist::wmacros, inputlist::wpoloidal, inputlist::wreadin, and inputlist::wwrtend.

Referenced by xspech().

Here is the caller graph for this function:



9.1.2.3 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.

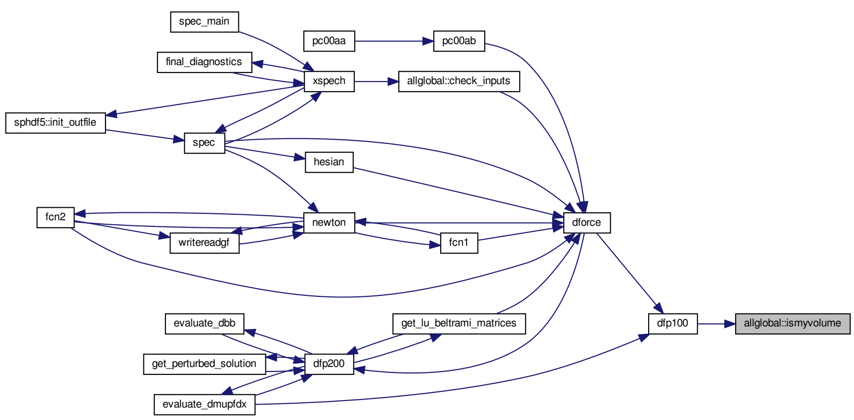
Parameters

vvol	volume to check

References ismyvolumevalue, myid, and ncpu.

Referenced by dfp100().

Here is the caller graph for this function:



9.2 constants Module Reference

some constants used throughout the code

Variables

- real, parameter zero = 0.0

  0
- real, parameter one = 1.0

  1
- real, parameter two = 2.0

  2
- real, parameter three = 3.0

  3
- real, parameter four = 4.0

  4
- real, parameter five = 5.0

  5
- real, parameter six = 6.0

  6
- real, parameter seven = 7.0

  7
- real, parameter eight = 8.0

  8
- real, parameter nine = 9.0

  9
- real, parameter ten = 10.0

  10
- real, parameter eleven = 11.0

  11
- real, parameter twelve = 12.0

  12
- real, parameter hundred = 100.0

  100
- real, parameter thousand = 1000.0

  1000
- real, parameter half = one / two

  1/2
- real, parameter third = one / three

  1/3
- real, parameter quart = one / four

  1/4
- real, parameter fifth = one / five

  1/5
- real, parameter sixth = one / six

  1/6
- real, parameter pi2 = 6.28318530717958623

  2π
- real, parameter pi = pi2 / two

  π
- real, parameter mu0 = 2.0E-07 $*$ pi2

  $4\pi \cdot 10^{-7}$
- real, parameter goldenmean = 1.618033988749895

  golden mean = $(1+\sqrt{5})/2$ *;*
- real, parameter version = 3.10

  version of SPEC

9.2.1 Detailed Description

some constants used throughout the code

9.3 cputiming Module Reference

timing variables

Variables

- real treadin = 0.0
  timing of readin()
- real twrtend = 0.0
  timing of wrtend()

9.3.1 Detailed Description

timing variables

9.4 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 (?)

9.4.1 Detailed Description

Interface to FFTW library.

9.5 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;

9.5.1 Detailed Description

central definition of file units to avoid conflicts

9.6 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

  eventually redundant; 24 Oct 12;

9.6.1 Detailed Description

...todo...

9.7 newtontime Module Reference

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 (?)

9.7.1 Detailed Description

timing of Newton iterations

9.8 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;

9.8.1 Detailed Description

platform-dependant numerical resolution

9.9 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 θ 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 θ 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 θ 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 R coordinate of field line following.
- integer(hid_t) memspace_z

  Dataspace identifier in memory for 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.

9.9.1 Detailed Description

writing the HDF5 output file

9.10 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...*

9.10.1 Detailed Description

type definitions for custom datatypes

9.10.2 Data Type Documentation

9.10.2.1 type typedefns::subgrid

used for quantities which have different resolutions in different volumes, e.g. the vector potential

Class Members

real, dimension(:), allocatable	s	coefficients
integer, dimension(:), allocatable	i	indices

Class Members

real, dimension(:,:), allocatable	mat	
integer, dimension(:), allocatable	ipivot	

9.10.2.2 type typedefns::matrixlu

9.10.2.3 type typedefns::derivative

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

Class Members

logical	l	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?

10 Data Type Documentation

10.1 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 **kjreal**
- real, dimension(:,:,:), allocatable **bloweremn**
- real, dimension(:,:,:), allocatable **bloweromn**
- real, dimension(:,:,:), allocatable **gbupper**
- real, dimension(:,:,:), allocatable **blower**
- real, dimension(:,:,:,:), allocatable **basis**

10.1.1 Detailed Description

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

Todo Zhisong might need to update the documentation of this type.

10.1.2 Member Data Documentation

10.1.2.1 efmn `real, dimension(:,:), allocatable intghs_module::intghs_workspace::efmn`

This is efmn.

10.1.2.2 ofmn `real, dimension(:,:), allocatable intghs_module::intghs_workspace::ofmn`

This is ofmn.

10.1.2.3 cfmn `real, dimension(:,:), allocatable intghs_module::intghs_workspace::cfmn`

10.1.2.4 sfmn `real, dimension(:,:), allocatable intghs_module::intghs_workspace::sfmn`

10.1.2.5 evmn `real, dimension(:,:), allocatable intghs_module::intghs_workspace::evmn`

10.1.2.6 odmn `real, dimension(:,:), allocatable intghs_module::intghs_workspace::odmn`

10.1.2.7 ijreal `real, dimension(:,:), allocatable intghs_module::intghs_workspace::ijreal`

10.1.2.8 jireal `real, dimension(:,:), allocatable intghs_module::intghs_workspace::jireal`

10.1.2.9 jkreal `real, dimension(:,:), allocatable intghs_module::intghs_workspace::jkreal`

10.1.2.10 kjreal `real, dimension(:,:), allocatable intghs_module::intghs_workspace::kjreal`

10.1.2.11 bloweremn `real, dimension(:,:,:), allocatable intghs_module::intghs_workspace↩ ::bloweremn`

10.1.2.12 bloweromn `real, dimension(:,:,:), allocatable intghs_module::intghs_workspace↩ ::bloweromn`

10.1.2.13 gbupper `real, dimension(:,:,:), allocatable intghs_module::intghs_workspace::gbupper`

10.1.2.14 blower `real, dimension(:,:,:), allocatable intghs_module::intghs_workspace::blower`

10.1.2.15 basis `real, dimension(:,:,:,:), allocatable intghs_module::intghs_workspace::basis`

The documentation for this type was generated from the following file:

- intghs.f90

11 File Documentation

11.1 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, lrad, mpol, zernike)

  Get the Zernike polynomials $\hat{R}^m_l$ with zeroth, first derivatives.
- subroutine get_zernike_d2 (r, lrad, mpol, zernike)

  Get the Zernike polynomials $\hat{R}^m_l$ with zeroth, first, second derivatives.
- subroutine get_zernike_rm (r, lrad, mpol, zernike)

  Get the Zernike polynomials $\hat{R}^m_l/r^m$.

11.1.1 Detailed Description

Polynomials evaluation.

11.1.2 Function/Subroutine Documentation

11.1.2.1 get_cheby()

```
subroutine get_cheby (
        real, intent(in) lss,
        integer, intent(in) lrad,
        real, dimension(0:lrad,0:1), intent(inout) cheby )
```

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.

$$T_0(s) = 1,$$
$$T_1(s) = s,$$
$$T_{l+1}(s) = 2sT_l(s) - T_{l-1}(s).$$

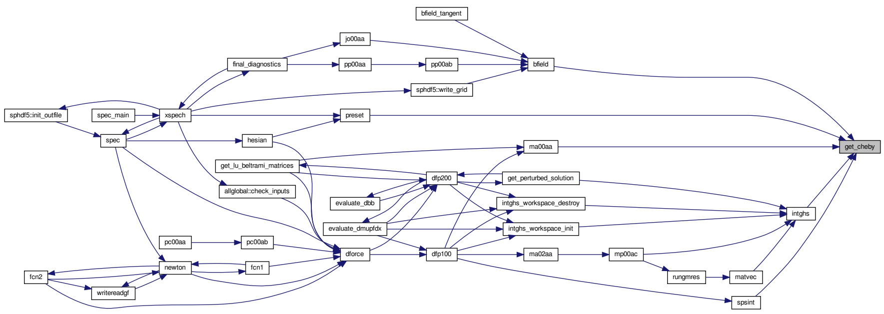
Parameters

in	*lss*	coordinate input lss
in	*lrad*	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:



11.1.2.2 get_cheby_d2()

```
subroutine get_cheby_d2 (
    real, intent(in) lss,
    integer, intent(in) lrad,
    real, dimension(0:lrad,0:2), intent(inout) 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.

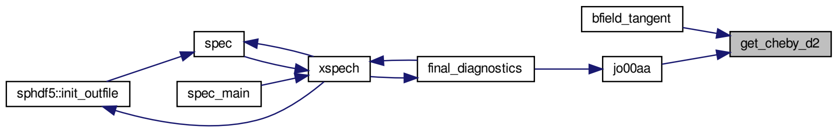
Parameters

in	*lss*	coordinate input lss
in	*lrad*	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:



11.1.2.3 get_zernike()

```
subroutine get_zernike (
    real, intent(in) r,
    integer, intent(in) lrad,
    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

$$\begin{aligned} Z_l^{-m}(s,\theta) &= R_l^m(s)\sin m\theta, \\ Z_l^{m}(s,\theta) &= R_l^m(s)\cos m\theta, \end{aligned}$$

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

$$\begin{aligned} \hat{R}_0^0 &= 1, \hat{R}_l^0 &= \frac{1}{l+1}R_l^0 - \frac{(-1)^{l/2}}{l+1}, \\ \hat{R}_1^1 &= s, \hat{R}_l^1 &= \frac{1}{l+1}R_l^1 - \frac{(-1)^{(l-1)/2}}{2}s. \end{aligned}$$

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

$$\hat{R}_l^m = \frac{1}{l+1}R_l^m.$$

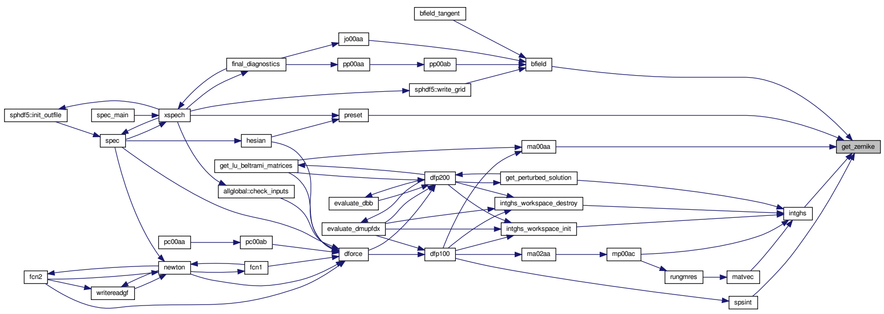
Parameters

in	*r*	coordinate input, note that this is normalized to $[0,1]$
in	*lrad*	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:



11.1.2.4 get_zernike_d2()

```
subroutine get_zernike_d2 (
        real, intent(in) r,
        integer, intent(in) lrad,
        integer, intent(in) mpol,
        real, dimension(0:lrad,0:mpol,0:2), intent(inout) zernike )
```

Get the Zernike polynomials $\hat{R}_l^m$ with zeroth, first, second derivatives.

See get_zernike for more detail.

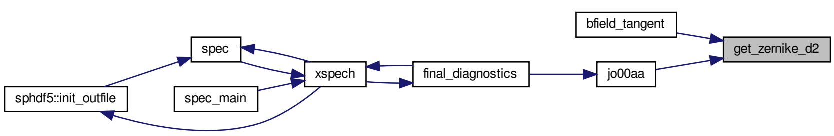
Parameters

in	*r*	coordinate input, note that this is normalized to $[0, 1]$
in	*lrad*	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:



11.1.2.5 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.

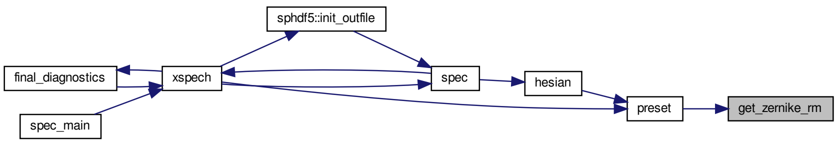
Parameters

in	*r*	coordinate input, note that this is normalized to $[0, 1]$
in	*lrad*	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:



11.2 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

11.2.1 Detailed Description

Returns $\dot{s} \equiv B^s / B^\zeta$ and $\dot{\theta} \equiv B^\theta / B^\zeta$.

11.2.2 Function/Subroutine Documentation

11.2.2.1 bfield_tangent()

```
subroutine bfield_tangent (
        real, intent(in) zeta,
        real, dimension(1:6), intent(in) st,
        real, dimension(1:6), intent(out) Bst )
```

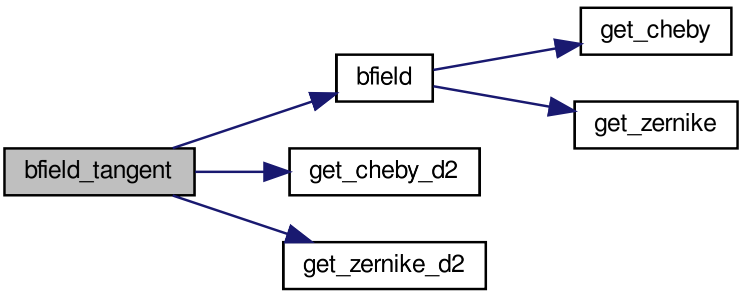
compute the tangential magnetic field

Parameters

in	*zeta*	toroidal angle
in	*st*	radial(s) and poloidal(theta) positions
out	*Bst*	tangential magnetic field

References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, 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:



11.3 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)

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

11.3.1 Detailed Description

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

11.4 brcast.f90 File Reference

Broadcasts Beltrami fields, profiles, . . .

Functions/Subroutines

- subroutine brcast (lvol)

  Broadcasts Beltrami fields, profiles, . . .

11.4.1 Detailed Description

Broadcasts Beltrami fields, profiles, . . .

11.5 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.

11.5.1 Detailed Description

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

11.6 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 (lvol, lss, Lcurvature, Ntz, mn)

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

11.6.1 Detailed Description

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

11.7 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 (lvol, mn, Nt, Nz, iflag, ldItGp)
  Computes the plasma current, $I \equiv \int B_\theta \, d\theta$, and the "linking" current, $G \equiv \int B_\zeta \, d\zeta$.

11.7.1 Detailed Description

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

11.8 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.

11.8.1 Detailed Description

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

11.9 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 $\mathbf{F}(\mathbf{x})$, 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 $\nabla\mathbf{F}$.
- subroutine **fndiff_dforce** (NGdof)

11.9.1 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 $\nabla\mathbf{F}$.

11.10 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.

11.10.1 Detailed Description

Split the work between MPI nodes and evaluate the global constraint.

11.10.2 Function/Subroutine Documentation

11.10.2.1 dfp100()

```
subroutine dfp100 (
    integer Ndofgl,
    real, dimension(1:mvol-1) x,
    real, dimension(1:ndofgl) Fvec,
    logical LComputeDerivatives )
```

Split the work between MPI nodes and evaluate the global constraint.

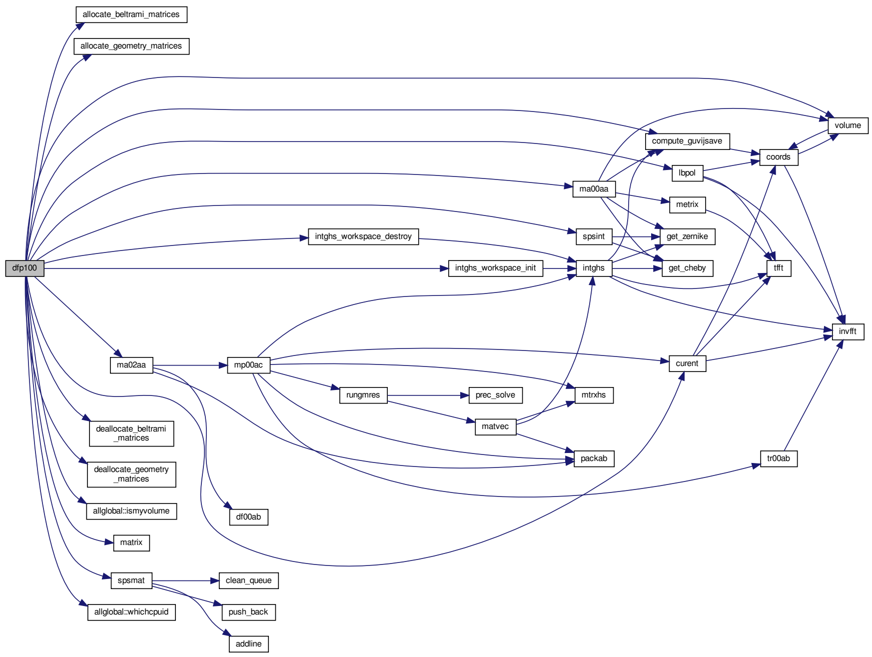
Parameters

Ndofgl	
x	
Fvec	
LComputeDerivatives	

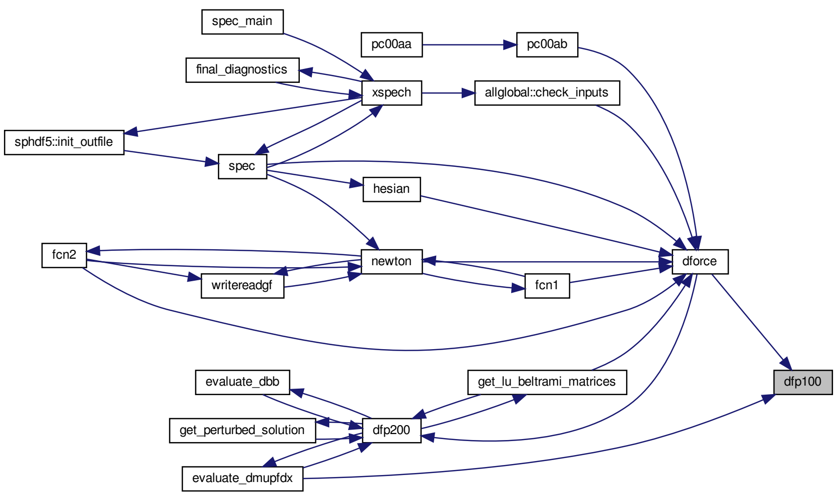
References allocate_beltrami_matrices(), allocate_geometry_matrices(), compute_guvijsave(), allglobal::cpus, curent(), inputlist::curpol, allglobal::dbdx, allglobal::ddttcc, allglobal::ddttcs, allglobal::ddttsc, allglobal::ddttss, allglobal::ddtzcc, allglobal::ddtzcs, allglobal::ddtzsc, allglobal::ddtzss, allglobal::ddzzcc, allglobal::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::iquad, allglobal::ismyvolume(), allglobal::ismyvolumevalue, inputlist::isurf, allglobal::izbs, lbpol(), 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, allglobal::tdszsc, allglobal::tdszss, allglobal::ttsscc, allglobal::ttsscs, allglobal::ttsssc, allglobal::ttssss, 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:



11.11 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 (lvol, 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.

11.11.1 Detailed Description

Given the field consistent with the constraints and the geometry, computes local quantites related to the force evaluation.

11.11.2 Function/Subroutine Documentation

11.11.2.1 dfp200()

```
subroutine dfp200 (
    logical, intent(in) LcomputeDerivatives,
    integer vvol )
```

Given the field consistent with the constraints and the geometry, computes local quantites related to the force evaluation.

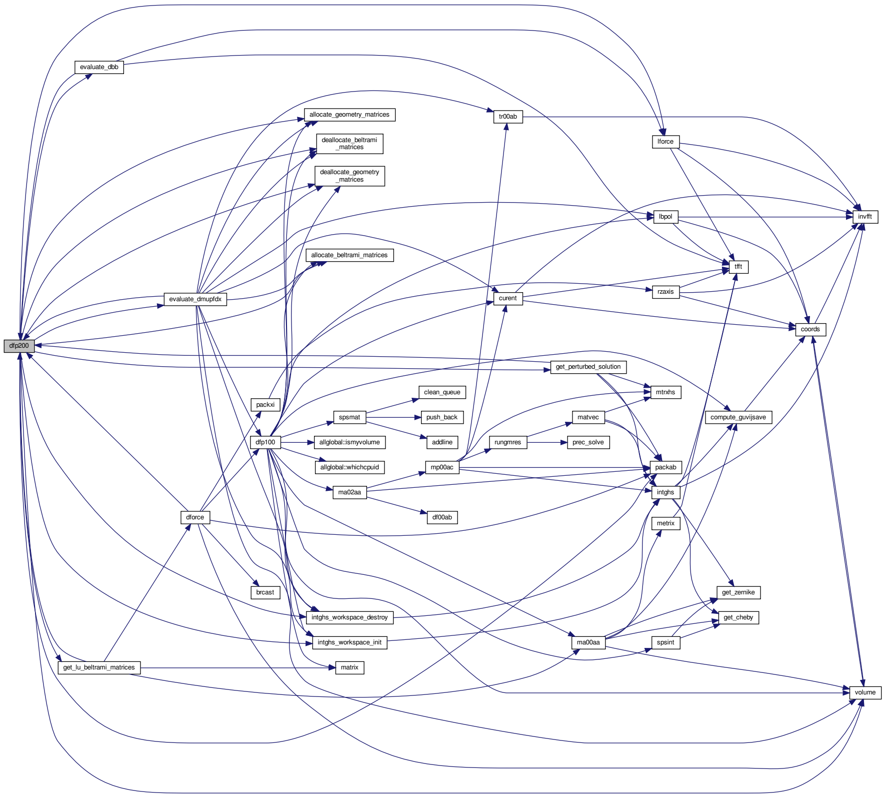
Parameters

LcomputeDerivatives	
vvol	

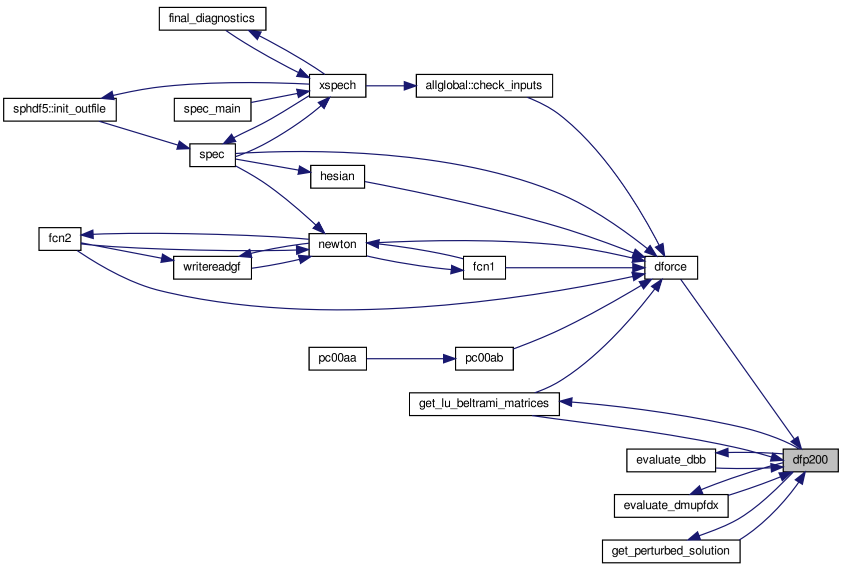
References inputlist::adiabatic, allocate_beltrami_matrices(), allocate_geometry_matrices(), allglobal::cpus, deallocate_beltrami_matrices(), deallocate_geometry_matrices(), inputlist::epsilon, evaluate_dbb(), evaluate_dmupfdx(), inputlist::gamma, get_lu_beltrami_matrices(), get_perturbed_solution(), 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:



11.11.2.2 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

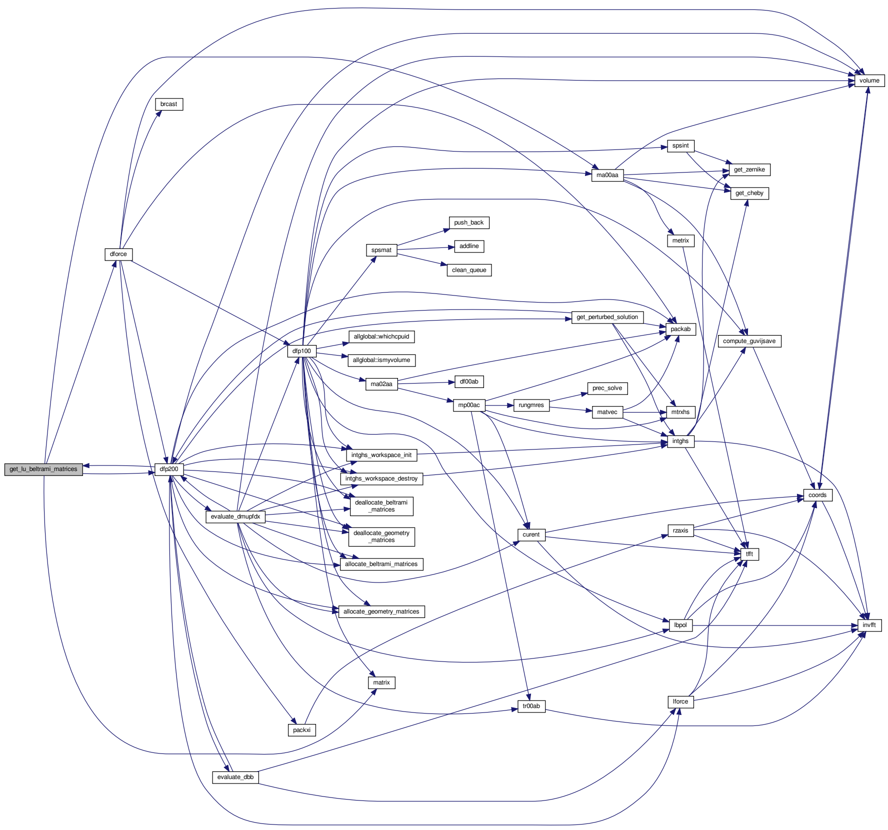
Parameters

vvol	
oBI	
NN	

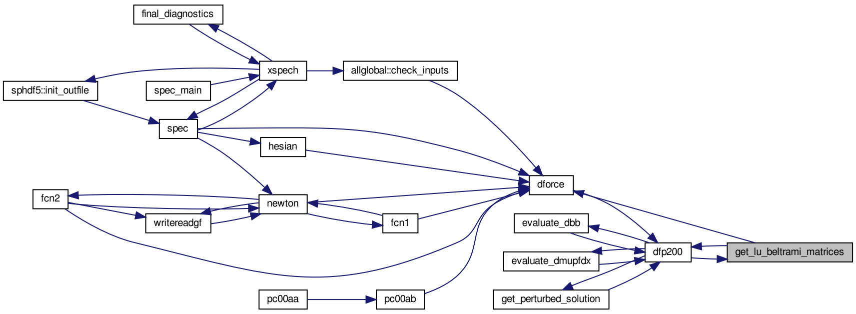
References allglobal::cpus, allglobal::dbdx, dforce(), dfp200(), allglobal::dma, allglobal::dmb, allglobal::dmd, allglobal::dmg, constants::half, allglobal::iquad, inputlist::lconstraint, allglobal::lcoordinatesingularity, allglobal::lplasmaregion, inputlist::lrad, allglobal::lsavedguvij, allglobal::lvacuumregion, ma00aa(), matrix(), allglobal::mn, allglobal::mne, allglobal::mpi_comm_spec, inputlist::mu, allglobal::myid, allglobal::ncpu, allglobal::nt, allglobal::nz, constants::one, fileunits::ounit, allglobal::solution, 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:



11.11.2.3 get_perturbed_solution()

```
subroutine get_perturbed_solution (
        integer, intent(in) vvol,
        type(matrixlu), intent(inout) oBI,
        integer, intent(in) NN )
```

This routine evaluates the value of the magnetic field once the interface is perturbed using matrix perturbation theory.

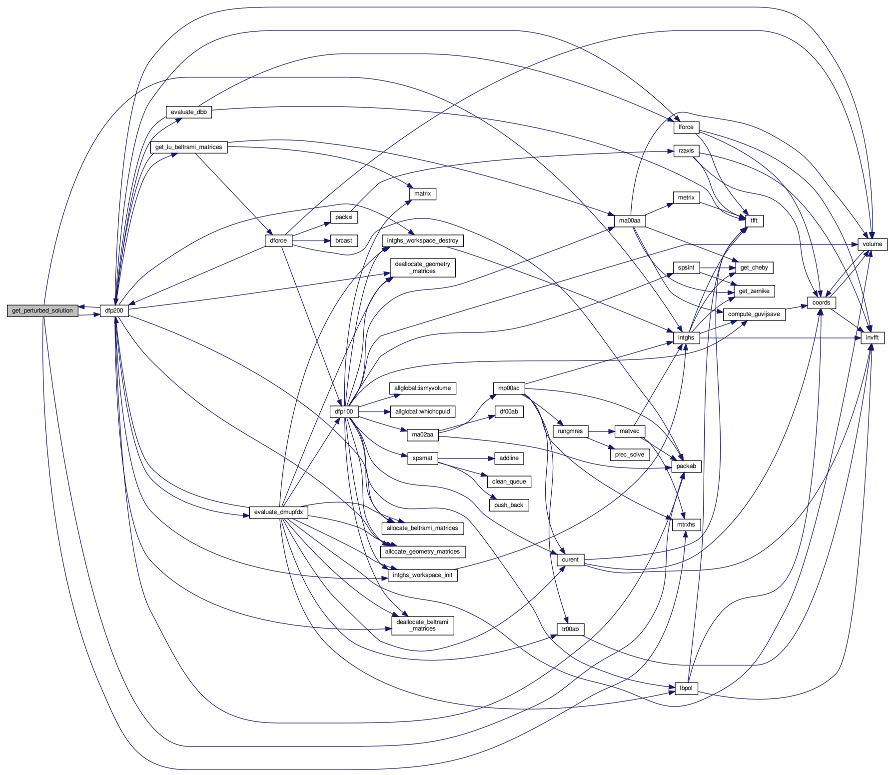
Parameters

vvol	
oBI	
NN	

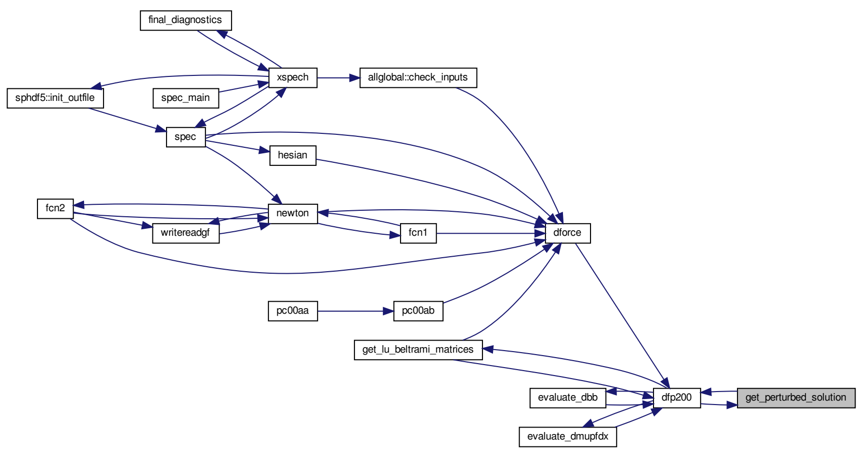
References allglobal::cpus, allglobal::dbdx, dfp200(), allglobal::dma, allglobal::dmb, allglobal::dmd, allglobal::dmg, allglobal::dpflux, allglobal::dtflux, constants::half, intghs(), allglobal::iquad, inputlist::lconstraint, inputlist::lrad, allglobal::mn, allglobal::mpi_comm_spec, mtrxhs(), inputlist::mu, 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 call graph for this function:



Here is the caller graph for this function:



11.11.2.4 evaluate_dmupfdx()

```
subroutine evaluate_dmupfdx (
        integer innout,
        integer idof,
```

```
integer ii,
integer issym,
integer irz )
```

Evaluate mu and psip derivatives and store them in dmupfdx.

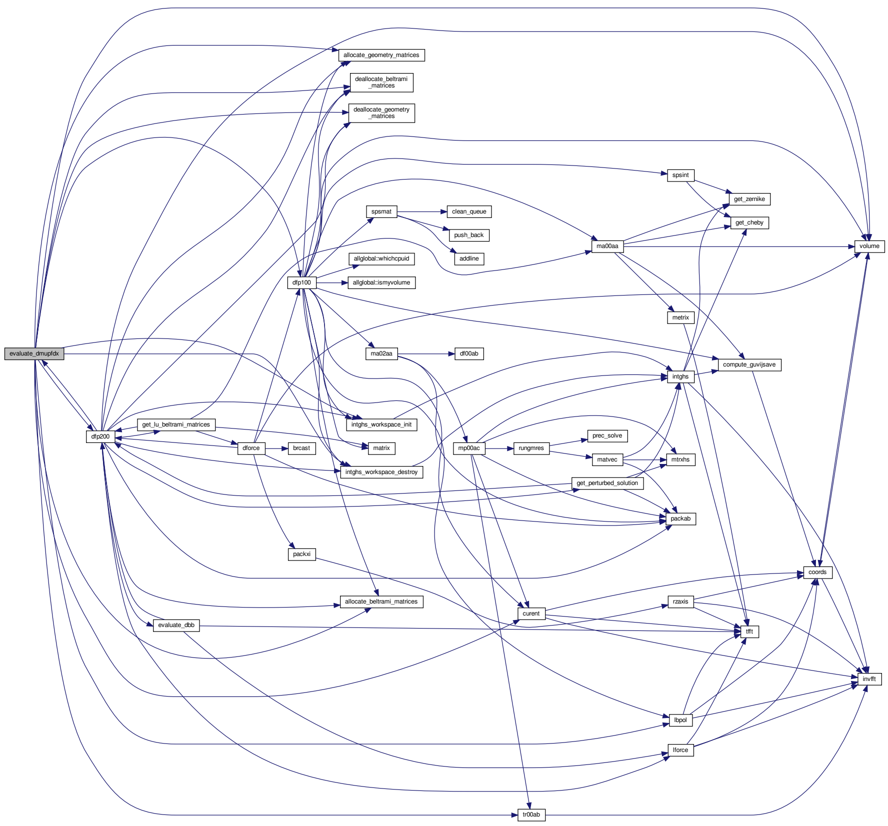
Parameters

innout	
idof	
ii	
issym	
irz	

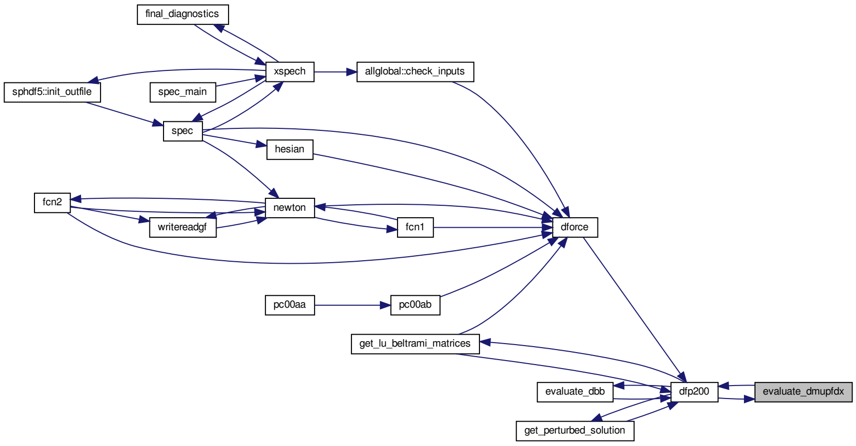
References allocate_beltrami_matrices(), allocate_geometry_matrices(), allglobal::cpus, curent(), deallocate_beltrami_matrices(), deallocate_geometry_matrices(), dfp100(), dfp200(), inputlist::drz, constants::half, inputlist::igeometry, intghs_workspace_destroy(), intghs_workspace_init(), allglobal::iquad, allglobal::irbc, allglobal::irbs, allglobal::izbc, allglobal::izbs, lbpol(), inputlist::lcheck, inputlist::lconstraint, allglobal::lcoordinatesingularity, inputlist::lfreebound, allglobal::lplasmaregion, inputlist::lrad, allglobal::lvacuumregion, allglobal::mpi_comm_spec, inputlist::mu, inputlist::mupftol, allglobal::myid, allglobal::ncpu, allglobal::ngdof, inputlist::nvol, constants::one, fileunits::ounit, numerical::small, tr00ab(), constants::two, volume(), inputlist::wmacros, and constants::zero.

Referenced by dfp200().

Here is the call graph for this function:



Here is the caller graph for this function:



11.11.2.5 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

lvol	
idof	
innout	
issym	
irz	
ii	
dBB	
XX	
YY	
length	

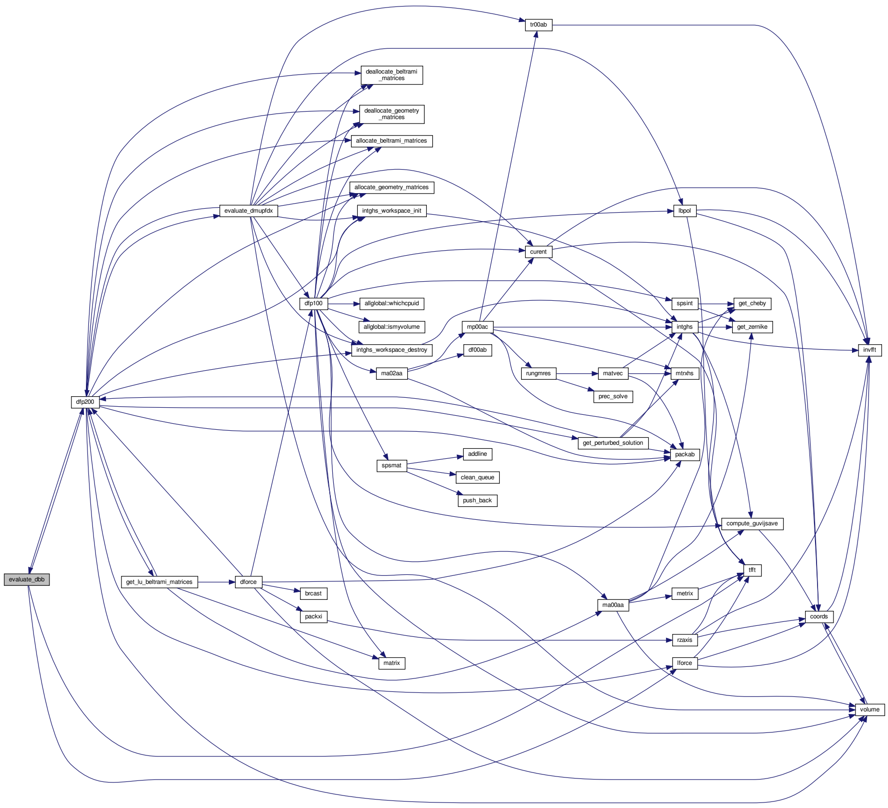
Parameters

dRR	
dZZ	
dII	
dLL	
dPP	
Ntz	
LcomputeDerivatives	

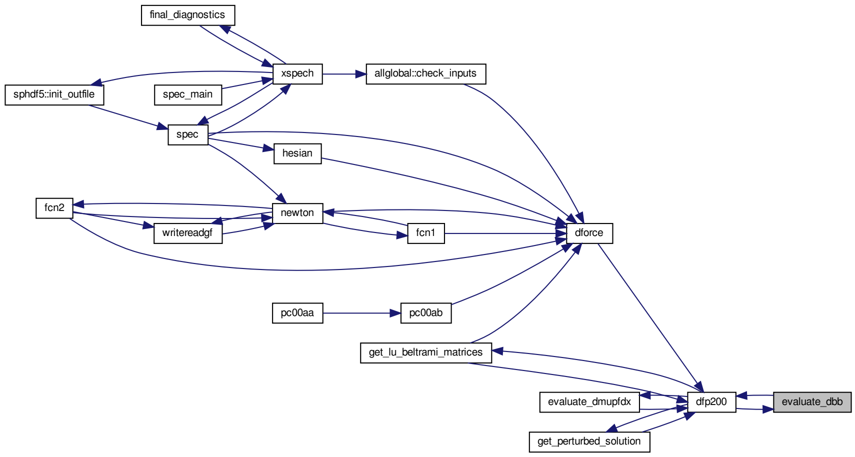
References inputlist::adiabatic, allglobal::cpus, dfp200(), allglobal::dpflux, inputlist::drz, inputlist::epsilon, inputlist::gamma, constants::half, inputlist::igeometry, allglobal::irbc, allglobal::irbs, allglobal::izbc, allglobal::izbs, inputlist::lcheck, inputlist::lconstraint, allglobal::lcoordinatesingularity, 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, tfft(), 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:



11.12 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** (lvol, 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

    0
- real, parameter constants::one = 1.0

    1
- real, parameter constants::two = 2.0

    2
- real, parameter constants::three = 3.0

    3
- real, parameter constants::four = 4.0

    4
- real, parameter constants::five = 5.0

    5
- real, parameter constants::six = 6.0

    6
- real, parameter constants::seven = 7.0

    7
- real, parameter constants::eight = 8.0

    8
- real, parameter constants::nine = 9.0

    9
- real, parameter constants::ten = 10.0

    10
- real, parameter constants::eleven = 11.0

    11
- real, parameter constants::twelve = 12.0

    12
- real, parameter constants::hundred = 100.0

    100
- real, parameter constants::thousand = 1000.0

    1000
- real, parameter constants::half = one / two

    1/2
- real, parameter constants::third = one / three

    1/3

- real, parameter constants::quart = one / four

  1/4
- real, parameter constants::fifth = one / five

  1/5
- real, parameter constants::sixth = one / six

  1/6
- real, parameter constants::pi2 = 6.28318530717958623

  2π
- real, parameter constants::pi = pi2 / two

  π
- 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::treadin = 0.0

  timing of readin()
- real cputiming::twrtend = 0.0

  timing of wrtend()
- 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

  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::lmpol

  what is this?

- integer allglobal::lntor

  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 $|curlB\text{-}mu*B|$ *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

  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

- 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 θ of grid in real space
- integer allglobal::nz

  discrete resolution along ζ 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
- real, dimension(:,:,:), allocatable allglobal::bsupvmn

  tangential field on interfaces; ζ -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::lmd

  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::lmbvalue

  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::lmfvalue

  what is this?
- real, dimension(:,:), allocatable allglobal::lmgvalue

  what is this?
- real, dimension(:,:), allocatable allglobal::lmhvalue

  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?
- 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(Itor,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 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
- 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, 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 θ ?
- real, dimension(:), allocatable allglobal::gzeta

  something related to $\sqrt{g}$ and ζ ?
- 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
- real allglobal::gbzeta

  toroidal (contravariant) field; calculated in bfield; required to convert $\dot{\theta}$ to B^θ, $\dot{s}$ 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, θ, ζ) given (R, Z, φ)
- type(derivative) allglobal::dbdx

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

  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
- 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

  FFTW-related (?)
- complex(c_double_complex), dimension(:,:,:), allocatable fftw_interface::cplxout

  FFTW-related (?)

11.12.1 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 $N \equiv$ Nvol, is described by a set of Fourier harmonics, using an arbitrary poloidal angle,

$$R_l(\theta,\zeta) = \sum_j R_{j,l} \cos(m_j\theta - n_j\zeta), \tag{289}$$

$$Z_l(\theta,\zeta) = \sum_j Z_{j,l} \sin(m_j\theta - n_j\zeta). \tag{290}$$

- These harmonics are read from the `ext.sp` file and come directly after the namelists described above. The required format is as follows:

$$\begin{array}{cccccccc} m_1 & n_1 & R_{1,0} & Z_{1,0} & R_{1,1} & Z_{1,1} & \dots & R_{1,N} & Z_{1,N} \\ m_2 & n_2 & R_{2,0} & Z_{2,0} & R_{2,1} & Z_{2,1} & \dots & R_{2,N} & Z_{2,N} \\ \dots \\ m_j & n_j & R_{j,0} & Z_{j,0} & R_{j,1} & Z_{j,1} & \dots & R_{j,N} & Z_{j,N} \\ \dots \end{array} \tag{291}$$

- The coordinate axis corresponds to $j = 0$ and the outermost boundary corresponds to $j =$ 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.

11.12.2 Data Type Documentation

11.12.2.1 type typedefns::subgrid

used for quantities which have different resolutions in different volumes, e.g. the vector potential

Class Members

real, dimension(:), allocatable	s	coefficients
integer, dimension(:), allocatable	i	indices

Class Members

real, dimension(:,:), allocatable	mat	
integer, dimension(:), allocatable	ipivot	

11.12.2.2 type typedefns::matrixlu

11.12.2.3 type typedefns::derivative $\mathrm{d}\mathbf{B}/\mathrm{d}\mathbf{X}$ (?)

Class Members

logical	l	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?

11.13 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, $\nabla_{\xi}\mathbf{F}$*.*

11.13.1 Detailed Description

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

11.14 inputlist.f90 File Reference

Input namelists.

Functions/Subroutines

- subroutine **inputlist::initialize_inputs**

Variables

- integer, parameter inputlist::mnvol = 256

  The maximum value of $\mathtt{Nvol}$ *is* $\mathtt{MNvol{=}256}$.
- integer, parameter inputlist::mmpol = 64

  The maximum value of $\mathtt{Mpol}$ *is* $\mathtt{MNpol{=}64}$.
- integer, parameter inputlist::mntor = 64

  The maximum value of $\mathtt{Ntor}$ *is* $\mathtt{MNtor{=}64}$.
- integer inputlist::igeometry = 3

  selects Cartesian, cylindrical or toroidal geometry;
- integer inputlist::istellsym = 1

  stellarator symmetry is enforced if $\mathtt{Istellsym{=}{=}1}$
- 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, ψ_t*, enclosed by each interface*
- real, dimension(1:mnvol+1) inputlist::pflux = 0.0

  poloidal flux, ψ_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, μ*, in each volume*
- real, dimension(1:mnvol+1) inputlist::ivolume = 0.0

Toroidal current constraint normalized by μ_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 μ_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 γ 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 γ 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 γ 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 γ is the golden mean, $\gamma = (1 + \sqrt{5})/2$.
- real, dimension(0:mnvol) inputlist::iota = 0.0

  rotational-transform, ι, 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 γ 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 γ 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 γ 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 γ is the golden mean, $\gamma = (1 + \sqrt{5})/2$.
- real, dimension(0:mnvol) inputlist::oita = 0.0

  rotational-transform, ι, on outer side of each interface
- real inputlist::mupftol = 1.0e-14

  accuracy to which μ 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;
- 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.ge.1` .

- 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
- 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 `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 casing()

- 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 π) 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 $\nabla \mathbf{F}$

- 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::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

11.14.1 Detailed Description

Input namelists.

11.15 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 (lquad, mn, lvol, lrad, idx)

  Calculates volume integrals of Chebyshev polynomials and covariant field products.

- subroutine intghs_workspace_init (lvol)

  init workspace

- subroutine intghs_workspace_destroy ()

  free workspace

Variables

- type(intghs_workspace) intghs_module::wk

  This is an instance of the intghs_workspace type.

11.15.1 Detailed Description

Calculates volume integrals of Chebyshev-polynomials and covariant field for Hessian computation.

11.15.2 Function/Subroutine Documentation

11.15.2.1 intghs()

```
subroutine intghs (
        integer, intent(in) lquad,
        integer, intent(in) mn,
        integer, intent(in) lvol,
        integer, intent(in) lrad,
        integer, intent(in) idx )
```

Calculates volume integrals of Chebyshev polynomials and covariant field products.

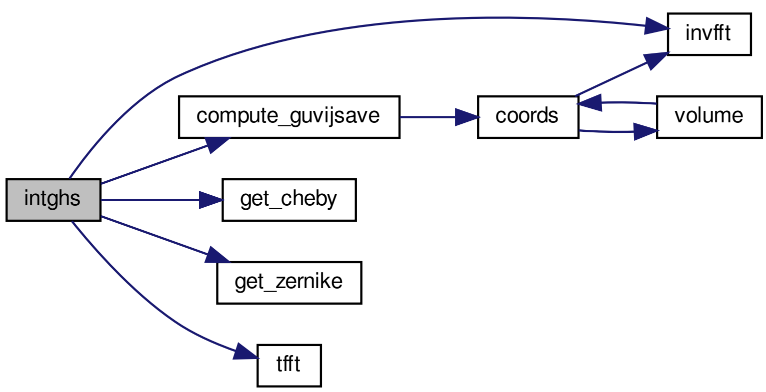
Parameters

lquad	
mn	
lvol	
lrad	
idx	

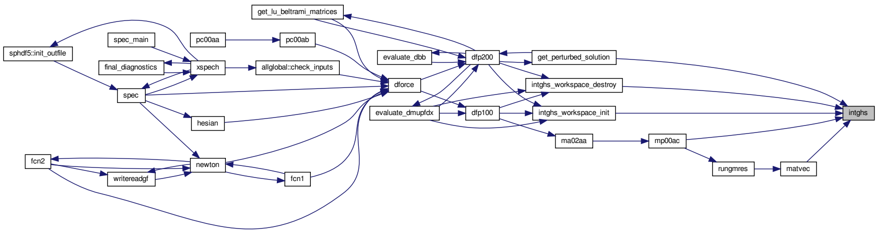
References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, compute_guvijsave(), allglobal::cpus, allglobal::dbdx, allglobal::dtc, allglobal::dts, allglobal::dzc, allglobal::dzs, allglobal::gaussianabscissae, allglobal↩ ::gaussianweight, get_cheby(), get_zernike(), allglobal::guvij, allglobal::guvijsave, constants::half, allglobal::im, allglobal::in, invfft(), allglobal::lcoordinatesingularity, allglobal::lsavedguvij, allglobal::mne, allglobal::mpi_comm_↩ spec, inputlist::mpol, allglobal::myid, allglobal::ncpu, allglobal::notstellsym, allglobal::nt, allglobal::ntz, allglobal↩ ::nz, constants::one, fileunits::ounit, constants::pi, constants::pi2, allglobal::sg, numerical::small, numerical↩ ::sqrtmachprec, tfft(), allglobal::tsc, allglobal::tss, allglobal::ttc, allglobal::tts, constants::two, allglobal::tzc, allglobal↩ ::tzs, numerical::vsmall, inputlist::wmacros, allglobal::yesstellsym, and constants::zero.

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:



11.15.2.2 intghs_workspace_init() `subroutine intghs_workspace_init ( integer, intent(in) lvol )`

init workspace

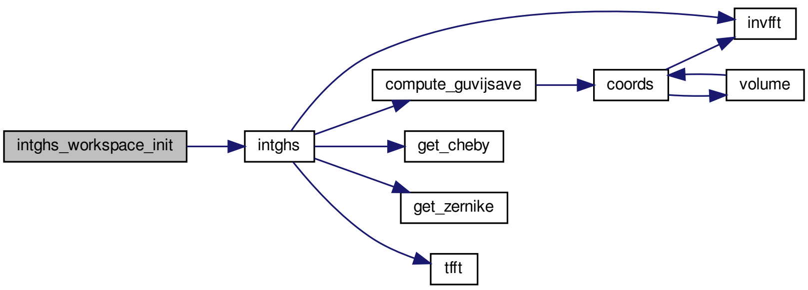
Parameters

lvol	

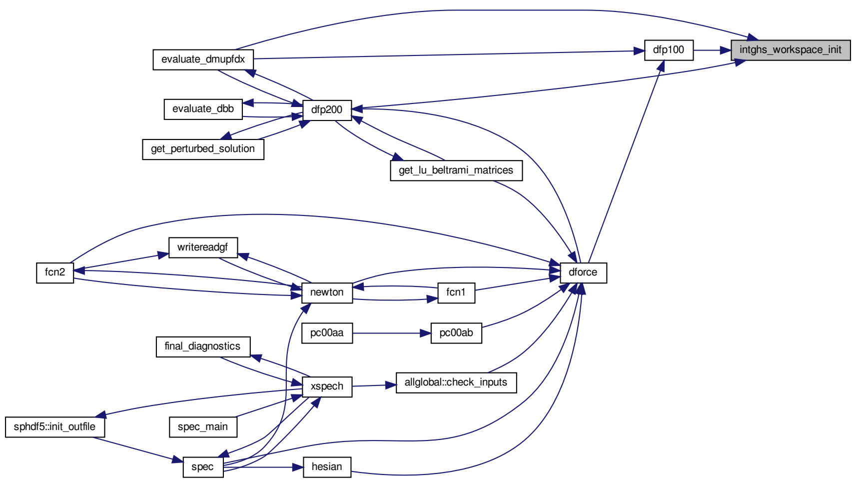
References allglobal::cpus, intghs(), allglobal::iquad, inputlist::lrad, allglobal::mn, allglobal::mpi_comm_spec, inputlist::mpol, allglobal::myid, allglobal::ncpu, allglobal::ntz, fileunits::ounit, inputlist::wmacros, and constants::zero.

Referenced by dfp100(), dfp200(), and evaluate_dmupfdx().

Here is the call graph for this function:



Here is the caller graph for this function:



11.15.2.3 intghs_workspace_destroy() `subroutine intghs_workspace_destroy`

free workspace

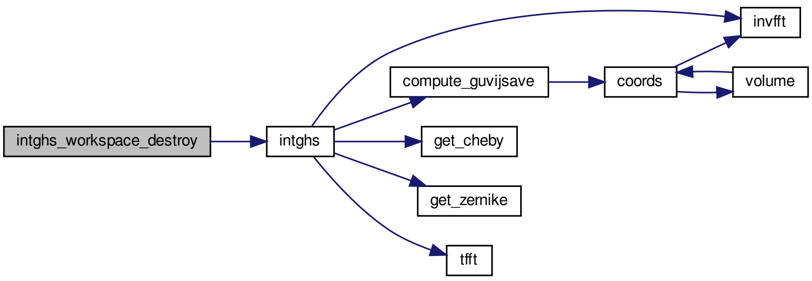
Parameters

lvol	

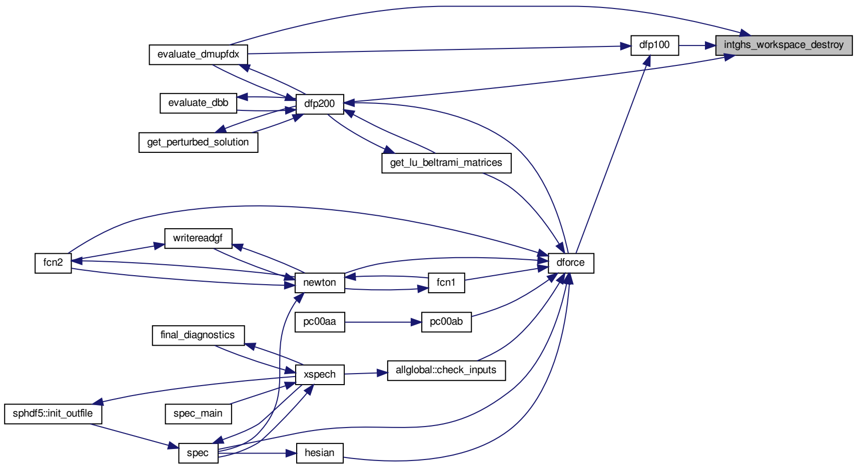
References allglobal::cpus, intghs(), allglobal::mpi_comm_spec, allglobal::myid, allglobal::ncpu, fileunits::ounit, and inputlist::wmacros.

Referenced by dfp100(), dfp200(), and evaluate_dmupfdx().

Here is the call graph for this function:



Here is the caller graph for this function:



11.16 jo00aa.f90 File Reference

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

Functions/Subroutines

- subroutine jo00aa (lvol, Ntz, lquad, mn)

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

11.16.1 Detailed Description

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

11.17 lbpol.f90 File Reference

Computes $B_{\theta,e,0,0}$ at the interface.

Functions/Subroutines

- subroutine lbpol (lvol, Bt00, ideriv, iocons)

  Computes $B_{\theta,e,0,0}$ *at the interface.*

11.17.1 Detailed Description

Computes $B_{\theta,e,0,0}$ at the interface.

11.17.2 Function/Subroutine Documentation

11.17.2.1 lbpol()

```
subroutine lbpol (
    integer, intent(in) lvol,
    real, dimension(1:mvol, 0:1, -1:2), intent(inout) Bt00,
    integer, intent(in) ideriv,
    integer, intent(in) iocons )
```

Computes $B_{\theta,e,0,0}$ at the interface.

Parameters

in	*lvol*	
in,out	*Bt00*	
in	*ideriv*	
in	*iocons*	
in	*ideriv*	lbpol will return $B_{\theta,e,0,0}$ (0) or its derivative with respect to the geometry (-1), mu (1) or the poloidal flux (2). ideriv $\in \{-1, \ldots, 2\}$
in	*lvol*	Volume index. lvol $\in \{1, \ldots,$ Mvol$\}$
in	*iocons*	$B_{\theta,e,0,0}$ is evaluated on the inner (iocons=0) or outer (iocons=1) volume boundary. iocons $\in \{0, 1\}$
in,out	*bt00*	$B_{\theta,e,0,0}$, with indices Bt00(lvol, iocons, ideriv).

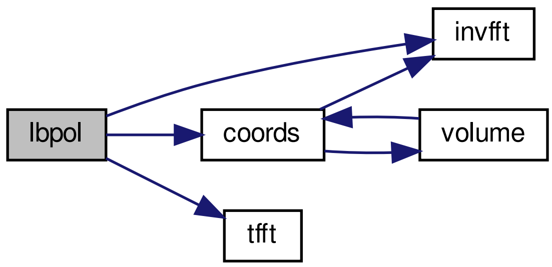
Computes $B_{\theta,e,0,0}$ at the volume interfaces. This is used by dfp100 to evaluate the toroidal current at the volume interfaces, and by dfp200 to construct the force gradient when the current constraint (Lconstraint=3) is used. This is also used by xspech to compute the toroidal current at the volume interfaces, written in the output.

1. Call coords() to compute the metric coefficients and the jacobian.
2. Build coefficients efmn, ofmn, cfmn, sfmn from the field vector potential Ate, Ato, Aze and Azo, and radial derivatives of the polynomial basis TT(ll,innout,1). These variables are the derivatives with respect to s of the magnetic field vector potential in Fourier space. If ideriv $\neq 0$, construct the relevant derivatives of the vector potential.
3. Take the inverse Fourier transform of efmn, ofmn, cfmn, sfmn. These are the covariant components of $\frac{\partial A}{\partial s}$, *i.e.* the contravariant components of $\mathbf{B}$.
4. Build covariant components of the field using the metric coefficients guvij and the jacobian sg.
5. If ideriv=-1 (derivatives with respect to the geometry), need to add derivatives relative to the metric elements
   (a) Get derivatives of metric element by calling coords()
   (b) Compute vector potential without taking any derivatives
   (c) Add to $\frac{\partial B_\theta}{\partial x_i}$ the contributions from $\frac{\partial}{\partial x_i} \frac{g_{\mu\nu}}{\sqrt{g}}$
6. Fourier transform the field and store it in the variables efmn, ofmn, cfmn and sfmn.
7. Save first even fourier mode into Bt00(lvol, iocons, ideriv)

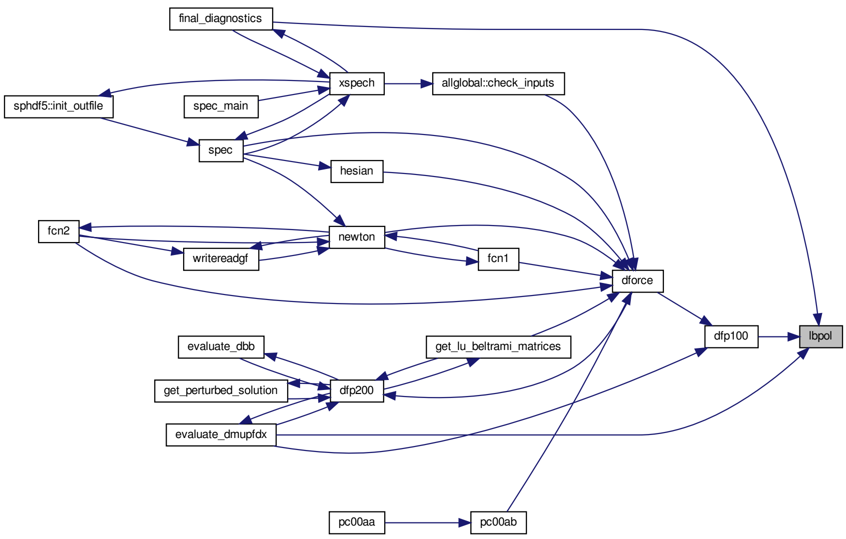
References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::cfmn, allglobal::comn, coords(), allglobal::cpus, allglobal::dbdx, allglobal::efmn, allglobal::evmn, allglobal::guvij, constants::half, inputlist::igeometry, allglobal::im, allglobal::ime, allglobal::in, allglobal::ine, invfft(), inputlist::lcheck, allglobal::lcoordinatesingularity, inputlist::lrad, allglobal::mn, allglobal::mne, constants::mu0, allglobal::myid, allglobal::notstellsym, allglobal::nt, allglobal::ntz, allglobal::nz, allglobal::odmn, allglobal::ofmn, constants::one, fileunits::ounit, constants::pi, constants::pi2, allglobal::regumm, allglobal::sfmn, allglobal::sg, allglobal::simn, tfft(), allglobal::tt, constants::two, allglobal::yesstellsym, and constants::zero.

Referenced by dfp100(), evaluate_dmupfdx(), and final_diagnostics().

Here is the call graph for this function:



Here is the caller graph for this function:



11.18 lforce.f90 File Reference

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

Functions/Subroutines

- subroutine lforce (lvol, iocons, ideriv, Ntz, dBB, XX, YY, length, DDl, MMl, iflag)

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

11.18.1 Detailed Description

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

11.19 ma00aa.f90 File Reference

Calculates volume integrals of Chebyshev polynomials and metric element products.

Functions/Subroutines

- subroutine ma00aa (lquad, mn, lvol, lrad)

  Calculates volume integrals of Chebyshev polynomials and metric element products.

11.19.1 Detailed Description

Calculates volume integrals of Chebyshev polynomials and metric element products.

11.20 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 (lvol, NN)

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

11.20.1 Detailed Description

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

11.21 manual.f90 File Reference

Code development issues and future physics applications.

11.21.1 Detailed Description

Code development issues and future physics applications.

See also

Manual / Documentation

11.22 matrix.f90 File Reference

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

Functions/Subroutines

- subroutine matrix (lvol, mn, lrad)

  Constructs energy and helicity matrices that represent the Beltrami linear system.
  gauge conditions
- subroutine **matrixbg** (lvol, mn, lrad)

11.22.1 Detailed Description

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

11.23 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

11.23.1 Detailed Description

memory management module

11.23.2 Function/Subroutine Documentation

11.23.2.1 allocate_beltrami_matrices()

```
subroutine allocate_beltrami_matrices (
        integer, intent(in) vvol,
        logical, intent(in) LcomputeDerivatives )
```

allocate Beltrami matrices

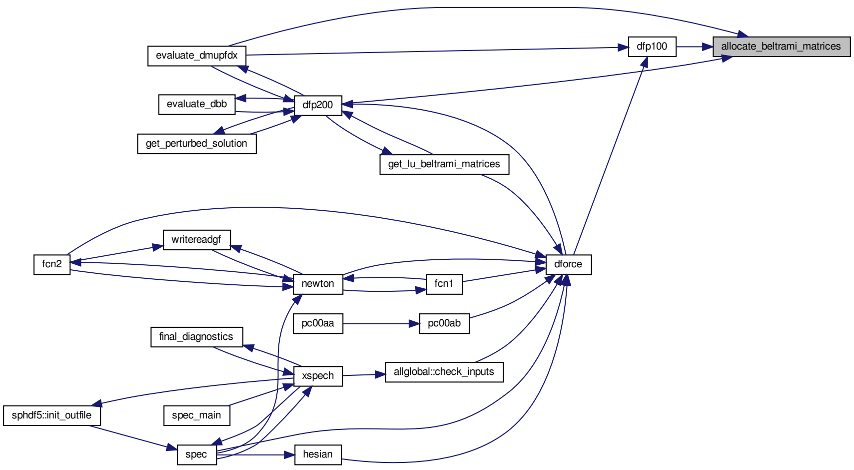
Parameters

vvol	
LcomputeDerivatives	

References allglobal::adotx, allglobal::ddotx, allglobal::dma, allglobal::dmas, allglobal::dmb, allglobal::dmd, allglobal::dmds, allglobal::dmg, allglobal::idmas, allglobal::jdmas, allglobal::liluprecond, allglobal::mbpsi, allglobal↩ ::nadof, allglobal::ndmasmax, allglobal::notmatrixfree, allglobal::solution, and inputlist::wmacros.

Referenced by dfp100(), dfp200(), and evaluate_dmupfdx().

Here is the caller graph for this function:



11.23.2.2 deallocate_beltrami_matrices() `subroutine deallocate_beltrami_matrices ( logical, intent(in) LcomputeDerivatives )`

deallocate Beltrami matrices

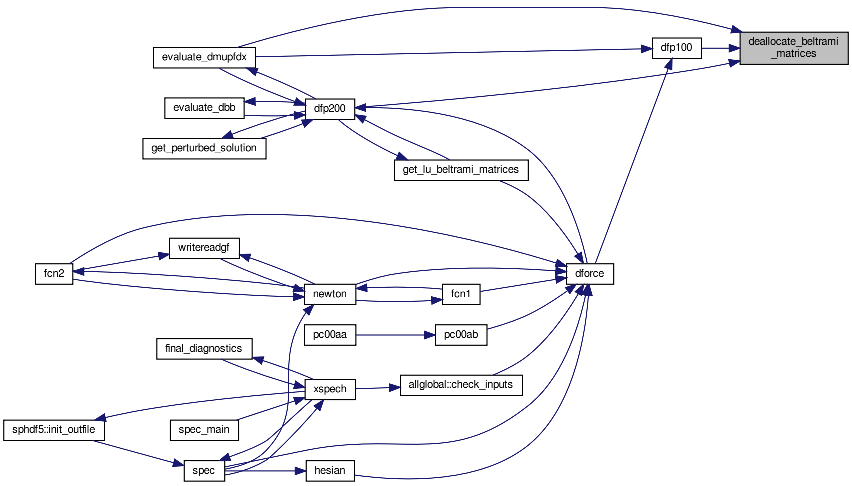
Parameters

LcomputeDerivatives	

References allglobal::adotx, allglobal::ddotx, allglobal::dma, allglobal::dmas, allglobal::dmb, allglobal::dmd, allglobal::dmds, allglobal::dmg, allglobal::idmas, allglobal::jdmas, allglobal::liluprecond, allglobal::mbpsi, allglobal↩ ::notmatrixfree, allglobal::solution, and inputlist::wmacros.

Referenced by dfp100(), dfp200(), and evaluate_dmupfdx().

Here is the caller graph for this function:



11.23.2.3 allocate_geometry_matrices()

```
subroutine allocate_geometry_matrices (
        integer vvol,
        logical, intent(in) LcomputeDerivatives )
```

allocate geometry matrices

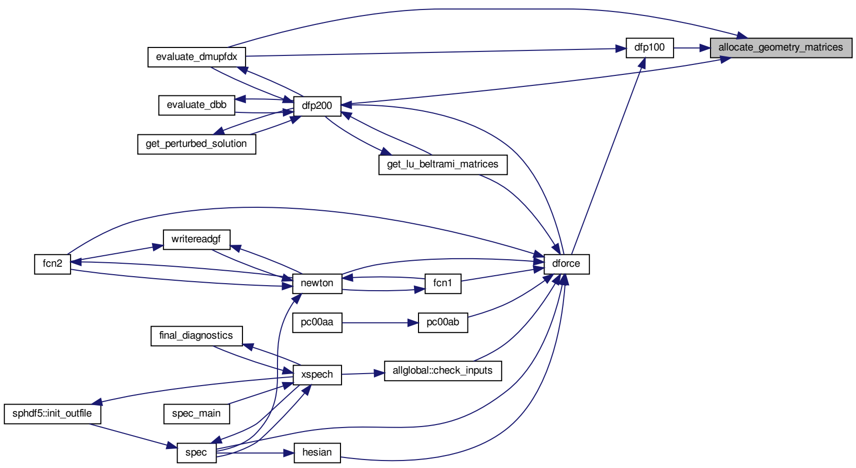
Parameters

vvol	
LcomputeDerivatives	

References allglobal::ddttcc, allglobal::ddttcs, allglobal::ddttsc, allglobal::ddttss, allglobal::ddtzcc, allglobal::ddtzcs, allglobal::ddtzsc, allglobal::ddtzss, allglobal::ddzzcc, allglobal::ddzzcs, allglobal::ddzzsc, allglobal::ddzzss, allglobal::dtc, allglobal::dtoocc, allglobal::dtoocs, allglobal::dtoosc, allglobal::dtooss, allglobal::dts, allglobal::dzc, allglobal::dzs, allglobal::guvijsave, allglobal::iquad, allglobal::lcoordinatesingularity, inputlist::lrad, allglobal::mn, inputlist::mpol, allglobal::notstellsym, allglobal::ntz, allglobal::tdstcc, allglobal::tdstcs, allglobal::tdstsc, allglobal::tdstss, allglobal::tdszcc, allglobal::tdszcs, allglobal::tdszsc, allglobal::tdszss, allglobal::tsc, allglobal::tss, allglobal::ttc, allglobal::tts, allglobal::ttsscc, allglobal::ttsscs, allglobal::ttsssc, allglobal::ttssss, allglobal::tzc, allglobal::tzs, inputlist::wmacros, and constants::zero.

Referenced by dfp100(), dfp200(), and evaluate_dmupfdx().

Here is the caller graph for this function:



11.23.2.4 deallocate_geometry_matrices() `subroutine deallocate_geometry_matrices ( logical, intent(in) LcomputeDerivatives )`

deallocate geometry matrices

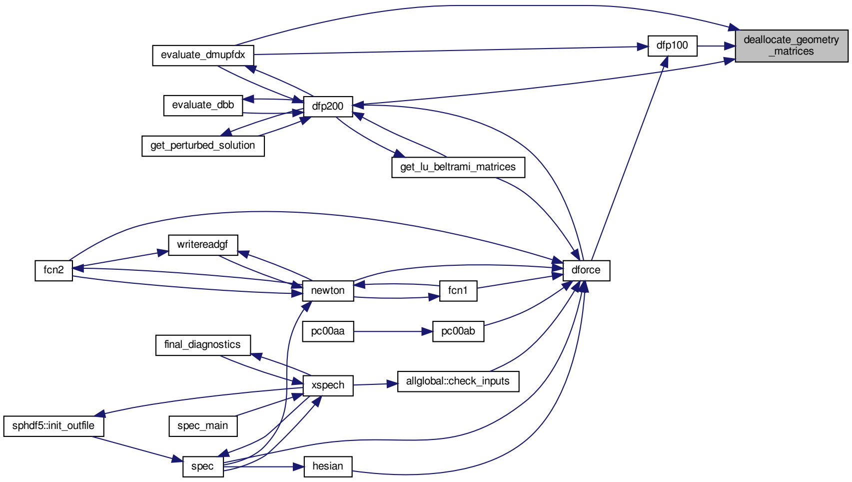
Parameters

LcomputeDerivatives	

References allglobal::ddttcc, allglobal::ddttcs, allglobal::ddttsc, allglobal::ddttss, allglobal::ddtzcc, allglobal::ddtzcs, allglobal::ddtzsc, allglobal::ddtzss, allglobal::ddzzcc, allglobal::ddzzcs, allglobal::ddzzsc, allglobal::ddzzss, allglobal::dtc, allglobal::dtoocc, allglobal::dtoocs, allglobal::dtoosc, allglobal::dtooss, allglobal::dts, allglobal::dzc, allglobal::dzs, allglobal::guvijsave, allglobal::lsavedguvij, allglobal::notstellsym, allglobal::tdstcc, allglobal::tdstcs, allglobal::tdstsc, allglobal::tdstss, allglobal::tdszcc, allglobal::tdszcs, allglobal::tdszsc, allglobal::tdszss, allglobal::tsc, allglobal::tss, allglobal::ttc, allglobal::tts, allglobal::ttsscc, allglobal::ttsscs, allglobal::ttsssc, allglobal::ttssss, allglobal::tzc, allglobal::tzs, inputlist::wmacros, and constants::zero.

Referenced by dfp100(), dfp200(), and evaluate_dmupfdx().

Here is the caller graph for this function:



11.24 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 (lquad, lvol)

  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

11.24.1 Detailed Description

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

11.24.2 Function/Subroutine Documentation

11.24.2.1 compute_guvijsave()

```
subroutine compute_guvijsave (
        integer, intent(in) lquad,
        integer, intent(in) vvol,
        integer, intent(in) ideriv,
        integer, intent(in) Lcurvature )
```

compute guvijsave

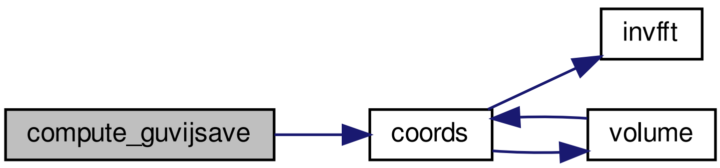
Parameters

lquad	
vvol	
ideriv	
Lcurvature	

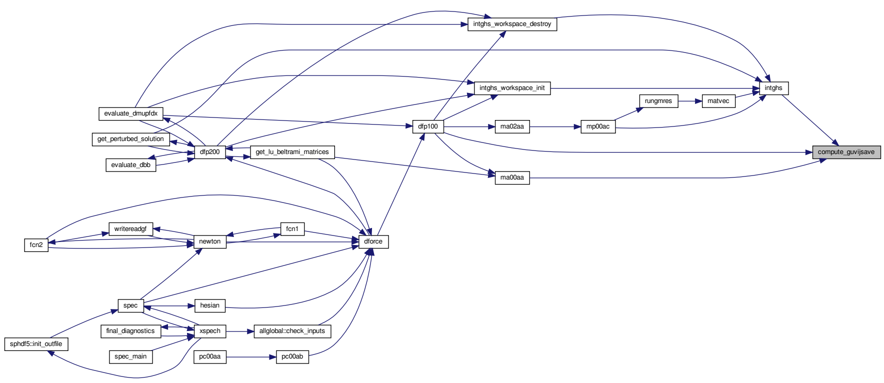
References coords(), allglobal::gaussianabscissae, allglobal::guvij, allglobal::guvijsave, allglobal::mn, allglobal::ntz, and allglobal::sg.

Referenced by dfp100(), intghs(), and ma00aa().

Here is the call graph for this function:



Here is the caller graph for this function:



11.25 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

11.25.1 Detailed Description

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

11.25.2 Function/Subroutine Documentation

11.25.2.1 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	
mu	
vvol	
rhs	
sol	
ipar	
fpar	
wk	

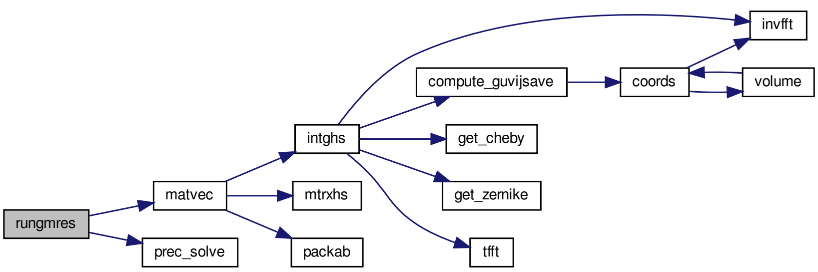
Parameters

nw	
guess	
a	
au	
jau	
ju	
iperm	
ierr	

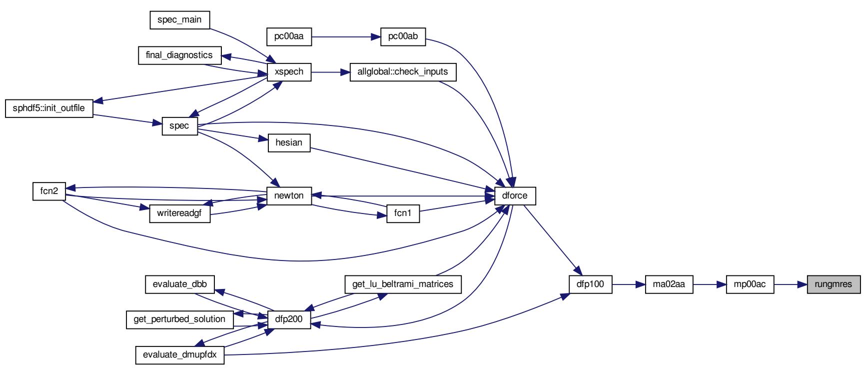
References inputlist::epsgmres, allglobal::liluprecond, matvec(), inputlist::nitergmres, constants::one, prec_solve(), and constants::zero.

Referenced by mp00ac().

Here is the call graph for this function:



Here is the caller graph for this function:



11.25.2.2 matvec()

```
subroutine matvec (
        integer, intent(in) n,
        real, dimension(1:n) x,
        real, dimension(1:n) ax,
        real, dimension(*) a,
        real mu,
        integer, intent(in) vvol )
```

compute a.x by either by coumputing it directly, or using a matrix free method

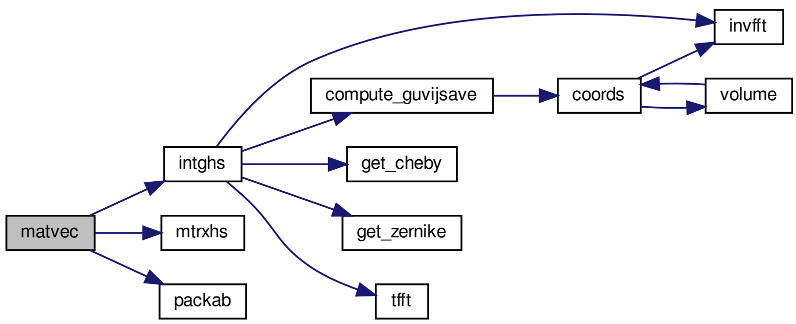
Parameters

n	
x	
ax	
a	
mu	
vvol	

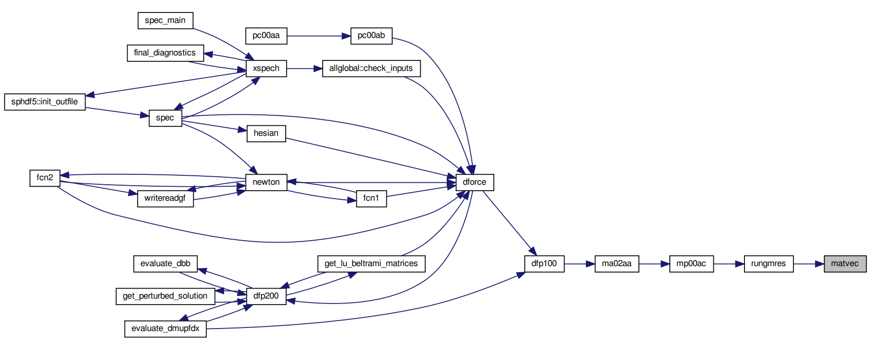
References allglobal::dmd, intghs(), allglobal::iquad, inputlist::lrad, allglobal::mn, mtrxhs(), allglobal::notmatrixfree, constants::one, packab(), and constants::zero.

Referenced by rungmres().

Here is the call graph for this function:



Here is the caller graph for this function:



11.25.2.3 prec_solve()

```
subroutine prec_solve (
        integer n,
        real, dimension(*) vecin,
        real, dimension(*) vecout,
        real, dimension(*) au,
        integer, dimension(*) jau,
        integer, dimension(*) ju,
        integer, dimension(*) iperm )
```

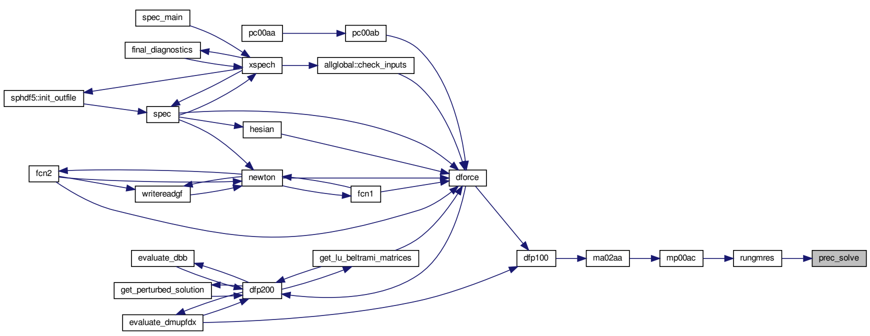
apply the preconditioner

Parameters

n	
vecin	
vecout	
au	
jau	
ju	
iperm	

Referenced by rungmres().

Here is the caller graph for this function:



11.26 mtrxhs.f90 File Reference

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

Functions/Subroutines

- subroutine mtrxhs (lvol, mn, lrad, resultA, resultD, idx)

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

11.26.1 Detailed Description

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

11.27 newton.f90 File Reference

Employs Newton method to find $\mathbf{F}(\mathbf{x}) = 0$, where $\mathbf{x} \equiv \{\mathrm{geometry}\}$ 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 $\mathbf{x} \equiv \{\mathrm{geometry}\}$ and $\mathbf{F}$ is defined in dforce() .
- subroutine writereadgf (readorwrite, NGdof, ireadhessian)
  read or write force-derivative matrix
- subroutine fcn1 (NGdof, xx, fvec, irevcm)
  fcn1
- 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 (?)

11.27.1 Detailed Description

Employs Newton method to find $\mathbf{F}(\mathbf{x}) = 0$, where $\mathbf{x} \equiv \{\mathrm{geometry}\}$ and $\mathbf{F}$ is defined in dforce() .

11.28 numrec.f90 File Reference

Various miscellaneous "numerical" routines.

Functions/Subroutines

- subroutine gi00ab (Mpol, Ntor, Nfp, mn, im, in)
  Assign Fourier mode labels.
- subroutine getimn (Mpol, Ntor, Nfp, mi, ni, idx)
  convert m and n to index
- subroutine tfft (Nt, Nz, ijreal, ijimag, mn, im, in, efmn, ofmn, cfmn, sfmn, ifail)
  Forward Fourier transform (fftw wrapper)
- subroutine invfft (mn, im, in, efmn, ofmn, cfmn, sfmn, Nt, Nz, ijreal, ijimag)
  Inverse Fourier transform (fftw wrapper)
- subroutine gauleg (n, weight, abscis, ifail)
  Gauss-Legendre weights and abscissae.

11.28.1 Detailed Description

Various miscellaneous "numerical" routines.

11.28.2 Function/Subroutine Documentation

11.28.2.1 getimn()

```
subroutine getimn (
        integer, intent(in) Mpol,
        integer, intent(in) Ntor,
        integer, intent(in) Nfp,
        integer, intent(in) mi,
        integer, intent(in) ni,
        integer, intent(out) idx )
```

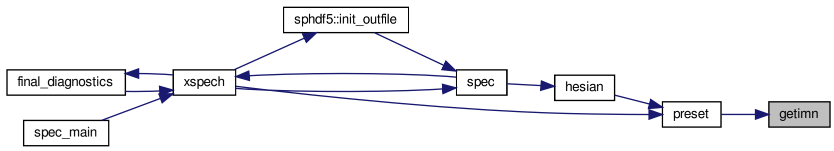
convert m and n to index

Parameters

Mpol	
Ntor	
Nfp	
mi	
ni	
idx	

Referenced by preset().

Here is the caller graph for this function:



11.29 packab.f90 File Reference

Packs, and unpacks, Beltrami field solution vector; $\mathbf{a} \equiv \{A_{\theta,e,i,l}, A_{\zeta,e,i,l}, \mathrm{etc.}\}$.

Functions/Subroutines

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

  Packs and unpacks Beltrami field solution vector.

11.29.1 Detailed Description

Packs, and unpacks, Beltrami field solution vector; $\mathbf{a} \equiv \{A_{\theta,e,i,l}, A_{\zeta,e,i,l}, \mathrm{etc.}\}$.

11.30 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.

11.30.1 Detailed Description

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

11.31 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.

11.31.1 Detailed Description

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

11.32 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.

11.32.1 Detailed Description

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

11.33 pp00aa.f90 File Reference

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

Functions/Subroutines

- subroutine pp00aa
  Constructs Poincaré plot and "approximate" rotational-transform (driver).

11.33.1 Detailed Description

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

11.34 pp00ab.f90 File Reference

Follows magnetic fieldline using ode-integration routine from rksuite.f .

Functions/Subroutines

- subroutine pp00ab (lvol, sti, Nz, nPpts, poincaredata, fittedtransform, utflag)
  Constructs Poincaré plot and "approximate" rotational-transform (for single field line).

11.34.1 Detailed Description

Follows magnetic fieldline using ode-integration routine from rksuite.f .

11.35 preset.f90 File Reference

Allocates and initializes internal arrays.

Functions/Subroutines

- subroutine preset
  Allocates and initializes internal arrays.

11.35.1 Detailed Description

Allocates and initializes internal arrays.

11.36 ra00aa.f90 File Reference

Writes vector potential to .ext.sp.A .

Functions/Subroutines

- subroutine ra00aa (writeorread)
  Writes vector potential to .ext.sp.A .

11.36.1 Detailed Description

Writes vector potential to .ext.sp.A .

11.37 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)

11.37.1 Detailed Description

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

11.38 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 θ 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 θ 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 θ 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 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.

11.38.1 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.

11.39 spsint.f90 File Reference

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

Functions/Subroutines

- subroutine spsint (lquad, mn, lvol, lrad)
  Calculates volume integrals of Chebyshev-polynomials and metric elements for preconditioner.

11.39.1 Detailed Description

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

11.40 spsmat.f90 File Reference

Constructs matrices for the precondtioner.

Functions/Subroutines

- subroutine spsmat (lvol, mn, lrad)
  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 (nq, NN, qA, qD, qjA, ns, nrow, dMAS, dMDS, jdMAS, idMAS)
  add the content from the queue to the real matrices

11.40.1 Detailed Description

Constructs matrices for the precondtioner.

11.40.2 Function/Subroutine Documentation

11.40.2.1 push_back()

```
subroutine push_back (
    integer, intent(in) iq,
    integer, dimension(4), intent(inout) nq,
    integer, intent(in) NN,
    real, intent(in) vA,
    real, intent(in) vD,
    integer, intent(in) vjA,
    real, dimension(nn,4), intent(inout) qA,
    real, dimension(nn,4), intent(inout) qD,
    integer, dimension(nn,4), intent(inout) qjA )
```

push a new element at the back of the queue

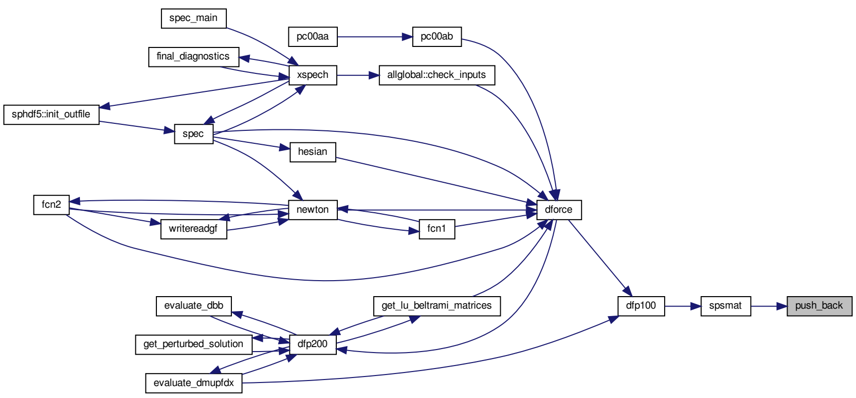
Parameters

iq	
nq	
NN	
vA	
vD	
vjA	
qA	
qD	
qjA	

References constants::zero.

Referenced by spsmat().

Here is the caller graph for this function:



11.40.2.2 clean_queue()

```
subroutine clean_queue (
    integer, dimension(4), intent(inout) nq,
    integer, intent(in) NN,
    real, dimension(nn,4), intent(inout) qA,
    real, dimension(nn,4), intent(inout) qD,
    integer, dimension(nn,4), intent(inout) qjA )
```

clean the queue

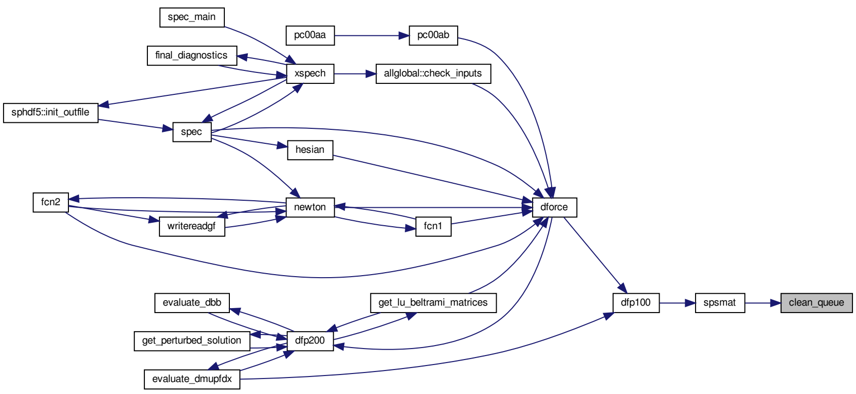
Parameters

nq	
NN	
qA	
qD	
qjA	

References constants::zero.

Referenced by spsmat().

Here is the caller graph for this function:



11.40.2.3 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 )
```

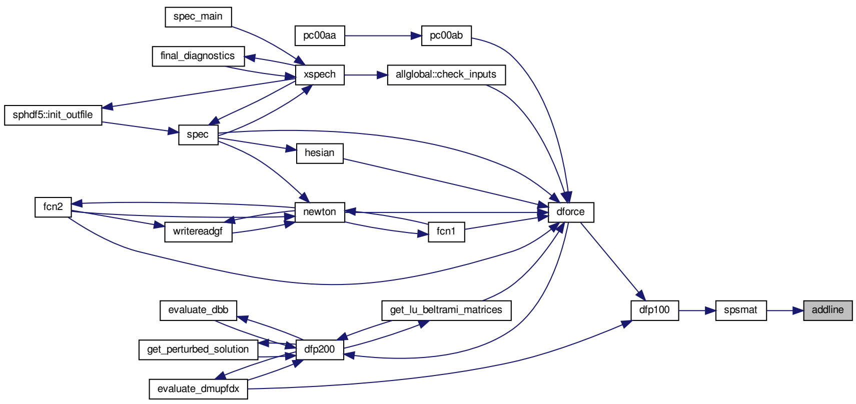
add the content from the queue to the real matrices

Parameters

nq	
NN	
qA	
qD	
qjA	
ns	
nrow	
dMAS	
dMDS	
jdMAS	
idMAS	

Referenced by spsmat().

Here is the caller graph for this function:



11.41 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,θ,ζ).

Functions/Subroutines

- subroutine stzxyz (lvol, stz, RpZ)

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

11.41.1 Detailed Description

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

11.42 tr00ab.f90 File Reference

Calculates rotational transform given an arbitrary tangential field.

Functions/Subroutines

- subroutine tr00ab (lvol, mn, NN, Nt, Nz, iflag, ldiota)

  Calculates rotational transform given an arbitrary tangential field.

11.42.1 Detailed Description

Calculates rotational transform given an arbitrary tangential field.

11.43 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 (lvol, vflag)

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

11.43.1 Detailed Description

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

11.44 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;

11.44.1 Detailed Description

Constructs smooth approximation to wall.

11.45 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.

11.45.1 Detailed Description

Main program.

11.45.2 Function/Subroutine Documentation

11.45.2.1 spec_main() `program spec_main`

Main program of SPEC.

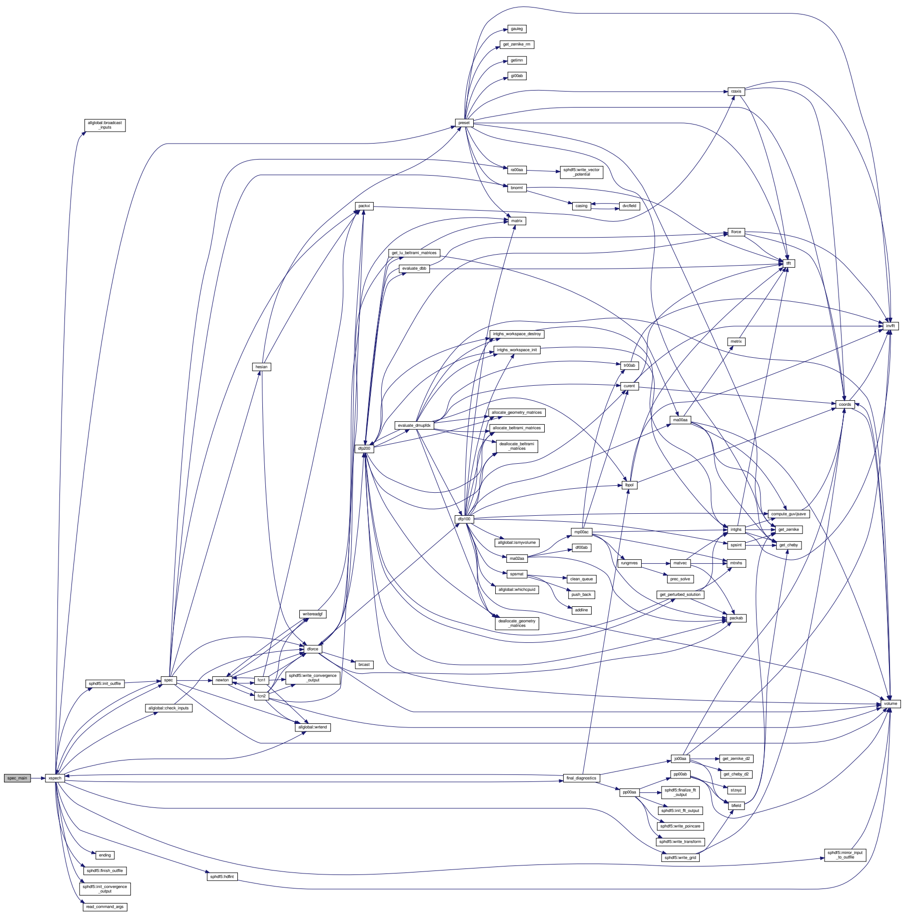
This only calls the xpech() subroutine to do a stand-alone SPEC run.

Returns

none

References xspech().

Here is the call graph for this function:



11.45.2.2 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";
}
```

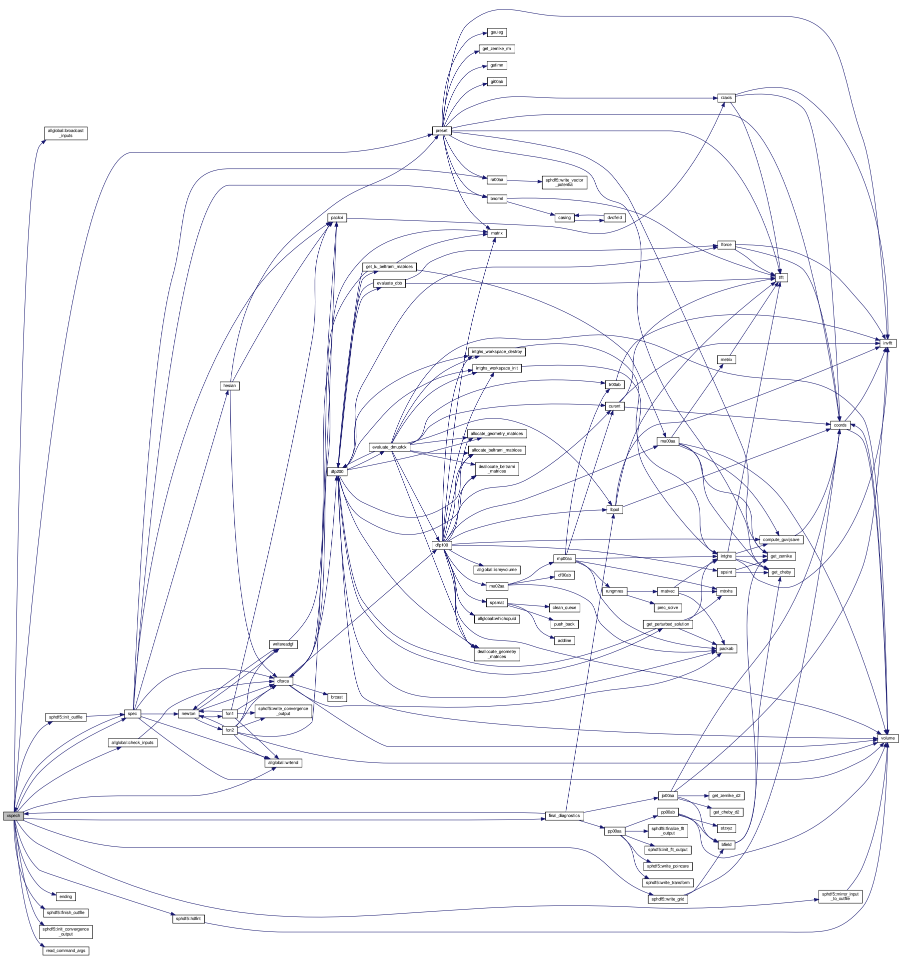
restart files

- wrtend() is called to write the restart files.

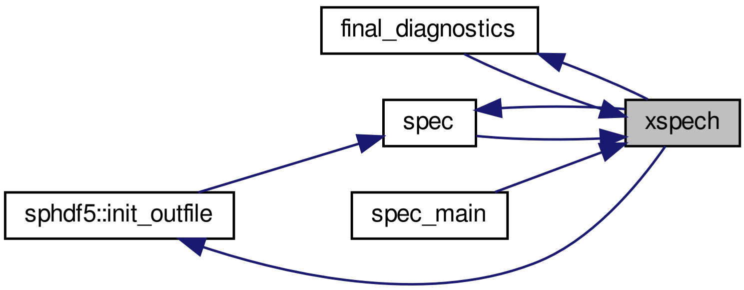
References allglobal::broadcast_inputs(), allglobal::check_inputs(), allglobal::cpus, ending(), final_diagnostics(), sphdf5::finish_outfile(), sphdf5::hdfint(), sphdf5::init_convergence_output(), sphdf5::init_outfile(), numerical::machprec, sphdf5::mirror_input_to_outfile(), allglobal::mpi_comm_spec, 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:



11.45.2.3 read_command_args() `subroutine read_command_args`

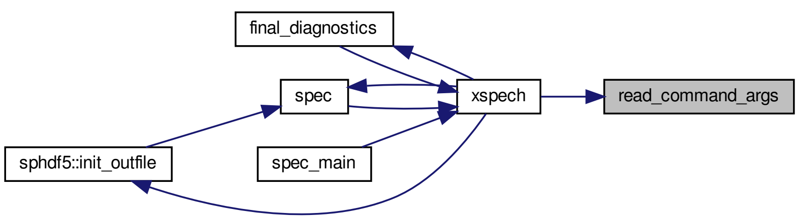
Read command-line arguments; in particular, determine input file (name or extension).

- 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 `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 allglobal::cpus, allglobal::mpi_comm_spec, allglobal::myid, fileunits::ounit, and inputlist::wreadin.

Referenced by xspech().

Here is the caller graph for this function:



11.45.2.4 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

$$P_v \equiv p_v V_v^\gamma, \tag{292}$$

where $p_v \equiv$ `pressure(vvol)` , the volume V_v of each region is computed by volume() , and the adiabatic index $\gamma \equiv$ `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. (292), 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:

$$\mathtt{Bns}_i^j = \lambda \, \mathtt{Bns}_i^{j-1} + (1-\lambda)\mathtt{Bns}_i, \tag{293}$$

where j labels free-boundary iterations, the "blending parameter" is $\lambda \equiv$ `gBnbld` , and `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

$$\sum_i |\mathtt{Bns}_i^{j-1} - \mathtt{Bns}_i|/N, \tag{294}$$

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 [9] 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. (293), and the free-boundary iterations will continue until either the tolerance condition is met (see `gBntol` and Eqn. (294)) 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.)

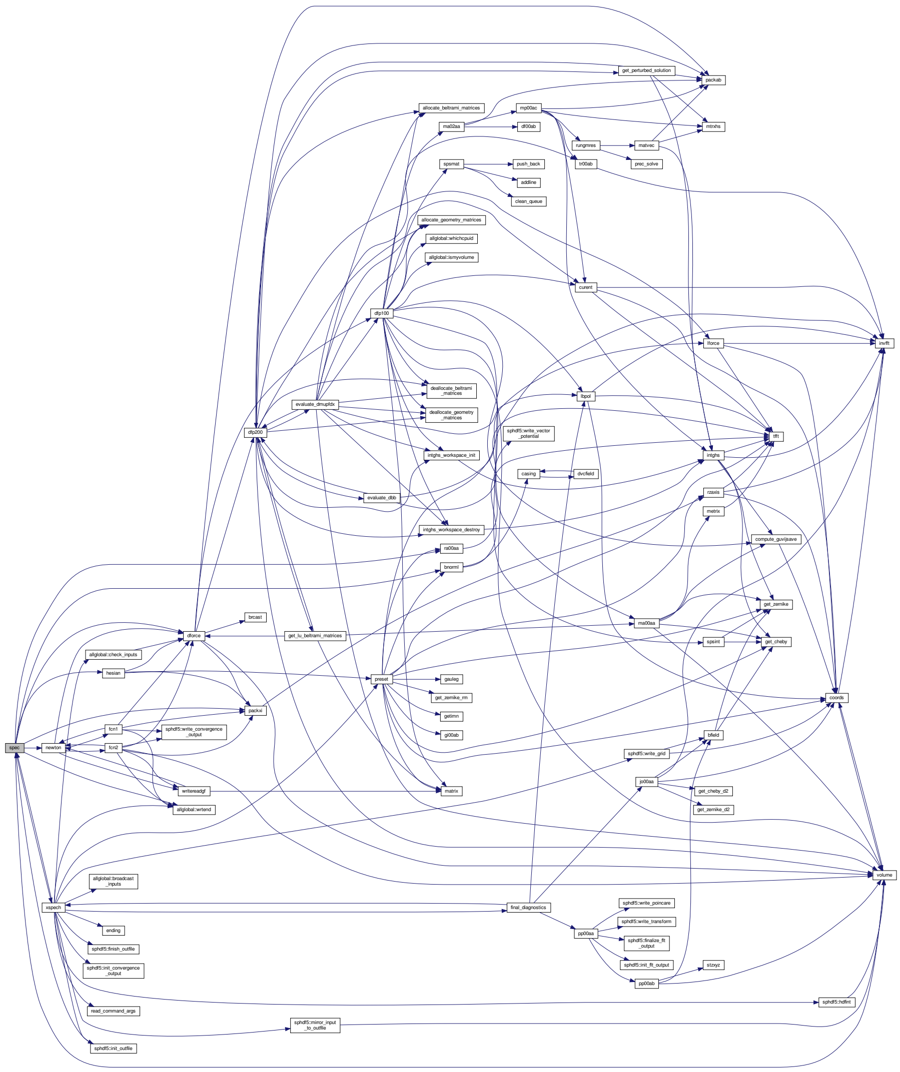
output files: vector potential

- The vector potential is written to file using ra00aa() .

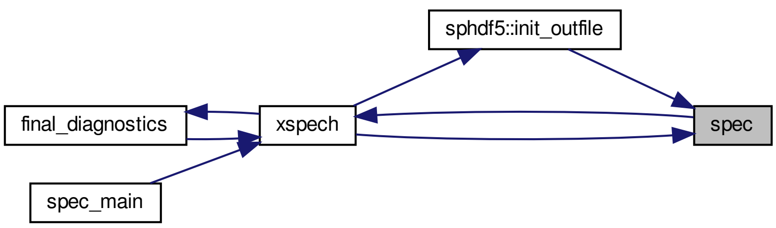
References inputlist::adiabatic, allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::bbe, allglobal::bbo, bnorml(), allglobal::cfmn, allglobal::cpus, dforce(), allglobal::dpflux, allglobal::dtflux, allglobal::efmn, allglobal::forceerr, inputlist::gamma, inputlist::gbnbld, inputlist::gbntol, inputlist::helicity, hesian(), allglobal::ibnc, allglobal::ibns, inputlist::igeometry, allglobal::iie, allglobal::iio, allglobal::im, allglobal::imagneticok, allglobal::in, allglobal::irbc, allglobal::irbs, inputlist::isurf, allglobal::ivnc, allglobal::ivns, inputlist::ivolume, allglobal::izbc, allglobal::izbs, inputlist::ladiabatic, inputlist::lautoinitbn, inputlist::lcheck, inputlist::lconstraint, allglobal::lcoordinatesingularity, inputlist::lfindzero, inputlist::lfreebound, allglobal::lgdof, inputlist::lhevalues, inputlist::lhevectors, inputlist::lhmatrix, numerical::logtolerance, inputlist::lperturbed, allglobal::lplasmaregion, 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:



11.45.2.5 final_diagnostics() `subroutine final_diagnostics`

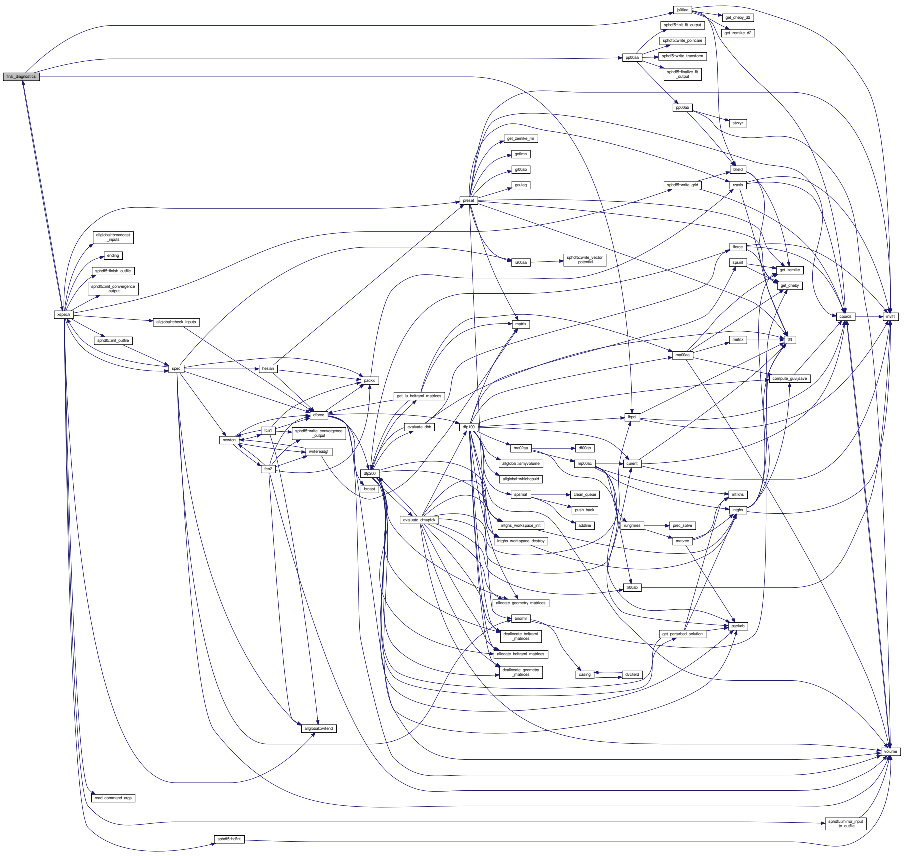
Final diagnostics.

- 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.

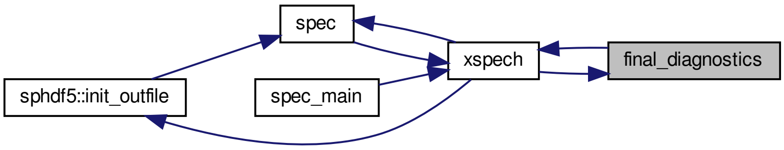
References allglobal::beltramierror, allglobal::btemn, allglobal::btomn, allglobal::bzemn, allglobal::bzomn, allglobal::cfmn, allglobal::cpus, allglobal::dtflux, allglobal::efmn, inputlist::igeometry, allglobal::imagneticok, allglobal::iquad, inputlist::isurf, inputlist::ivolume, jo00aa(), lbpol(), inputlist::lcheck, allglobal::lcoordinatesingularity, allglobal::lplasmaregion, allglobal::lvacuumregion, allglobal::mn, allglobal::mpi_comm_spec, inputlist::mu, allglobal::myid, allglobal::ncpu, inputlist::nppts, inputlist::nptrj, allglobal::ntz, 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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[2] S. P. Hirshman and J. Breslau. Explicit spectrally optimized Fourier series for nested magnetic surfaces. *Phys. Plas.*, 5(7):2664–2675, 1998. 41

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