SPEC

Generated on Fri Oct 27 2023 09:10:35 for SPEC by Doxygen 1.9.2

Fri Oct 27 2023 09:10:35

1 The Stepped Pressure Equilibrium Code

All relevant publications and presentations are given on the MRxMHD website.

A BibTex file is available: spec_refs.bib.

- There is also a brief description of SPEC on the Princeton Plasma Physics Laboratory Theory Department website.
- An overview of the algorithm is given in a Flow Chart.
- Please direct questions/suggestions to Stuart Hudson.
- Online documentation for SPEC is available on Github pages.
  A PDF version of this manual is available in SPEC_manual.pdf.
- Instructions for compiling and testing SPEC are in Compile.md.

2 Compilation hints for SPEC

This document tries to summarize the steps necessary to setup SPEC on your machine. Two approaches are discussed. The first one is the CMake setup. The second one is the more classical `Makefile` setup.

2.1 CMake and Anaconda

The Anaconda system provides an ecosystem of compilers, precompiled libraries and python packages ready to be used. The main goal is to decouple the conda environment from the host system, so that you can use modern software and tools also on machines with outdated local software.

This guide was written while testing the commands on a Debian 9 x86_64 Linux system. This should be deemed old enough to demonstrate the weirdest errors if something is not under control, hence facilitating the correctness of these instructions.

2.1.1 Install Anaconda

The Anaconda installer is available from the Anaconda website. At the time of writing, the URL to the actual file is: https://repo.anaconda.com/archive/Anaconda3-2021.11-Linux-x86_64.sh

Go into folder where the anaconda installer will be downloaded to and download the Anaconda installer:
```
cd ~/Downloads
wget https://repo.anaconda.com/archive/Anaconda3-2021.11-Linux-x86_64.sh
```

Launch the Anaconda installer:
```
bash Anaconda3-2021.11-Linux-x86_64.sh
```

- press ENTER to contine
- Accept License Agreement: `yes`
- Confirm the default installation location (here: `/home/IPP-HGW/jons/anaconda3` == `~/anaconda3`)
- Allow the installer to run `conda init`: `yes`

At this point, the Anaconda installer will modify your `~/.bashrc`. In order to make these changes take effect, you can logout and log back in, close and re-open your Terminal window or do:
```
source ~/.bashrc
```

Disable the activation of the Anaconda base environment on login:
```
conda config --set auto_activate_base False
```

Anaconda works in so-called virtual environments, where environment variables get managed by Anaconda to setup paths to compilers, libraries and include directories semi-automagically.

For SPEC, it is suggested to create a new conda environment. A setup script to perform these actions is provided in the SPEC repository. Thus, we need to clone the SPEC repository now.

2.1.2 Clone the SPEC repository

In this guide, we assume that your copy of SPEC will be located at ~/SPEC.

If you want to upload your changes to the SPEC repository, you should setup your SSH key in your GitHub Settings and use the following URL for the repository instead: git@github.com:PrincetonUniversity/SPEC.git

Clone the repository from GitHub into a folder SPEC in your home directory::
```
cd ~
git clone https://github.com/PrincetonUniversity/SPEC.git
```

2.1.3 Setup a Conda Environment for SPEC

The conda environment setup needed to compile and run SPEC is in setup_conda.sh. This scripts takes a specification of the conda packages to install from spec_conda_env.yml and created a conda environment called spec_env. Also, two scripts are created in etc/conda/activate.d and etc/conda/deactivate.d of the spec_env environment to mask the system's LD_LIBRARY_PATH when entering the conda environment and to restore it to its previous value when leaving the spec_env environment. Also, the environment variable FFTW_ROOT is set to the conda environment to tell SPEC to use the conda-provided version of FFTW.

Change into the freshly-cloned SPEC repository and run this script:
```
cd ~/SPEC
./setup_conda.sh
```

This might take a while, but at the end you should end up with a message similar to this:
```
... lots of stuff above here ...
done
#
# To activate this environment, use
#
#     $ conda activate spec_env
#
# To deactivate an active environment, use
#
#     $ conda deactivate
~/anaconda3/envs/spec_env ~/SPEC
~/SPEC
```

Activate the conda environment for SPEC:
```
conda activate spec_env
```

A forked version of f90wrap is required to build the SPEC Python wrapper (for now). Install that next (inside the spec_env conda environment !!!):
```
pip install -U git+https://github.com/zhucaoxiang/f90wrap
```

The CMake setup is controlled via the setup.py Python script from the SPEC repository. It parses the CMAKE_ARGS environment variable provided by conda.

Additional machine-dependent CMake options are loaded from cmake_config.json. This is a soft-link to a file in cmake_machines. Anaconda provides all libraries required to build SPEC, but we still need to make sure that the cmake_config.json link points to cmake_machines/conda_debian.json. Note that conda.json in cmake_machines is outdated, as it includes machine-dependent options (-DHDF5_ROOT=~/opt/miniconda3/envs/simsopt/).

Now force the cmake_config.json link to point to the correct file:
```
ln -sf cmake_machines/conda_debian.json cmake_config.json
```

This concludes the preliminary setup steps and we can progress by starting the build process:
```
python setup.py bdist_wheel
```

This step also takes quite a while. At the end, the SPEC python package (spec-0.0.1-cp310-cp310-linux_x86_64.whl or similar) should be available in dist.

Install it now:
```
pip install dist/*.whl
```

Note that the Python package you just installed also contains the regular stand-alone SPEC executable xspec, which gets installed into bin/xspec of your conda environment. Verify this by calling which xspec. You should get a message similar to:
```
/home/IPP-HGW/jons/anaconda3/envs/spec_env/bin/xspec
```

2.1.4 Testing your SPEC installation

First, verify that the stand-alone executable is usable. A few test cases are provided in `InputFiles/TestCases`.

Create a new directory for SPEC runs and change into it
```
mkdir ~/SPEC_runs
cd ~/SPEC_runs
```

Copy a demo input file into the current working directory:
```
cp ~/SPEC/InputFiles/TestCases/G3V01L0Fi.001.sp .
```

Call SPEC with an input file (`*.sp`) as argument on the command line:
```
xspec G3V01L0Fi.001.sp
```

You should see the screen output of the SPEC run. Among the last lines should be something similar to this:
```
ending :       0.88 : myid=  0 ; completion ; time=      0.88s =     0.01m =   0.00h =  0.00d ; date=
       2022/02/17 ; time= 17:35:33 ; ext = G1V02L0Fi.001
ending :            :
xspech :            :
xspech :       0.88 : myid=  0 : time=    0.01m =   0.00h =  0.00d ;
```

This indicates that the stand-alone executable is usable.

Next, the python wrapper is tested.

1. Check that the SPEC version can be found:
   ```
   python -c "from spec import spec_f90wrapped as spec; print('SPEC version:
    {:}'.format(spec.constants.version))"
   ```
   This should print a message like "SPEC version: 3.1" on the screen.

2. Check that the Python wrapper can be used as a stand-alone code:
   ```
   OMP_NUM_THREADS=1 python ~/SPEC/Utilities/python_wrapper/spec/core.py G3V01L0Fi.001.sp
   ```
   This should conclude with the message `SPEC called from python finished!`.

3. Run the optimization example code:
   ```
   OMP_NUM_THREADS=1 python ~/SPEC/Utilities/python_wrapper/examples/example.py
   ```
   This should run a basic optimization problem, where the SPEC inputs are controlled via `scipy.optimize`.

4. Run the interactive re-convergence example code:
   ```
   OMP_NUM_THREADS=1 python ~/SPEC/Utilities/python_wrapper/examples/example_2.py
   ```
   This should compute a SPEC equilibrium, then change the central pressure, re-converge SPEC, etc. for a set of five values of the central pressure in a two-volume classical Stellarator case. After the pressure scan with re-convergence, a plot of the MHD energy vs. the central pressure is shown.

2.1.5 Acknowledgements

Here are a few links that proved useful in setting this up:

- https://docs.anaconda.com/anaconda/install/linux/
- https://www.anaconda.com/products/individual
- https://www.rosehosting.com/blog/how-to-install-anaconda-python-on-debian-9/
- https://github.com/RcppCore/Rcpp/issues/770#issuecomment-346716808
- https://computing.docs.ligo.org/conda/compiling/
- https://stackoverflow.com/a/64253999
- https://stackoverflow.com/a/46833531
- https://stackoverflow.com/a/49238956
- https://conda.io/projects/conda-build/en/latest/resources/use-shared-libraries.html

2.2 BELOW INSTRUCTIONS ARE OUTDATED

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In order to run SPEC, you need a copy of the HDF5 libraries installed, which has the Fortran interface enabled.

2.4.1 Installation with CMake

Using CMake, SPEC can be built as a stand-alone executable and as a python extension, where SPEC can be run directly from python, with all variables passed directly in memory.

Download the package from git. And change to the root directory of SPEC source code by running
```
cd <SPEC_ROOT>
```

2.4.2 Stand-alone Executable Compiling

Compiling SPEC requires MPI, HDF5, and numerical libraries such as BLAS, LAPACK, FFTW. For numerical libraries, you could use system supplied libraries or you could use intel math kernel library (MKL).

Machine-specific settings when building the python wrapper are put into separate `json` files in the `cmake_machines` directory. For building the regular SPEC executable, the default settings should work.

In order to select a machine-specific settings file, create a soft link to the indented file in `cmake_machines`:
```
ln -sf cmake_machines/gfortran_ubuntu.json cmake_config.json
```

2.4.2.1 CentOS Here instructions are given for CentOS 7

2.4.2.1.1 Dependencies Install OpenBLAS, FFTW3, and hdf5 using the command
```
yum install -y  gcc-gfortran openmpi openmpi-devel hdf5 hdf5-devel fftw3 fftw3-devel openblas openblas-devel
       python3 python3-devel cmake ninja-build
```

If you don't have the latest version of cmake avaialable on your system, you can create a python virtual environment (instructions are here), activate it, and then install cmake in that virtual environment using pip
```
pip install cmake ninja
```

2.4.2.1.2 Configure When using cmake to build SPEC, the first step is to configure compilers and the locations of libraries. Cmake can detect compilers and libraries at standard locations easily but needs hand-holding when the required libraries are non-standard locations.

The following command was used to configure cmake build setup for SPEC on Centos
```
cmake -S. -Bbuild -GNinja -DCMAKE_Fortran_COMPILER=mpifort -DBLA_VENDOR=OpenBLAS
       -DHDF5_NO_FIND_PACKAGE_CONFIG_FILE=TRUE -DHDF5_PREFER_PARALLEL=TRUE
       -DCMAKE_INSTALL_PREFIX=${SPEC_ROOT}/install --trace-source=CMakeLists.txt 2>&1 | tee log
```

There are few points to note on the above command

- All the build related files will be in build folder.
- Ninja build system is used. If your system doesn't have ninja installed, remove the -G option. The default is the standard `make` tool.
- We ae using OpenBLAS for BLAS and LAPACK and MPI fortran compiler
- Since most of the libraries are in standard location, we don't have to specify them. We are giving couple of options related to HDF5 libraries.
- The installation path is install subfolder location within SPEC folder.
- We are interested in a verbose output and also want to store the output in `log` file.

2.4.2.1.3 Build After successful completion of cmake configuration step, building is trivial

```
cmake --build build
""
#### Install
The last step is to install the executable by running
"'bash
cmake --install build
```

That's it! If all the above steps completed without errors, you have the SPEC executable `xspec` installed at `install/bin` folder

2.4.3 Python Extension Compiling

Building the SPEC python extension will also build the SPEC executable. In the SPEC root folder, edit the `cmake_config.json` as necessary for your system. Few example `.json` files are provided in the `cmake_machines` folder.

2.4.3.1 Dependencies It is strongly suggested to use a python virtual environment either conda or python venv. After virtual environment is installed and activated, install the python related dependencies. Please note that these are in addition to the dependencies listed earlier in stand-alone installation steps. If you are using conda virtual environment try installing the dependencies using `conda install` command

```
conda  install -n <your_venv> numpy f90nml scikit-build cmake ninja
```

If you are using venv virtual environment, run

```
pip install numpy f90nml scikit-build cmake ninja
```

Now install f90wrap. Please keep in mind that numpy has to be installed before installing f90wrap.

```
pip install -U git+https://github.com/zhucaoxiang/f90wrap
```

Now install the SPEC extension by running the setup.py script present in the SPEC root folder.

```
python setup.py bdist_wheel; cd dist/;  pip install *.whl
```

in succession. At this point, you should be able to import the `spec` module in python. To test this, you can try the following command from the shell:

```
python -c "import spec; print('success')"
```

If you want editable install, run

```
python setup.py develop
```

2.4.4 Stellar cluster at PPPL

2.4.4.1 Python wrapper Below are the steps to build python wrappers for SPEC on stellar.

1. Needed modules are

    i. hdf5/gcc/1.10.6 ii. intel-mkl/2021.1.1 iii. openmpi/gcc/4.1.0 iv. anaconda3/2021.5.

    — **Note**

    FFTW is supplied as part of Intel MKL and we just need to link against MKL.

Load the modules by running

```
module load hdf5/gcc/1.10.6 intel-mkl/2021.1.1 openmpi/gcc/4.1.0 anaconda3/2021.5
```

1. Create conda virtual environment.

    ```
    conda create -n spec_ve python=3.8
    ```

    You have to press enter twice. Here a conda virtual environment named `spec_ve` is created with python version 3.8 and lot of packages are installed. Activate by running

    ```
    conda activate spec_ve
    ```

2. Install `cmake`, `ninja`, `scikit-build`, `numpy` using either conda or pip.
   ```
   conda install cmake ninja scikit-build numpy
   ```
   or
   ```
   pip install cmake ninja scikit-build numpy
   ```
3. Install `f90wrap` by running
   ```
   pip install git+https://github.com/zhucaoxiang/f90wrap.git
   ```
4. Clone the spec repo from github
   ```
   git clone https://github.com/PrincetonUniversity/SPEC.git
   ```
   Change the working directory by running `cd SPEC`.
5. Edit the cmake_config.json to populate correct cmake_flags. For stellar, cmake_config.json should look like
   ```
   {
     "cmake_args": [
       "-DCMAKE_C_COMPILER=mpicc",
       "-DCMAKE_CXX_COMPILER=mpicxx",
       "-DCMAKE_Fortran_COMPILER=mpifort",
       "-DBLA_VENDOR=Intel10_64lp",
       "-DHDF5_ROOT=/usr/local/hdf5/gcc/1.10.6",
       "-DHDF5_PREFER_PARALLEL=False"]
   }
   ```
6. Then build the python wheel for SPEC wrapper using
   ```
   python setup.py bdist_wheel
   ```
   The resulting wheel is located in `dist` folder. Install SPEC python wrapper by running
   ```
   pip install dist/spec*.whl
   ```
7. Install mpi4py using pip/conda. If using pip, don't forget to use `--no-cache-dir` flag
   ```
   pip install --no-cache-dir mpi4py
   ```
   or
   ```
   conda install mpi4py
   ```

2.4.4.2 SPEC executable.

The python wrapper builds spec executable but it gets installed at an obscure location. If you mainly want SPEC executable `xspec`, the steps are similar.

1. Load the required modules. Refer to the first step in the python wrapper instructions.
2. Clone the SPEC repo and make SPEC as working directory. Refer to the 5th step above.
3. Run the cmake configuration by running
   ```
   cmake -Bbuild -S . -DCMAKE_C_COMPILER=mpicc -DCMAKE_CXX_COMPILER=mpicxx
    -DCMAKE_Fortran_COMPILER=mpifort -DBLA_VENDOR=Intel10_64lp \
   -DHDF5_ROOT=/usr/local/hdf5/gcc/1.10.6 -DHDF5_PREFER_PARALLEL=False
    -DCMAKE_INSTALL_PREFIX=<SPEC_install_location>
   ```
   Please note SPEC gets installed at `<SPEC_install_location>/bin`, where `<SPEC_install_location>` is the folder of your choice. Building of SPEC library will be done in the folder `build`, where all the intermediary compilation files will be located.
4. Compile the code by running
   ```
   cmake --build build
   ```
   This command will invoke `make` build generator. Alternatively, you can switch to build folder and run make utility manually.
   ```
   cd build
   make
   ```
5. Install the SPEC executable by running
   ```
   cmake --install build
   ```
   SPEC library gets installed `<SPEC_install_location>/lib` and SPEC executable get installed at `<SPEC_install_location>/bin`

2.4.5 Mac

Here is how to build the HDF5 library :

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`

3. cd into source folder: `cd hdf5-1.10.5`
4. make a build folder: `mkdir build`
5. cd into build folder: `cd build`
6. run cmake with options for the Fortran interface: `cmake -DHDF5_BUILD_FORTRAN:BOOL=ON ..`
7. 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. See e.g. this document for more detailed instructions: https://support.hdfgroup.org/ftp/HDF5/current/src/unpacked/release_docs/INSTALL_CMake.txt
The compilation of SPEC itself then proceeds as usual. You then only need to specify the HDF5 folder in the Makefile, which will likely be `/Applications/HDF_Group/HDF5/1.10.5`.

3 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, ldltGp)

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.

4 Module Index

4.1 Modules

Here is a list of all modules:

5 Data Type Index

5.1 Data Types List

Here are the data types with brief descriptions:

6 File Index

6.1 File List

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

7 Module Documentation

7.1 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).

7.1.1 Detailed Description

7.1.2 Function/Subroutine Documentation

7.1.2.1 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.

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

Representation of magnetic field

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

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

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

  where $\overline{T}_{l,i}(s) \equiv \bar{s}^{m_i/2}\, T_l(s)$, $T_l(s)$ 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

$$\begin{aligned}
\sqrt{g}\,\mathbf{B} &= \mathbf{e}_s \textstyle\sum_{i,l}[(\; -m_i A_{\zeta,e,i,l} \; - \; n_i A_{\theta,e,i,l} \;)\overline{T}_{l,i}\sin\alpha_i + (\; +m_i A_{\zeta,o,i,l} \; + \; n_i A_{\theta,o,i,l} \;)\overline{T}_{l,i}\cos\alpha_i] \\
&+ \mathbf{e}_\theta \textstyle\sum_{i,l}[(\; \; - \; A_{\zeta,e,i,l} \;)\overline{T}'_{l,i}\cos\alpha_i + (\; \; - \; A_{\zeta,o,i,l} \;)\overline{T}'_{l,i}\sin\alpha_i] \\
&+ \mathbf{e}_\zeta \textstyle\sum_{i,l}[(\; A_{\theta,e,i,l} \;)\overline{T}'_{l,i}\cos\alpha_i + (\; A_{\theta,o,i,l} \;)\overline{T}'_{l,i}\sin\alpha_i]
\end{aligned} \tag{4}$$

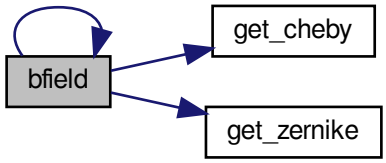
- In Eqn. (1) , the coordinate Jacobian, $\sqrt{g}$, cancels. No coordinate metric information is required to construct the fieldline equations from the magnetic vector potential.

IT IS REQUIRED TO SET IVOL THROUGH GLOBAL MEMORY BEFORE CALLING BFIELD.
The format of this subroutine is constrained by the NAG ode integration routines.

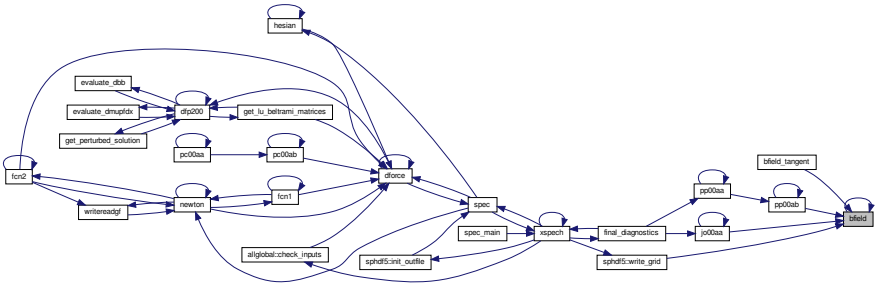
Parameters

in	*zeta*	toroidal angle 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, bfield(), 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(), bfield_tangent(), jo00aa(), pp00ab(), and sphdf5::write_grid().
Here is the call graph for this function:



Here is the caller graph for this function:



7.1.2.2 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

Parameters

in	*mn*	number of Fourier harmonics
in	*LGdof*	what is this?

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

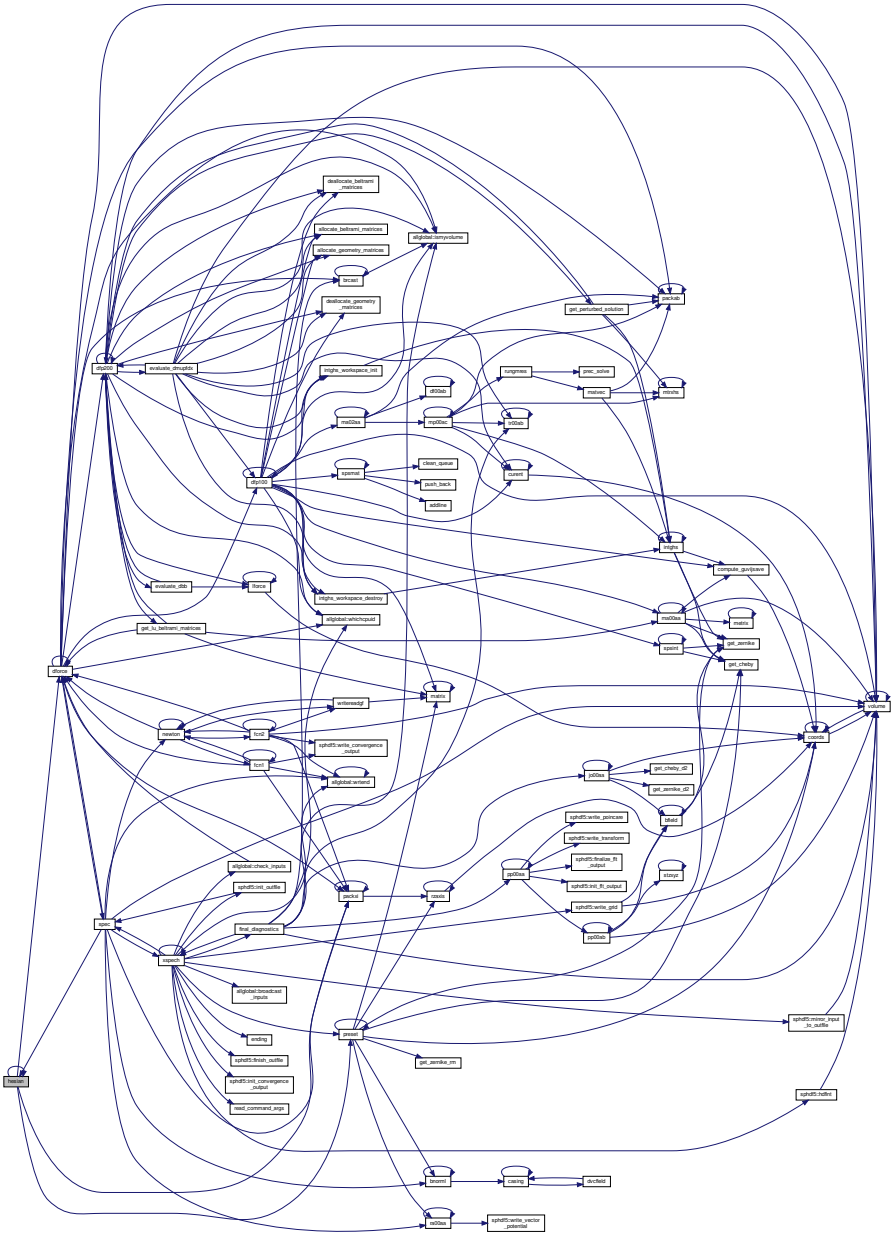
- If `LHevalues==T` then the eigenvalues of the Hessian are computed using the NAG routine `F02EBF`.
- If `LHevectors==T` then the eigenvalues *and* the eigenvectors of the Hessian are computed.
- Note that if `Igeometry==3`, then the derivative-matrix also contains information regarding how the "artificial" 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)
```

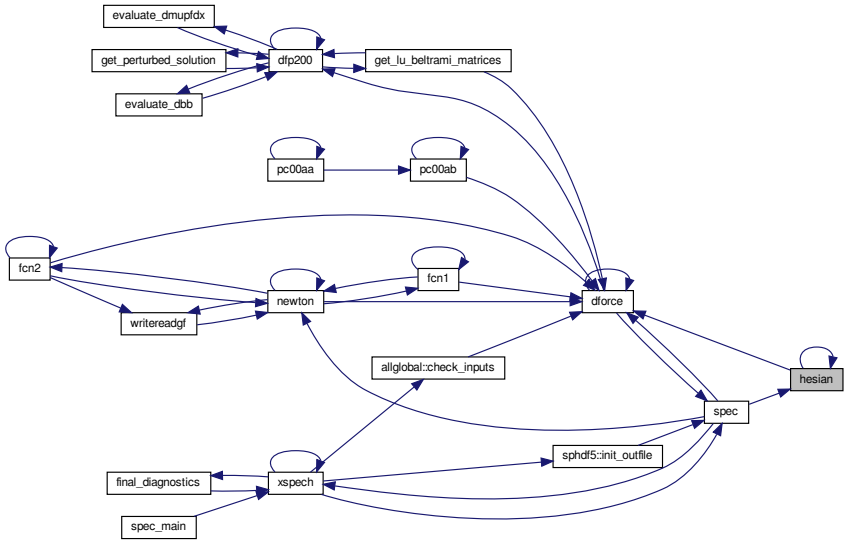
- The eigenvectors are saved in columns of `evecr`, `eveci`, as described by the NAG documentation for `F02EBF`.

References allglobal::cpus, allglobal::dbbdmp, allglobal::dbbdrz, allglobal::denergydrr, allglobal::denergydrz, allglobal::denergydzr, allglobal::denergydzz, allglobal::dessian, allglobal::dessian2d, allglobal::dffdrz, dforce(), allglobal::dmupfdx, inputlist::dpp, inputlist::dqq, allglobal::drbc, allglobal::drbs, allglobal::dzbc, allglobal::dzbs, allglobal::energy, constants::half, allglobal::hdffdrz, inputlist::helicity, hesian(), allglobal::hessian, allglobal::hessian2d, 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::lhessian2dallocated, allglobal::lhessian3dallocated, 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 hesian(), and spec().

Here is the call graph for this function:



Here is the caller graph for this function:



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

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

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

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

  where $\overline{T}_{l,i}(s) \equiv \bar{s}^{m_i/2}\, T_l(s)$, $T_l(s)$ 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

$$\begin{aligned}
\sqrt{g}\,\mathbf{B} &= \mathbf{e}_s \textstyle\sum_{i,l}[(\; -m_i A_{\zeta,e,i,l} - n_i A_{\theta,e,i,l}\;)\overline{T}_{l,i}\sin\alpha_i + (\; +m_i A_{\zeta,o,i,l} + n_i A_{\theta,o,i,l}\;)\overline{T}_{l,i}\cos\alpha_i] \\
&+ \mathbf{e}_\theta \textstyle\sum_{i,l}[(\; - A_{\zeta,e,i,l}\;)\overline{T}'_{l,i}\cos\alpha_i + (\; - A_{\zeta,o,i,l}\;)\overline{T}'_{l,i}\sin\alpha_i] \\
&+ \mathbf{e}_\zeta \textstyle\sum_{i,l}[(\; A_{\theta,e,i,l}\;)\overline{T}'_{l,i}\cos\alpha_i + (\; A_{\theta,o,i,l}\;)\overline{T}'_{l,i}\sin\alpha_i]
\end{aligned} \tag{7}$$

- The current is

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

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

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

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

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

quantification of the error

- The measures of the error are

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

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

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

comments

- Is there a better definition and quantification of the error? For example, should we employ an error measure that is dimensionless?
- If the coordinate singularity is in the domain, then $|\nabla\theta| \to \infty$ at the coordinate origin. What then happens to $||\left(\mathbf{j}-\mu\mathbf{B}\right)\cdot\nabla\theta||$ as defined in Eqn. (13)?
- What is the predicted scaling of the error in the Chebyshev-Fourier representation scale with numerical resolution? Note that the predicted error scaling for E^s, E^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) [4] , where the expected scaling of the error for a finite-element implementation is confirmed numerically.)
- Instead of using Gaussian integration to compute the integral over s, an adaptive quadrature algorithm may be preferable.

Parameters

in	*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

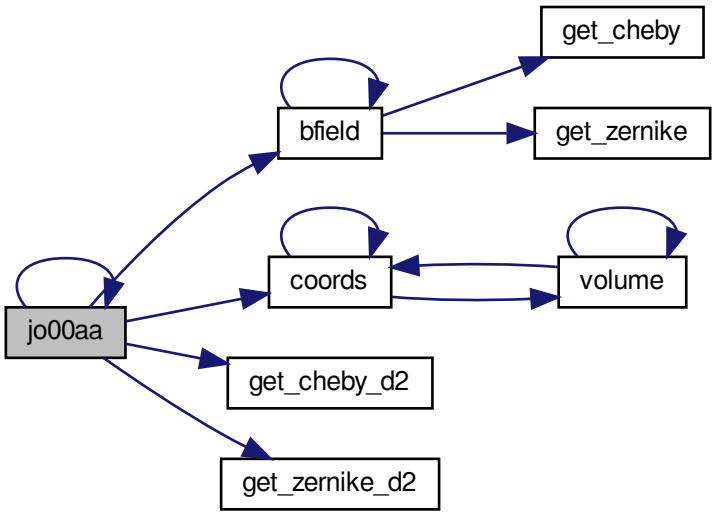
- The integration over s is performed using Gaussian integration, e.g., $\int f(s)ds \approx \sum_k \omega_k f(s_k)$; with the abscissae, s_k, and the weights, ω_k, for $k = 1$, `Iquad` $_v$, determined by `CDGQF`. The resolution, `N` $\equiv$ `Iquad` $_v$, is determined by `Nquad` (see global.f90 and 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. (5) and Eqn. (6), and their first and second radial derivatives, are summed.
  - The quantities $\sqrt{g}B^s$, $\sqrt{g}B^\theta$ and $\sqrt{g}B^\zeta$, and their first and second derivatives with respect to (s, θ, ζ), are computed on the regular angular grid (using FFTs).

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

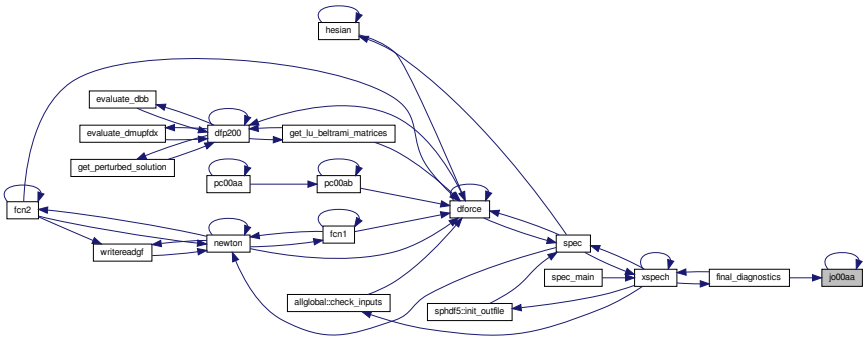
$$\begin{aligned}
\sqrt{g}j^s &= \sum_u \left[\partial_\theta(\sqrt{g}B^u)\, g_{u,\zeta} + (\sqrt{g}B^u)\, \partial_\theta g_{u,\zeta} - (\sqrt{g}B^u) g_{u,\zeta}\, \partial_\theta\sqrt{g}/\sqrt{g}\right]/\sqrt{g} \\
&- \sum_u \left[\partial_\zeta(\sqrt{g}B^u)\, g_{u,\theta} + (\sqrt{g}B^u)\, \partial_\zeta g_{u,\theta} - (\sqrt{g}B^u) g_{u,\theta}\, \partial_\zeta\sqrt{g}/\sqrt{g}\right]/\sqrt{g}, \qquad (15) \\
\sqrt{g}j^\theta &= \sum_u \left[\partial_\zeta(\sqrt{g}B^u)\, g_{u,s} + (\sqrt{g}B^u)\, \partial_\zeta g_{u,s} - (\sqrt{g}B^u) g_{u,s}\, \partial_\zeta\sqrt{g}/\sqrt{g}\right]/\sqrt{g} \\
&- \sum_u \left[\partial_s(\sqrt{g}B^u)\, g_{u,\zeta} + (\sqrt{g}B^u)\, \partial_s g_{u,\zeta} - (\sqrt{g}B^u) g_{u,\zeta}\, \partial_s\sqrt{g}/\sqrt{g}\right]/\sqrt{g}, \qquad (16) \\
\sqrt{g}j^\zeta &= \sum_u \left[\partial_s(\sqrt{g}B^u)\, g_{u,\theta} + (\sqrt{g}B^u)\, \partial_s g_{u,\theta} - (\sqrt{g}B^u) g_{u,\theta}\, \partial_s\sqrt{g}/\sqrt{g}\right]/\sqrt{g} \\
&- \sum_u \left[\partial_\theta(\sqrt{g}B^u)\, g_{u,s} + (\sqrt{g}B^u)\, \partial_\theta g_{u,s} - (\sqrt{g}B^u) g_{u,s}\, \partial_\theta\sqrt{g}/\sqrt{g}\right]/\sqrt{g}. \qquad (17)
\end{aligned}$$

- 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, allglobal::ivol, jo00aa(), 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(), and jo00aa().
Here is the call graph for this function:



Here is the caller graph for this function:



7.1.2.4 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)
```

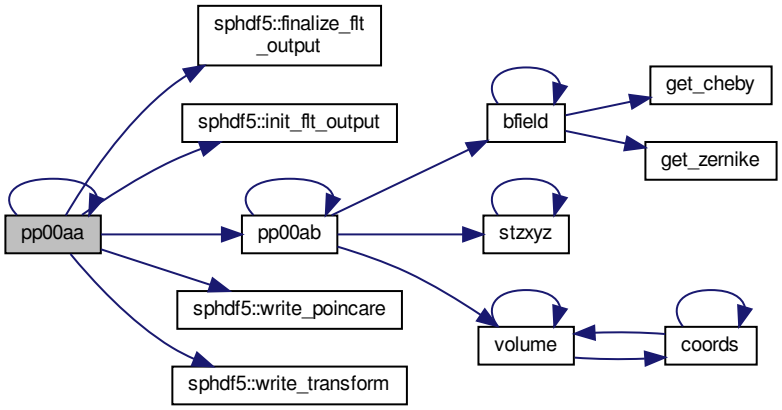
  where
  - $\theta \equiv$ `data(1,k,j)` is the poloidal angle,
  - $s \equiv$ `data(2,k,j)` is the radial coordinate,
  - $R \equiv$ `data(3,k,j)` is the cylindrical R,
  - $Z \equiv$ `data(4,k,j)` is the cylindrical Z,
- The integer `k`=0,Nz-1 labels toroidal planes, so that $\phi = (2\pi/\mathtt{Nfp})(k/\mathtt{Nz})$,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

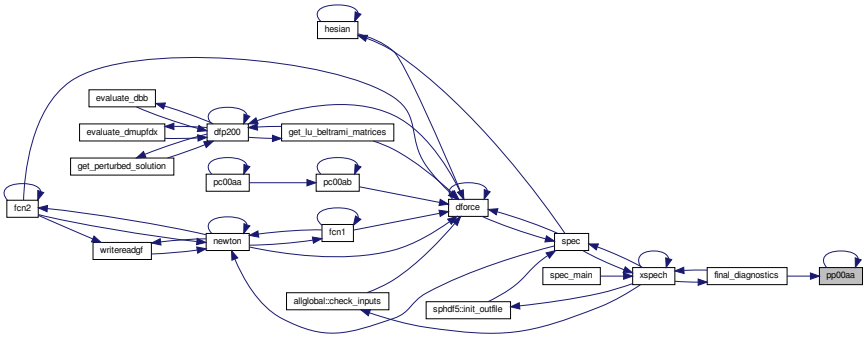
- The rotational-transform data is written to .ext.transform:xxxx , where xxxx is an integer indicating the volume. The format of this file is as follows:

```
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::lmns, 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, pp00aa(), pp00ab(), inputlist::ppts, constants::two, inputlist::wmacros, sphdf5::write_poincare(), sphdf5::write_transform(), and constants::zero.
Referenced by final_diagnostics(), and pp00aa().
Here is the call graph for this function:



Here is the caller graph for this function:



7.1.2.5 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() .

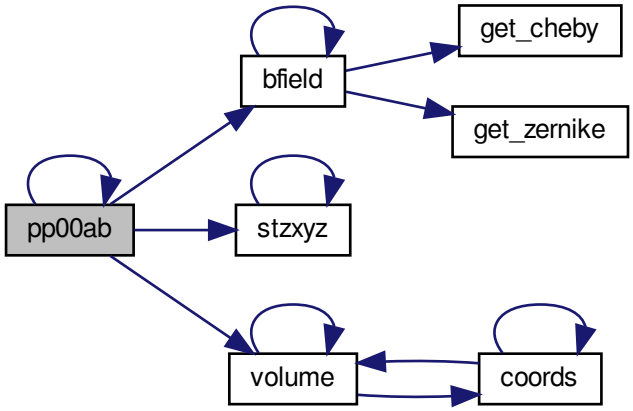
rotational-transform

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

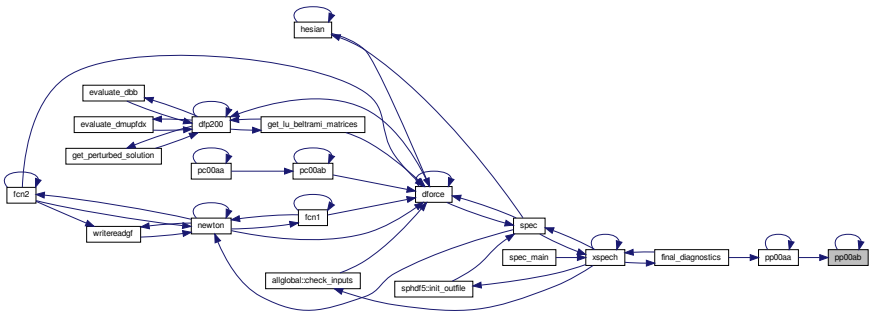
Parameters

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, pp00ab(), numerical::small, stzxyz(), constants::two, volume(), and constants::zero.
Referenced by pp00aa(), and pp00ab().
Here is the call graph for this function:



Here is the caller graph for this function:



7.1.2.6 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).

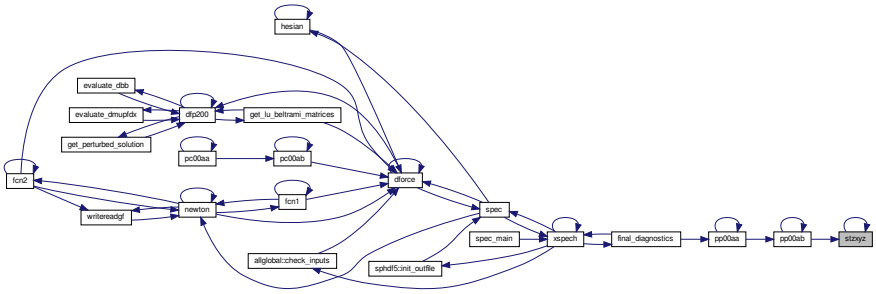
- This routine is a "copy" of co01aa(), which calculates the coordinate information on a regular, discrete grid in θ and ζ at given s whereas stzxyz() calculates the coordinate information at a single point (s,θ,ζ).
- **Todo** Please see co01aa() for documentation.

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, stzxyz(), numerical::vsmall, and constants::zero.
Referenced by pp00ab(), and stzxyz().
Here is the call graph for this function:

Here is the caller graph for this function:



7.2 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.

7.2.1 Detailed Description

7.2.2 Function/Subroutine Documentation

7.2.2.1 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.

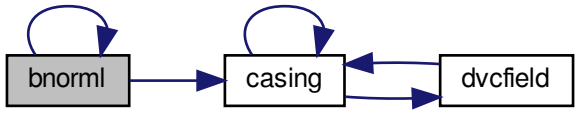
See also

casing.f90

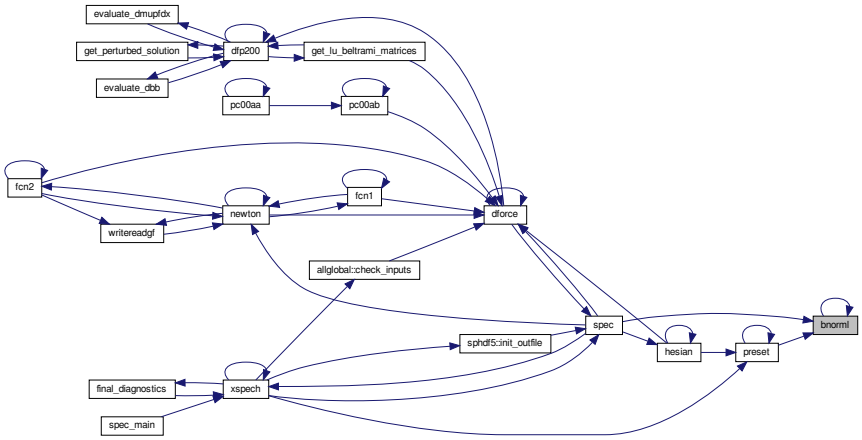
Parameters

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, bnorml(), 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, allglobal::tt, constants::two, inputlist::vcasingper, inputlist::vcasingtol, allglobal::virtualcasingfactor, inputlist::wmacros, constants::zero, and allglobal::zij.
Referenced by bnorml(), preset(), and spec().
Here is the call graph for this function:



Here is the caller graph for this function:



7.2.2.2 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,

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

  and the tangential field on this boundary,

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

  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) [7], Lazerson (2012) [5] and Hanson (2015) [1]) shows that the field outside/inside the plasma arising from plasma currents inside/outside the boundary is equivalent to the field generated by a surface current,

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

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

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

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

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

- For ease of notation introduce

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

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

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

$$j_x = \alpha\, x_\theta - \beta\, x_\zeta \tag{23}$$
$$j_y = \alpha\, y_\theta - \beta\, y_\zeta \tag{24}$$
$$j_z = \alpha\, z_\theta - \beta\, z_\zeta. \tag{25}$$

- Requiring that the current,

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

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

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

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

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

$$B^x = \oint\!\!\oint d\theta d\zeta\;\; (j_y r_z - j_z r_y)/r^3, \tag{28}$$
$$B^y = \oint\!\!\oint d\theta d\zeta\;\; (j_z r_x - j_x r_z)/r^3, \tag{29}$$
$$B^z = \oint\!\!\oint d\theta d\zeta\;\; (j_x r_y - j_y r_x)/r^3 \tag{30}$$

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

- When all is said and done, this routine calculates

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

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

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

Calculation of integrand

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

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

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

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

- The distance between the "evaluate" point, (X, Y, Z), and the given point on the surface, (x, y, z) is computed.

- If the computational boundary becomes too close to the plasma boundary, the distance is small and this causes problems for the numerics. I have tried to regularize this problem by introducing $\epsilon \equiv$inputvar vcasingeps. Let the "distance" be

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

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

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

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

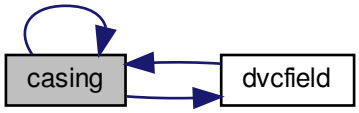
Todo This needs to be revised.

Parameters

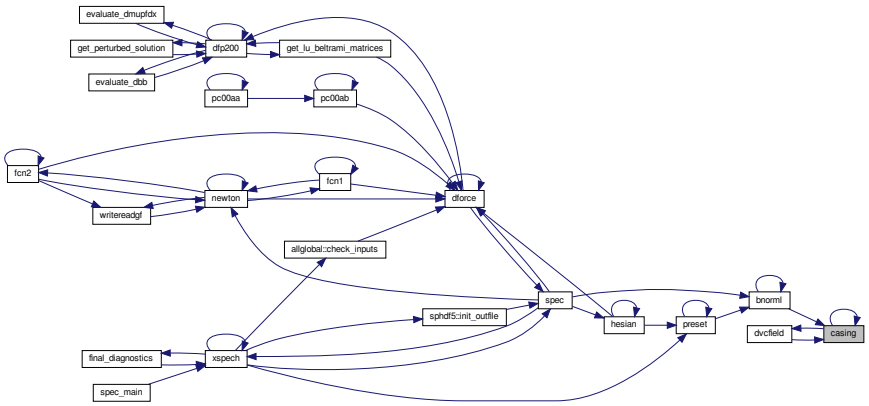
in	*teta*	θ
in	*zeta*	ζ
out	*gBn*	$\sqrt{g}\mathbf{B} \cdot \mathbf{n}$
out	*icasing*	return flag from dcuhre()

References casing(), 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(), casing(), and dvcfield().

Here is the call graph for this function:



Here is the caller graph for this function:



7.2.2.3 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 )
```

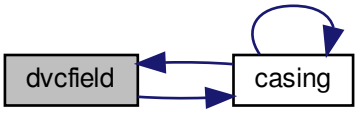
Differential virtual casing integrand.
Differential virtual casing integrand

Parameters

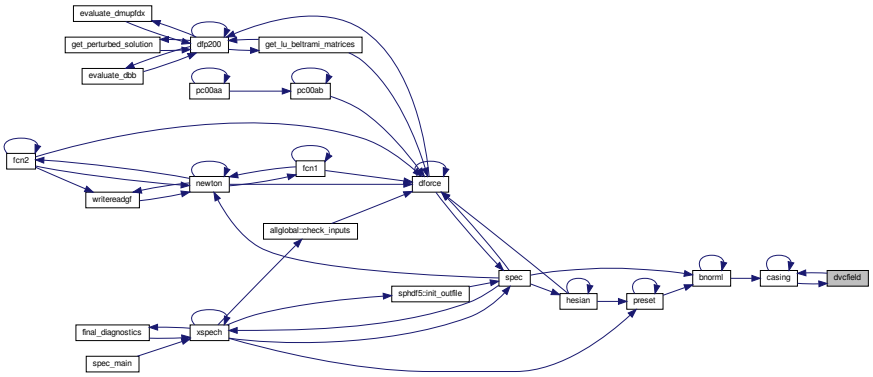
in	*Ndim*	number of parameters (==2)
in	*tz*	θ and ζ
in	*Nfun*	number of function values (==3)
out	*vcintegrand*	cartesian components of magnetic field

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:



7.3 Parallelization

Functions/Subroutines

- subroutine brcast (lvol)

  Broadcasts Beltrami fields, profiles, . . .

7.3.1 Detailed Description

7.3.2 Function/Subroutine Documentation

7.3.2.1 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,

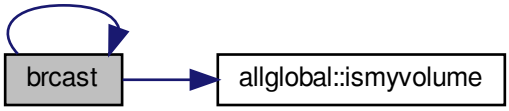
$$\mathbf{F}_i \equiv [[p + B^2/2]]_i = (p + B^2/2)_{v,i} - (p + B^2/2)_{v-1,i} \tag{34}$$

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

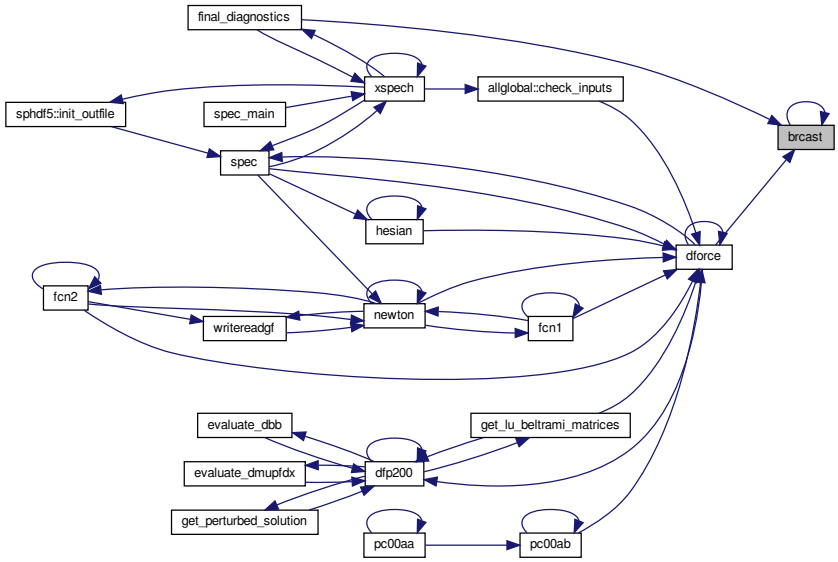
Parameters

in	*lvol*	index of nested volume

References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::bemn, allglobal::bomn, brcast(), allglobal::cpus, inputlist::curpol, inputlist::curtor, allglobal::dbbdmp, allglobal::denergydrr, allglobal::denergydzr, allglobal::dffdrz, allglobal::diotadxup, allglobal::ditgpdxtp, allglobal::dmupfdx, allglobal::dpflux, allglobal::dtflux, inputlist::helicity, allglobal::iemn, allglobal::imagneticok, allglobal::iomn, allglobal::ismyvolume(), allglobal::ismyvolumevalue, allglobal::labintegral, allglobal::lbbintegral, inputlist::lconstraint, inputlist::lfindzero, allglobal::lgdof, allglobal::lhessian3dallocated, allglobal::lhessianallocated, allglobal::localconstraint, inputlist::lrad, allglobal::mn, inputlist::mnvol, allglobal::mpi_comm_spec, inputlist::mu, allglobal::myid, allglobal::ncpu, allglobal::notstellsym, allglobal::ntz, inputlist::nvol, fileunits::ounit, allglobal::pemn, allglobal::pomn, allglobal::semn, allglobal::somn, allglobal::vvolume, inputlist::wmacros, and constants::zero.
Referenced by brcast(), dforce(), and final_diagnostics().
Here is the call graph for this function:



Here is the caller graph for this function:



7.4 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.

7.4.1 Detailed Description

7.4.2 Function/Subroutine Documentation

7.4.2.1 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

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

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

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

  - `Igeometry=3` : Toroidal

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

    where $\hat{\mathbf{r}} \equiv \cos\phi\,\hat{\mathbf{i}} + \sin\phi\,\hat{\mathbf{j}}$ and $\hat{\phi} \equiv -\sin\phi\,\hat{\mathbf{i}} + \cos\phi\,\hat{\mathbf{j}}$.
- The geometry of the ideal interfaces is given as Fourier summation: e.g., for stellarator-symmetry

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

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

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

interpolation between interfaces

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

$$\begin{aligned} R(s,\theta,\zeta) &\equiv \sum_j \left[\frac{(1-s)}{2}\,R_{j,v-1} + \frac{(1+s)}{2}\,R_{j,v}\right]\cos\alpha_j, \\ Z(s,\theta,\zeta) &\equiv \sum_j \left[\frac{(1-s)}{2}\,Z_{j,v-1} + \frac{(1+s)}{2}\,Z_{j,v}\right]\sin\alpha_j, \end{aligned} \tag{40}$$

coordinate singularity: regularized extrapolation

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

$$R_j(s) = R_{j,0} + (R_{j,1} - R_{j,0}) f_j, \tag{41}$$
$$Z_j(s) = Z_{j,0} + (Z_{j,1} - Z_{j,0}) f_j, \tag{42}$$

  where, in toroidal geometry,

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

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

Jacobian

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

$$\mathbf{e}_\theta \times \mathbf{e}_\zeta = -r_{tor} R_\theta \, \hat{\mathbf{i}} - r_{pol} R_\zeta \, \hat{\mathbf{j}} + r_{pol} r_{tor} \hat{\mathbf{k}} \tag{44}$$
$$\boldsymbol{\xi} \cdot \mathbf{e}_\theta \times \mathbf{e}_\zeta = \delta R \tag{45}$$
$$\sqrt{g} = R_s \, r_{pol} \, r_{tor} \tag{46}$$

  - `Igeometry=2` : Cylindrical

$$\mathbf{e}_\theta \times \mathbf{e}_\zeta = (R_\theta \sin\theta + R\cos\theta) \, \hat{\mathbf{i}} + (R \sin\theta - R_\theta \cos\theta) \, \hat{\mathbf{j}} - R R_\zeta \, \hat{\mathbf{k}} \tag{47}$$
$$\boldsymbol{\xi} \cdot \mathbf{e}_\theta \times \mathbf{e}_\zeta = \delta R \, R \tag{48}$$
$$\sqrt{g} = R_s \, R \tag{49}$$

  - `Igeometry=3` : Toroidal

$$\mathbf{e}_\theta \times \mathbf{e}_\zeta = -R \, Z_\theta \, \hat{r} + (Z_\theta \, R_\zeta - R_\theta \, Z_\zeta) \hat{\phi} + R \, R_\theta \, \hat{z} \tag{50}$$
$$\boldsymbol{\xi} \cdot \mathbf{e}_\theta \times \mathbf{e}_\zeta = R(\delta Z \, R_\theta - \delta R \, Z_\theta) \tag{51}$$
$$\sqrt{g} = R(Z_s \, R_\theta - R_s \, Z_\theta) \tag{52}$$

cartesian metrics

- The cartesian metrics are

$$g_{ss} = R_s R_s, \quad g_{s\theta} = R_s R_\theta, \quad g_{s\zeta} = R_s R_\zeta, \quad g_{\theta\theta} = R_\theta R_\theta + r_{pol}^2, \quad g_{\theta\zeta} = R_\theta R_\zeta, \quad g_{\zeta\zeta} = R_\zeta R_\zeta + r_{tor}^2 \tag{53}$$

cylindrical metrics

- The cylindrical metrics are

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

logical control

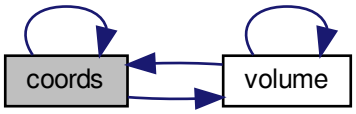
- The logical control is provided by `Lcurvature` as follows:
  - `Lcurvature=0` : only the coordinate transformation is computed, i.e. only R and Z are calculated, e.g. global()
  - `Lcurvature=1` : the Jacobian, $\sqrt{g}$, and "lower" metrics, $g_{\mu,\nu}$, are calculated , e.g. bnorml(), lforce(), curent(), metrix(), sc00aa()

- `Lcurvature=2` : the "curvature" terms are calculated, by which I mean the second derivatives of the position vector; this information is required for computing the current, $\mathbf{j} = \nabla \times \nabla \times \mathbf{A}$, e.g. jo00aa()
- `Lcurvature=3` : the derivative of the $g_{\mu,\nu}/\sqrt{g}$ w.r.t. the interface boundary geometry is calculated, e.g. metrix(), curent()
- `Lcurvature=4` : the derivative of the $g_{\mu,\nu}$ w.r.t. the interface boundary geometry is calculated, e.g. dforce()
- `Lcurvature=5` : the derivative of $\sqrt{g}$ w.r.t. the interface boundary geometry is calculated, e.g. rzaxis()

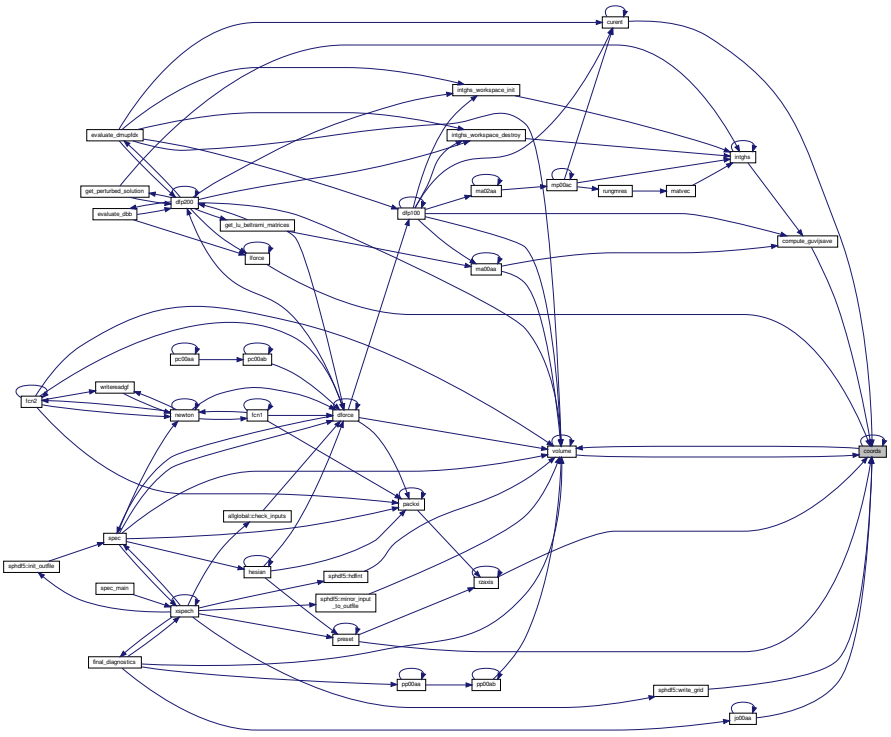
Parameters

in	*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 coords(), 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, 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, inputlist::zbc, inputlist::zbs, constants::zero, and allglobal::zij.
Referenced by compute_guvijsave(), coords(), curent(), jo00aa(), lforce(), preset(), rzaxis(), volume(), and sphdf5::write_grid().
Here is the call graph for this function:



Here is the caller graph for this function:



7.5 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, $G \equiv \int B_\zeta \, d\zeta$.

7.5.1 Detailed Description

7.5.2 Function/Subroutine Documentation

7.5.2.1 curent()

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

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

enclosed currents

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

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

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

- The magnetic field is given by the curl of the magnetic vector potential, as described in e.g. bfield() .

- The toroidal, plasma current is obtained by taking a "poloidal" loop, $d\mathbf{l} = \mathbf{e}_\theta \, d\theta$, on the plasma boundary, where $B^s = 0$, to obtain

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

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

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

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

Fourier integration

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

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

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

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

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

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

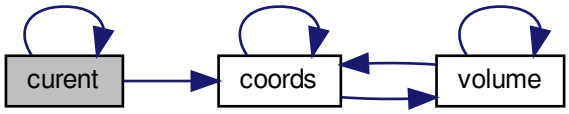
- The plasma current, Eqn. (58), should be independent of ζ, and the linking current, Eqn. (59), should be independent of θ.

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

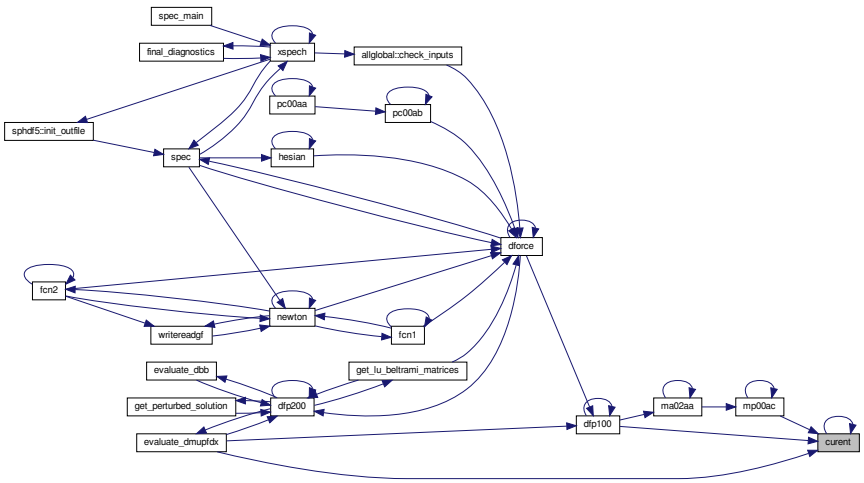
Parameters

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	*ldItGp*	plasma and linking current

References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::cfmn, allglobal::comn, coords(), allglobal::cpus, curent(), allglobal::efmn, allglobal::evmn, allglobal::guvij, allglobal::ijimag, allglobal::ijreal, allglobal::im, allglobal::ime, allglobal::in, allglobal::ine, 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, allglobal::tt, constants::two, inputlist::wmacros, allglobal::yesstellsym, and constants::zero.
Referenced by curent(), dfp100(), evaluate_dmupfdx(), and mp00ac().
Here is the call graph for this function:



Here is the caller graph for this function:



7.6 "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* $\nabla\mathbf{F}$*.*

7.6.1 Detailed Description

7.6.2 Function/Subroutine Documentation

7.6.2.1 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 $i = 1, \texttt{mn}$ labels the Fourier harmonic and $v = 1, \texttt{Mvol} - 1$ 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:

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

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

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

where the spectral condensation constraints, $I_{i,v}$, and the "star-like" poloidal angle constraints, $S_{i,v,\pm 1}$, are calculated and defined in 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

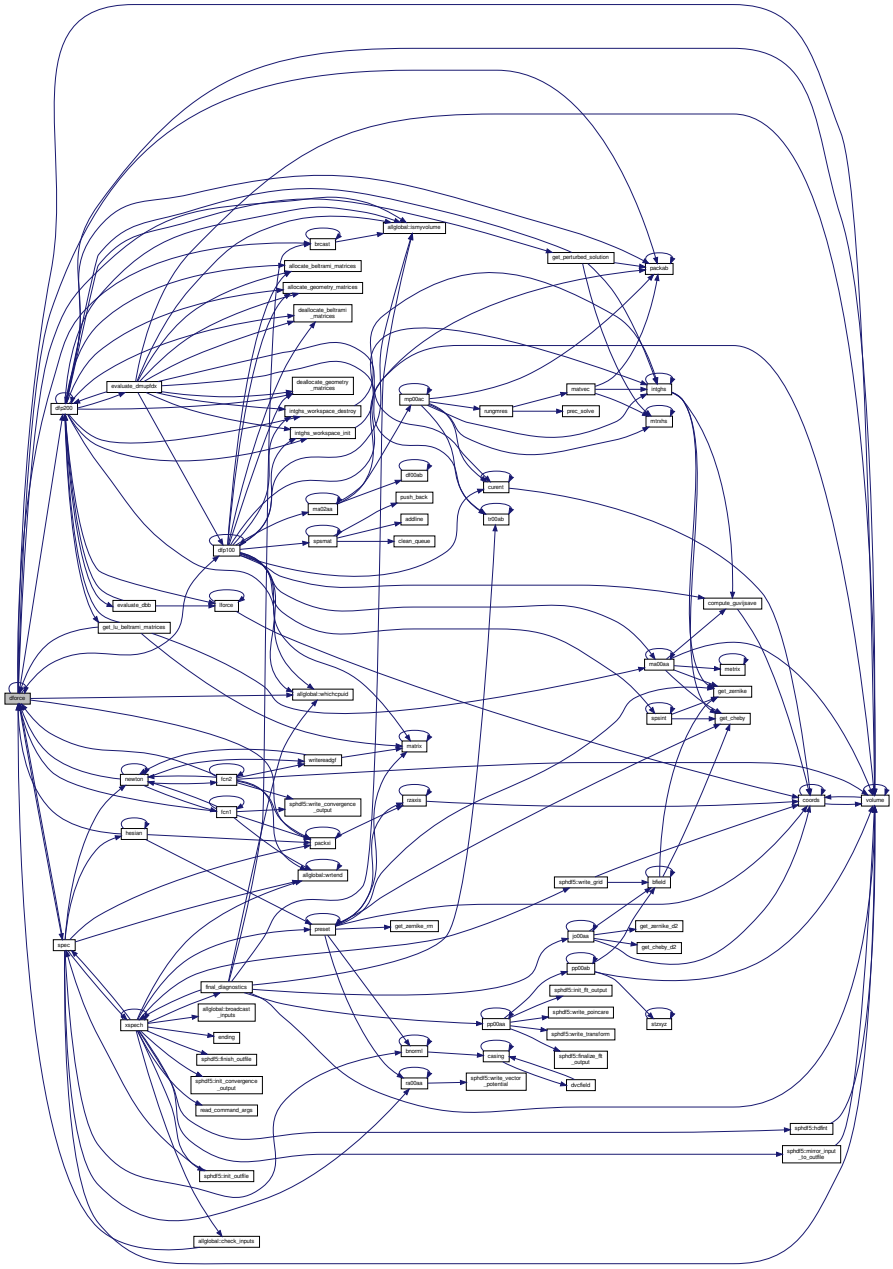
- Matrix perturbation theory is used to compute the derivatives of the solution, i.e. the Beltrami fields, as the geometry of the interfaces changes:

Parameters

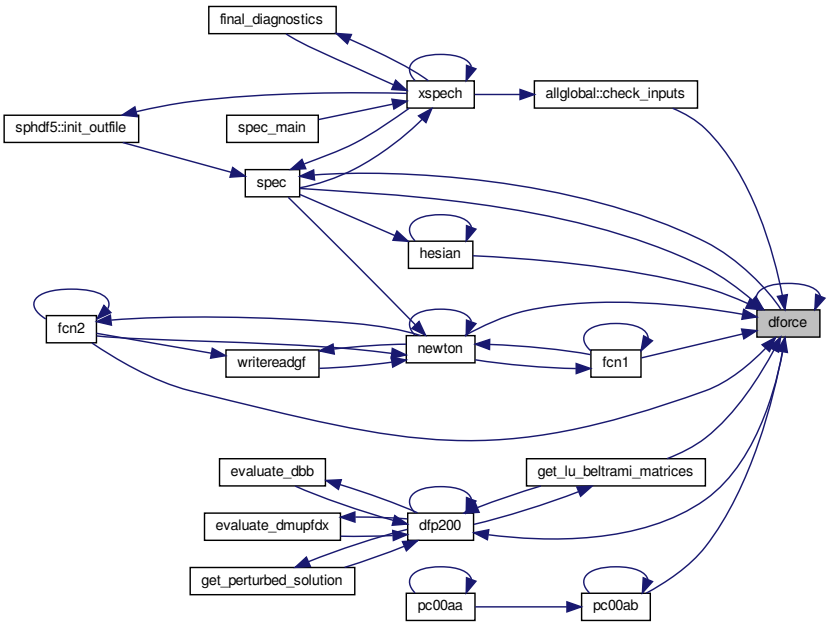
in	*NGdof*	number of global degrees of freedom
in	*position*	degrees-of-freedom = internal geometry (packed by packxi)
out	*force*	output: Fourier harmonics of B_mn^2 and spectral constraint forces
in	*LComputeDerivatives*	indicates whether derivatives are to be calculated; 0: no derivatives, 1:
in,out	*LComputeAxis*	

References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::bbe, allglobal::bbo, allglobal::bbweight, allglobal::bemn, allglobal::bomn, brcast(), allglobal::cpus, allglobal::dbbdmp, allglobal::dbdx, allglobal::denergydrr, allglobal::denergydrz, allglobal::denergydzr, allglobal::denergydzz, allglobal::dessian, allglobal::dessian2d, allglobal::dessian3d, allglobal::dffdrz, dforce(), dfp100(), dfp200(), allglobal::diotadxup, allglobal::ditgpdxtp, allglobal::dmupfdx, allglobal::dpflux, inputlist::drz, allglobal::dtflux, allglobal::energy, inputlist::epsilon, allglobal::forceerr, constants::half, allglobal::hdffdrz, allglobal::hessian, allglobal::hessian2d, allglobal::hessian3d, allglobal::iemn, inputlist::igeometry, allglobal::iie, allglobal::iio, allglobal::im, allglobal::imagneticok, allglobal::in, allglobal::iomn, allglobal::ipdtdpf, allglobal::iquad, allglobal::irbc, allglobal::irbs, allglobal::ismyvolume(), allglobal::ismyvolumevalue, allglobal::izbc, allglobal::izbs, allglobal::lbbintegral, inputlist::lcheck, inputlist::lconstraint, allglobal::lcoordinatesingularity, inputlist::lextrap, inputlist::lfreebound, allglobal::lgdof, allglobal::lhessian2dallocated, allglobal::lhessian3dallocated, allglobal::lhessianallocated, inputlist::lhmatrix, allglobal::localconstraint, numerical::logtolerance, allglobal::lplasmaregion, inputlist::lrad, allglobal::lvacuumregion, allglobal::mn, allglobal::mpi_comm_spec, inputlist::mu, 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, allglobal::semn, allglobal::solution, allglobal::somn, spec(), allglobal::sweight, constants::two, volume(), allglobal::whichcpuid(), inputlist::wmacros, allglobal::xoffset, allglobal::yesstellsym, and constants::zero.
Referenced by allglobal::check_inputs(), dforce(), fcn1(), fcn2(), get_lu_beltrami_matrices(), hesian(), newton(), pc00ab(), and spec().

Here is the call graph for this function:

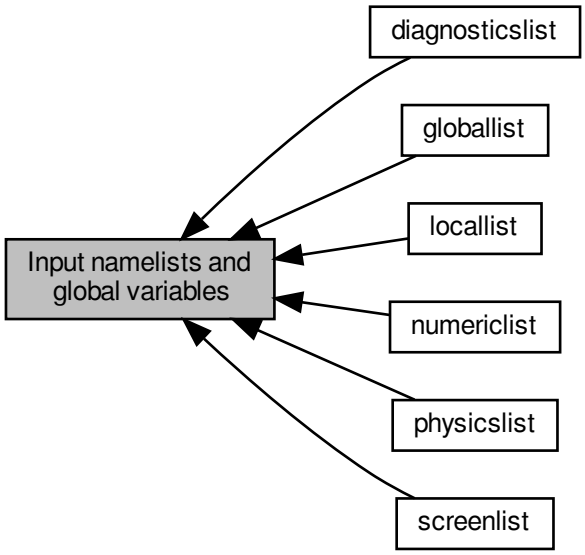


Here is the caller graph for this function:



7.7 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`.

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

Functions/Subroutines

- subroutine **inputlist::initialize_inputs**

Variables

- integer, parameter **inputlist::mnvol** = 256

  The maximum value of `Nvol` is `MNvol=256`.
- integer, parameter **inputlist::mmpol** = 128

  The maximum value of `Mpol` is `MNpol=64`.
- integer, parameter **inputlist::mntor** = 128

  The maximum value of `Ntor` is `MNtor=64`.

7.7.1 Detailed Description

Input namelists.

7.8 "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, $\mathcal{I}_i$.

7.8.1 Detailed Description

7.8.2 Function/Subroutine Documentation

7.8.2.1 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

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

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

- The quantity returned is

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

  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

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

  where i labels the interfaces, and

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

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

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

  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

$$x(\theta,\zeta) \equiv R_i(\theta,\zeta) - R_{i,0}(\zeta), \tag{68}$$
$$y(\theta,\zeta) \equiv Z_i(\theta,\zeta) - Z_{i,0}(\zeta), \tag{69}$$

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

$$R_{i,0} \equiv \int_0^{2\pi} d\theta\ R_i(\theta,\zeta)\sqrt{R_{i,\theta}(\theta,\zeta)^2 + Z_{i,\theta}(\theta,\zeta)^2}, \tag{70}$$
$$Z_{i,0} \equiv \int_0^{2\pi} d\theta\ Z_i(\theta,\zeta)\sqrt{R_{i,\theta}(\theta,\zeta)^2 + Z_{i,\theta}(\theta,\zeta)^2}, \tag{71}$$

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

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

$$\delta R_i(\theta,\zeta) \equiv R_{i,\theta}(\theta,\zeta)\,\delta u_i(\theta,\zeta), \tag{72}$$
$$\delta Z_i(\theta,\zeta) \equiv Z_{i,\theta}(\theta,\zeta)\,\delta u_i(\theta,\zeta), \tag{73}$$

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

$$\delta R_{j,i} = \oint\oint d\theta d\zeta\ \ R_{i,\theta}(\theta,\zeta)\,\delta u_i(\theta,\zeta)\ \cos(m_j\theta - n_j\zeta), \tag{74}$$
$$\delta Z_{j,i} = \oint\oint d\theta d\zeta\ \ Z_{i,\theta}(\theta,\zeta)\,\delta u_i(\theta,\zeta)\ \sin(m_j\theta - n_j\zeta), \tag{75}$$

and

$$\delta R_{i,\theta}(\theta,\zeta) \equiv R_{i,\theta\theta}(\theta,\zeta)\,\delta u_i(\theta,\zeta) + R_{i,\theta}(\theta,\zeta)\,\delta u_{i,\theta}(\theta,\zeta) \tag{76}$$
$$\delta Z_{i,\theta}(\theta,\zeta) \equiv Z_{i,\theta\theta}(\theta,\zeta)\,\delta u_i(\theta,\zeta) + Z_{i,\theta}(\theta,\zeta)\,\delta u_{i,\theta}(\theta,\zeta) \tag{77}$$

- The variation in F is

$$\begin{aligned}
\delta F = &\sum_{i=1}^{N-1} \alpha_i \oint\oint d\theta d\zeta \left(\frac{-2\Theta_{i,\theta\theta}}{\Theta_{i,\theta}^2}\right)\delta u_i \\
&+ \sum_{i=1}^{N-1} \beta_i \oint\oint d\theta d\zeta\ (R_{i,\theta}X_i + Z_{i,\theta}Y_i)\,\delta u_i \\
&+ \sum_{i=1}^{N-1} \gamma_i \int d\zeta\ (Z_i(0,\zeta) - Z_{i,0})\,Z_{i,\theta}\,\delta u_i \\
&+ \sum_{i=1}^{N-1} \delta_i \oint\oint d\theta d\zeta \left(\frac{\Delta R_i R_{i,\theta} + \Delta Z_i Z_{i,\theta}}{L_i}\right)\delta u_i \\
&- \sum_{i=1}^{N-1} \delta_{i+1} \oint\oint d\theta d\zeta \left(\frac{\Delta R_{i+1} R_{i,\theta} + \Delta Z_{i+1} Z_{i,\theta}}{L_{i+1}}\right)\delta u_i
\end{aligned} \tag{78}$$

where, for the stellarator symmetric case,

$$X_i \equiv \sum\nolimits_j (m_j^p - M_i)\,R_{j,i}\cos(m_j\theta - n_j\zeta), \tag{79}$$
$$Y_i \equiv \sum\nolimits_j (m_j^p - M_i)\,Z_{j,i}\sin(m_j\theta - n_j\zeta), \tag{80}$$

and

$$\Delta R_i \equiv R_i(\theta,\zeta) - R_{i-1}(\theta,\zeta), \tag{81}$$
$$\Delta Z_i \equiv Z_i(\theta,\zeta) - Z_{i-1}(\theta,\zeta), \tag{82}$$

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

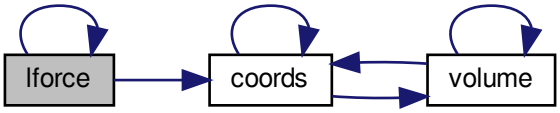
$$\begin{aligned} I_i(\theta,\zeta) &\equiv -2\alpha_i \frac{\Theta_{i,\theta\theta}}{\Theta_{i,\theta}^2} + \beta_i \left(R_{i,\theta}X_i + Z_{i,\theta}Y_i\right) + \gamma_i \left(Z_i(0,\zeta) - Z_{i,0}\right) Z_{i,\theta}(0,\zeta) \\ &+ \delta_i \frac{\Delta R_i R_{i,\theta} + \Delta Z_i Z_{i,\theta}}{L_i} - \delta_{i+1} \frac{\Delta R_{i+1} R_{i,\theta} + \Delta Z_{i+1} Z_{i,\theta}}{L_{i+1}} \end{aligned} \tag{83}$$

- Note that choosing $p = 2$ gives $X = -R_{\theta\theta}$ and $Y = -Z_{\theta\theta}$, and the spectrally condensed angle constraint, $R_\theta X + Z_\theta Y = 0$, becomes $\partial_\theta(R_\theta^2 + Z_\theta^2) = 0$, which defines the equal arc length angle.
- The poloidal-angle origin term, namely $\gamma_i \left(Z_i(0,\zeta) - Z_{i,0}\right) Z_{i,\theta}(0,\zeta)$ is only used to constrain the $m_j = 0$ harmonics.
- The construction of the angle functional was influenced by the following considerations:
  - The minimal spectral width constraint is very desirable as it reduces the required Fourier resolution, but it does not constrain the $m = 0$ harmonics and the minimizing spectral-width poloidal-angle may not be consistent with the poloidal angle used on adjacent interfaces.
  - The regularization of the vector potential and the coordinate interpolation near the coordinate origin (see elsewhere) assumes that the poloidal angle is the polar angle.
  - The user will provide the Fourier harmonics of the boundary, and thus the user will implicitly define the poloidal angle used on the boundary.
  - Minimizing the length term will ensure that the poloidal angle used on each interface is smoothly connected to the poloidal angle used on adjacent interfaces.
- A suitable choice of the weight factors, 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. (83) need to be differentiated with respect to the interface Fourier harmonics, $R_{j,i}$ and $Z_{j,i}$. The first and second terms lead to a block diagonal hessian, and the length term leads to a block tri-diagonal hessian.
- Including the poloidal-angle origin constraint means that the polar angle constraint can probably be ignored, i.e. $\alpha_i = 0$.

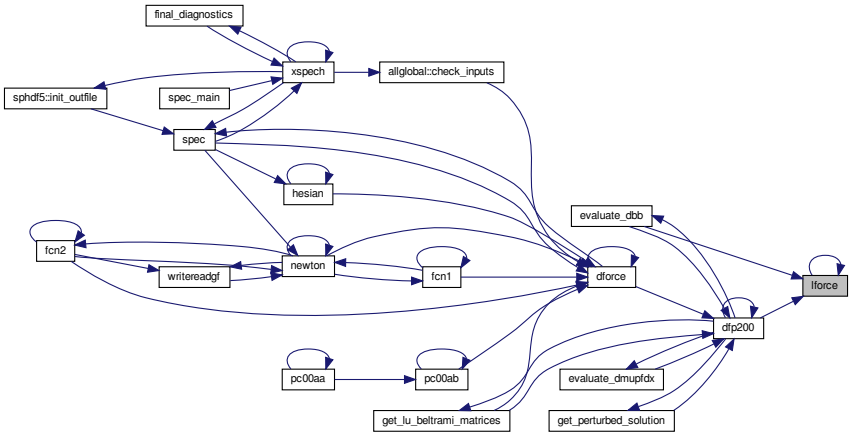
Parameters

in	*lvol*	
in	*iocons*	
in	*ideriv*	
in	*Ntz*	
	dBB	
	XX	
	YY	
	length	
	DDI	
	MMI	
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, allglobal::iomn, allglobal::irbc, allglobal::irbs, allglobal::irij, allglobal::izbc, allglobal::izbs, allglobal::izij, allglobal::jiimag, allglobal::jireal, inputlist::lcheck, allglobal::lcoordinatesingularity, lforce(), 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, allglobal::trij, allglobal::tt, constants::two, allglobal::tzij, allglobal::vvolume, allglobal::yesstellsym, and constants::zero.
Referenced by dfp200(), evaluate_dbb(), and lforce().
Here is the call graph for this function:



Here is the caller graph for this function:



7.9 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.

7.9.1 Detailed Description

7.9.2 Function/Subroutine Documentation

7.9.2.1 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 )
```

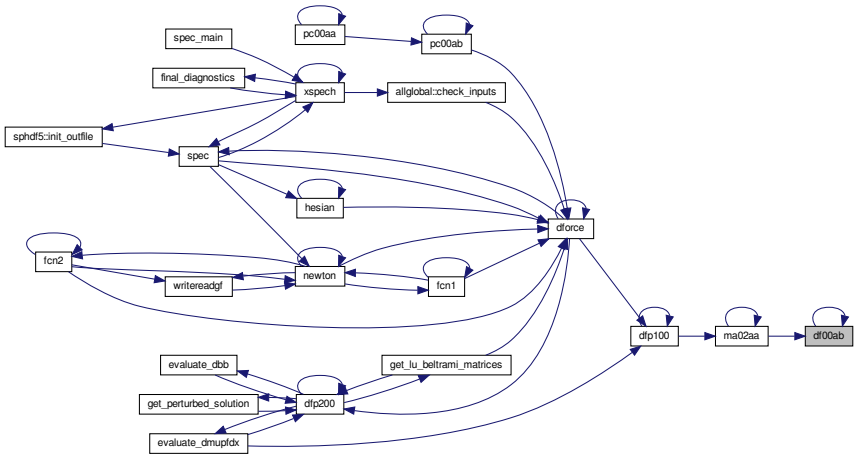
Evaluates volume integrals, and their derivatives w.r.t. interface geometry, using "packed" format.

Parameters

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

References allglobal::cpus, df00ab(), allglobal::dma, allglobal::dmd, constants::half, inputlist::helicity, allglobal::ivol, allglobal::mbpsi, allglobal::mpi_comm_spec, allglobal::myid, inputlist::nvol, constants::one, fileunits::ounit, numerical::small, constants::two, and constants::zero.
Referenced by df00ab(), and ma02aa().
Here is the call graph for this function:

Here is the caller graph for this function:



7.9.2.2 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:

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

$$\texttt{DToocs(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}_{p,j} \oint\!\!\oint d\theta d\zeta \;\; \cos\alpha_i \sin\alpha_j \tag{85}$$

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

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

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

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

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

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

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

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

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

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

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

$$\texttt{TDstcs(l,p,i,j)} \equiv \int ds\, \overline{T}_{l,i}\, \overline{T}'_{p,j} \oiint d\theta d\zeta \;\; \cos\alpha_i \sin\alpha_j\, \bar{g}_{s\zeta} \tag{97}$$

$$\texttt{TDstsc(l,p,i,j)} \equiv \int ds\, \overline{T}_{l,i}\, \overline{T}'_{p,j} \oiint d\theta d\zeta \;\; \sin\alpha_i \cos\alpha_j\, \bar{g}_{s\zeta} \tag{98}$$

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

$$\texttt{DDstcc(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oiint d\theta d\zeta \;\; \cos\alpha_i \cos\alpha_j\, \bar{g}_{\theta\theta} \tag{100}$$

$$\texttt{DDstcs(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oiint d\theta d\zeta \;\; \cos\alpha_i \sin\alpha_j\, \bar{g}_{\theta\theta} \tag{101}$$

$$\texttt{DDstsc(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oiint d\theta d\zeta \;\; \sin\alpha_i \cos\alpha_j\, \bar{g}_{\theta\theta} \tag{102}$$

$$\texttt{DDstss(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oiint d\theta d\zeta \;\; \sin\alpha_i \sin\alpha_j\, \bar{g}_{\theta\theta} \tag{103}$$

$$\texttt{DDstcc(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oiint d\theta d\zeta \;\; \cos\alpha_i \cos\alpha_j\, \bar{g}_{\theta\zeta} \tag{104}$$

$$\texttt{DDstcs(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oiint d\theta d\zeta \;\; \cos\alpha_i \sin\alpha_j\, \bar{g}_{\theta\zeta} \tag{105}$$

$$\texttt{DDstsc(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oiint d\theta d\zeta \;\; \sin\alpha_i \cos\alpha_j\, \bar{g}_{\theta\zeta} \tag{106}$$

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

$$\texttt{DDstcc(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oiint d\theta d\zeta \;\; \cos\alpha_i \cos\alpha_j\, \bar{g}_{\zeta\zeta} \tag{108}$$

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

$$\texttt{DDstsc(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oiint d\theta d\zeta \;\; \sin\alpha_i \cos\alpha_j\, \bar{g}_{\zeta\zeta} \tag{110}$$

$$\texttt{DDstss(l,p,i,j)} \equiv \int ds\, \overline{T}'_{l,i}\, \overline{T}'_{p,j} \oiint d\theta d\zeta \;\; \sin\alpha_i \sin\alpha_j\, \bar{g}_{\zeta\zeta} \tag{111}$$

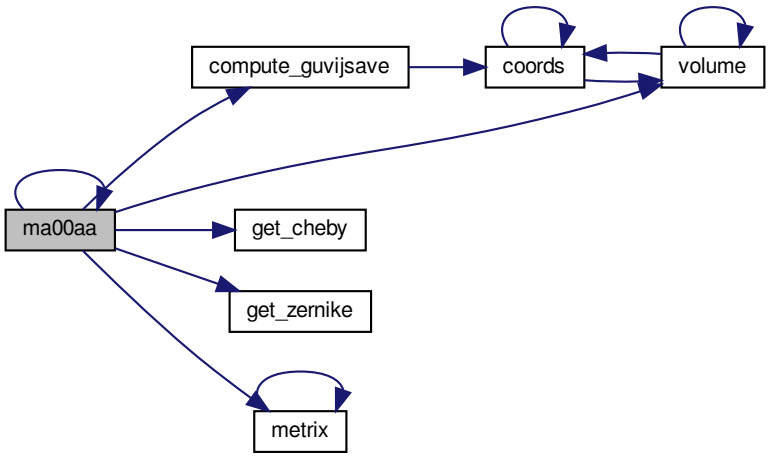
where $\overline{T}_{l,i} \equiv T_l\, \bar{s}^{m_i/2}$ if the domain includes the coordinate singularity, and $\overline{T}_{l,i} \equiv T_l$ if not; and $\bar{g}_{\mu\nu} \equiv g_{\mu\nu}/\sqrt{g}$.

- 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 .

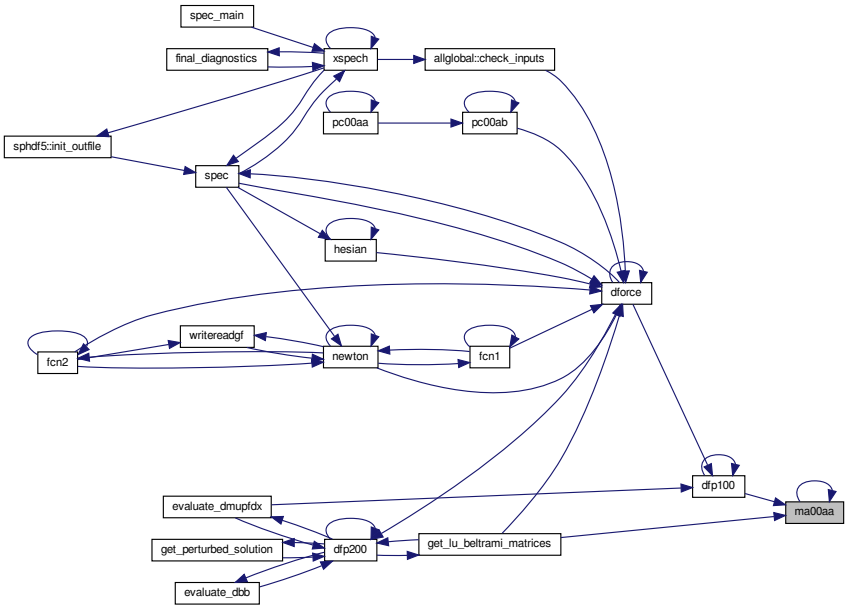
Parameters

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, ma00aa(), 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(), get_lu_beltrami_matrices(), and ma00aa().
Here is the call graph for this function:



Here is the caller graph for this function:



7.9.2.3 spsint() `subroutine spsint (`

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

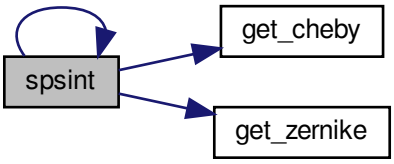
Calculates volume integrals of Chebyshev-polynomials and metric elements for preconditioner.
Computes the integrals needed for spsmat.f90. Same as ma00aa.f90, but only compute the relevant terms that are non-zero.

Parameters

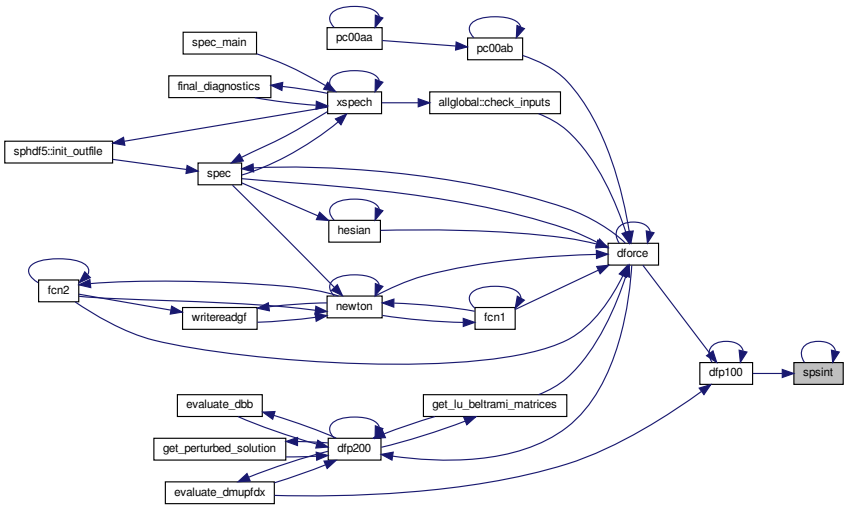
lquad	
mn	
lvol	
lrad	

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, spsint(), 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(), and spsint().

Here is the call graph for this function:



Here is the caller graph for this function:



7.10 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.

7.10.1 Detailed Description

7.10.2 Function/Subroutine Documentation

7.10.2.1 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

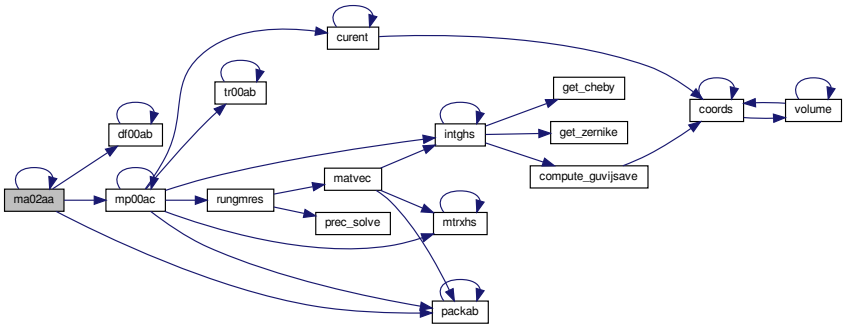
- Note that the rotational-transform (if required) is calculated by tr00ab(), which is called by mp00ac().
- If Lconstraint=1, then mp00ac() will ask tr00ab() to compute the derivatives of the transform with respect to variations in the helicity-multiplier, μ, and the enclosed poloidal-flux, $\Delta\psi_p$,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

$$\frac{\partial \iota}{\partial \mu} \tag{112}$$

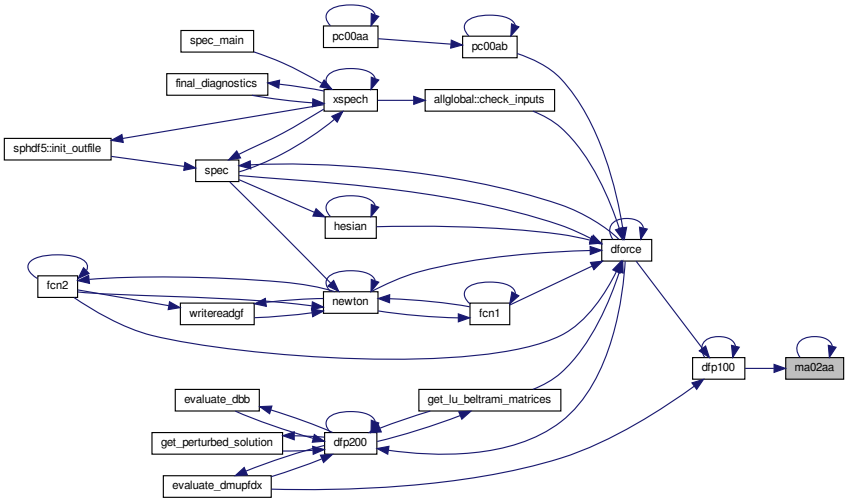
$$\frac{\partial \iota}{\partial \Delta\psi_p} \tag{113}$$

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

References allglobal::ate, allglobal::cpus, df00ab(), allglobal::dma, allglobal::dmb, allglobal::dmd, allglobal::dpflux, allglobal::dtflux, constants::half, inputlist::helicity, allglobal::im, allglobal::imagneticok, allglobal::in, allglobal::ivol, allglobal::labintegral, allglobal::lbbintegral, allglobal::lblinear, allglobal::lbnewton, allglobal::lbsequad, inputlist::lcheck, inputlist::lconstraint, allglobal::lcoordinatesingularity, allglobal::localconstraint, allglobal::lplasmaregion, inputlist::lrad, allglobal::lvacuumregion, ma02aa(), allglobal::mbpsi, allglobal::mn, mp00ac(), allglobal::mpi_comm_spec, inputlist::mu, inputlist::mupfits, inputlist::mupftol, allglobal::myid, allglobal::ncpu, allglobal::nfielddof, constants::one, fileunits::ounit, packab(), numerical::small, allglobal::solution, constants::ten, numerical::vsmall, inputlist::wmacros, allglobal::xoffset, and constants::zero.
Referenced by dfp100(), and ma02aa().
Here is the call graph for this function:



Here is the caller graph for this function:



7.11 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.

7.11.1 Detailed Description

7.11.2 Function/Subroutine Documentation

7.11.2.1 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

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

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

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

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

$$A_\theta(-1,\theta,\zeta) = 0 \tag{116}$$
$$A_\zeta(-1,0,\zeta) = 0 \tag{117}$$

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

boundary conditions

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

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

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

enclosed fluxes

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

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

Fourier-Chebyshev representation

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

$$A_\theta(s,\theta,\zeta) = \sum_{i,l} A_{\theta,e,i,l}\,\overline{T}_{l,i}(s)\cos\alpha_i + \sum_{i,l} A_{\theta,o,i,l}\,\overline{T}_{l,i}(s)\sin\alpha_i, \tag{120}$$
$$A_\zeta(s,\theta,\zeta) = \sum_{i,l} A_{\zeta,e,i,l}\,\overline{T}_{l,i}(s)\cos\alpha_i + \sum_{i,l} A_{\zeta,o,i,l}\,\overline{T}_{l,i}(s)\sin\alpha_i, \tag{121}$$

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

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

$$\begin{aligned}\sqrt{g}\,\mathbf{B} = {} & \mathbf{e}_s\ \textstyle\sum_{i,l}[(\ -m_i A_{\zeta,e,i,l}\ -\ n_i A_{\theta,e,i,l}\ )\overline{T}_{l,i}\sin\alpha_i + (\ +m_i A_{\zeta,o,i,l}\ +\ n_i A_{\theta,o,i,l}\ )\overline{T}_{l,i}\cos\alpha_i] \\ & + \mathbf{e}_\theta\ \textstyle\sum_{i,l}[(\ -\ A_{\zeta,e,i,l}\ )\overline{T}'_{l,i}\cos\alpha_i + (\ -\ A_{\zeta,o,i,l}\ )\overline{T}'_{l,i}\sin\alpha_i] \\ & + \mathbf{e}_\zeta\ \textstyle\sum_{i,l}[(\ A_{\theta,e,i,l}\ )\overline{T}'_{l,i}\cos\alpha_i + (\ A_{\theta,o,i,l}\ )\overline{T}'_{l,i}\sin\alpha_i]\end{aligned} \tag{122}$$

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

$$v_s(s,\theta,\zeta) = \sum_{i,l} v_{s,e,i,l}\,\overline{T}_{l,i}(s)\cos\alpha_i + \sum_{i,l} v_{s,o,i,l}\,\overline{T}_{l,i}(s)\sin\alpha_i, \tag{123}$$
$$v_\theta(s,\theta,\zeta) = \sum_{i,l} v_{\theta,e,i,l}\,\overline{T}_{l,i}(s)\cos\alpha_i + \sum_{i,l} v_{\theta,o,i,l}\,\overline{T}_{l,i}(s)\sin\alpha_i, \tag{124}$$
$$v_\zeta(s,\theta,\zeta) = \sum_{i,l} v_{\zeta,e,i,l}\,\overline{T}_{l,i}(s)\cos\alpha_i + \sum_{i,l} v_{\zeta,o,i,l}\,\overline{T}_{l,i}(s)\sin\alpha_i. \tag{125}$$

constrained energy functional

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

$$\mathcal{F} \equiv \mathcal{F}[A_{\theta,e,i,l}, A_{\zeta,e,i,l}, A_{\theta,o,i,l}, A_{\zeta,o,i,l}, v_{s,e,i,l}, v_{s,o,i,l}, v_{\theta,e,i,l}, v_{\theta,o,i,l}, v_{\zeta,e,i,l}, v_{\zeta,o,i,l}, \mu, a_i, b_i, c_i, d_i, e_i, f_i, g_1, h_1], \tag{126}$$

and is given by:

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

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

$$\frac{\partial}{\partial A_{\theta,e,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ \mathbf{B}\cdot\frac{\partial\mathbf{B}}{\partial A_{\theta,e,i,l}} = 2\int dv\ \mathbf{B}\cdot\left[-n_i\overline{T}_{l,i}\sin\alpha_i\,\mathbf{e}_s + \overline{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\zeta\right]/\sqrt{g} \tag{128}$$

$$\frac{\partial}{\partial A_{\theta,o,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ \mathbf{B}\cdot\frac{\partial\mathbf{B}}{\partial A_{\theta,o,i,l}} = 2\int dv\ \mathbf{B}\cdot\left[+n_i\overline{T}_{l,i}\cos\alpha_i\,\mathbf{e}_s + \overline{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\zeta\right]/\sqrt{g} \tag{129}$$

$$\frac{\partial}{\partial A_{\zeta,e,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ \mathbf{B}\cdot\frac{\partial\mathbf{B}}{\partial A_{\zeta,e,i,l}} = 2\int dv\ \mathbf{B}\cdot\left[-m_i\overline{T}_{l,i}\sin\alpha_i\,\mathbf{e}_s - \overline{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\theta\right]/\sqrt{g} \tag{130}$$

$$\frac{\partial}{\partial A_{\zeta,o,i,l}}\int dv\ \mathbf{B}\cdot\mathbf{B} = 2\int dv\ \mathbf{B}\cdot\frac{\partial\mathbf{B}}{\partial A_{\zeta,o,i,l}} = 2\int dv\ \mathbf{B}\cdot\left[+m_i\overline{T}_{l,i}\cos\alpha_i\,\mathbf{e}_s - \overline{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\theta\right]/\sqrt{g} \tag{131}$$

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

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

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

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

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

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

$$\frac{\partial}{\partial A_{\theta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left(\frac{\partial\mathbf{A}}{\partial A_{\theta,e,i,l}}\cdot\mathbf{B} + \mathbf{A}\cdot\frac{\partial\mathbf{B}}{\partial A_{\theta,e,i,l}}\right) = \int dv\ (\overline{T}_{l,i}\cos\alpha_i\nabla\theta\cdot\mathbf{B} + \mathbf{A}\cdot\overline{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\zeta/\sqrt{}) \quad (132)$$
$$\frac{\partial}{\partial A_{\theta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left(\frac{\partial\mathbf{A}}{\partial A_{\theta,o,i,l}}\cdot\mathbf{B} + \mathbf{A}\cdot\frac{\partial\mathbf{B}}{\partial A_{\theta,o,i,l}}\right) = \int dv\ (\overline{T}_{l,i}\sin\alpha_i\nabla\theta\cdot\mathbf{B} + \mathbf{A}\cdot\overline{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\zeta/\sqrt{}) \quad (133)$$
$$\frac{\partial}{\partial A_{\zeta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left(\frac{\partial\mathbf{A}}{\partial A_{\zeta,e,i,l}}\cdot\mathbf{B} + \mathbf{A}\cdot\frac{\partial\mathbf{B}}{\partial A_{\zeta,e,i,l}}\right) = \int dv\ (\overline{T}_{l,i}\cos\alpha_i\nabla\zeta\cdot\mathbf{B} - \mathbf{A}\cdot\overline{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\theta/\sqrt{}) \quad (134)$$
$$\frac{\partial}{\partial A_{\zeta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left(\frac{\partial\mathbf{A}}{\partial A_{\zeta,o,i,l}}\cdot\mathbf{B} + \mathbf{A}\cdot\frac{\partial\mathbf{B}}{\partial A_{\zeta,o,i,l}}\right) = \int dv\ (\overline{T}_{l,i}\sin\alpha_i\nabla\zeta\cdot\mathbf{B} - \mathbf{A}\cdot\overline{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\theta/\sqrt{}) \quad (135)$$

- 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

$$\frac{\partial}{\partial A_{\theta,e,j,p}}\frac{\partial}{\partial A_{\theta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[+\overline{T}_{l,i}\cos\alpha_i\cancel{\nabla\theta\cdot\overline{T}'_{p,j}}\cos\alpha_j\,\mathbf{e}_\zeta+\overline{T}_{p,j}\cos\alpha_j\cancel{\nabla\theta\cdot\overline{T}'_{l,i}}\cos\alpha_i\,\mathbf{e}_\zeta\right] \quad (136)$$

$$\frac{\partial}{\partial A_{\theta,o,j,p}}\frac{\partial}{\partial A_{\theta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[+\overline{T}_{l,i}\cos\alpha_i\cancel{\nabla\theta\cdot\overline{T}'_{p,j}}\sin\alpha_j\,\mathbf{e}_\zeta+\overline{T}_{p,j}\sin\alpha_j\cancel{\nabla\theta\cdot\overline{T}'_{l,i}}\cos\alpha_i\,\mathbf{e}_\zeta\right] \quad (137)$$

$$\frac{\partial}{\partial A_{\zeta,e,j,p}}\frac{\partial}{\partial A_{\theta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[-\overline{T}_{l,i}\cos\alpha_i\nabla\theta\cdot\overline{T}'_{p,j}\cos\alpha_j\,\mathbf{e}_\theta+\overline{T}_{p,j}\cos\alpha_j\nabla\zeta\cdot\overline{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\zeta\right] \quad (138)$$

$$\frac{\partial}{\partial A_{\zeta,o,j,p}}\frac{\partial}{\partial A_{\theta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[-\overline{T}_{l,i}\cos\alpha_i\nabla\theta\cdot\overline{T}'_{p,j}\sin\alpha_j\,\mathbf{e}_\theta+\overline{T}_{p,j}\sin\alpha_j\nabla\zeta\cdot\overline{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\zeta\right] \quad (139)$$

$$\frac{\partial}{\partial A_{\theta,e,j,p}}\frac{\partial}{\partial A_{\theta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[+\overline{T}_{l,i}\sin\alpha_i\cancel{\nabla\theta\cdot\overline{T}'_{p,j}}\cos\alpha_j\,\mathbf{e}_\zeta+\overline{T}_{p,j}\cos\alpha_j\cancel{\nabla\theta\cdot\overline{T}'_{l,i}}\sin\alpha_i\,\mathbf{e}_\zeta\right] \quad (140)$$

$$\frac{\partial}{\partial A_{\theta,o,j,p}}\frac{\partial}{\partial A_{\theta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[+\overline{T}_{l,i}\sin\alpha_i\cancel{\nabla\theta\cdot\overline{T}'_{p,j}}\sin\alpha_j\,\mathbf{e}_\zeta+\overline{T}_{p,j}\sin\alpha_j\cancel{\nabla\theta\cdot\overline{T}'_{l,i}}\sin\alpha_i\,\mathbf{e}_\zeta\right] \quad (141)$$

$$\frac{\partial}{\partial A_{\zeta,e,j,p}}\frac{\partial}{\partial A_{\theta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[-\overline{T}_{l,i}\sin\alpha_i\nabla\theta\cdot\overline{T}'_{p,j}\cos\alpha_j\,\mathbf{e}_\theta+\overline{T}_{p,j}\cos\alpha_j\nabla\zeta\cdot\overline{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\zeta\right] \quad (142)$$

$$\frac{\partial}{\partial A_{\zeta,o,j,p}}\frac{\partial}{\partial A_{\theta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[-\overline{T}_{l,i}\sin\alpha_i\nabla\theta\cdot\overline{T}'_{p,j}\sin\alpha_j\,\mathbf{e}_\theta+\overline{T}_{p,j}\sin\alpha_j\nabla\zeta\cdot\overline{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\zeta\right] \quad (143)$$

$$\frac{\partial}{\partial A_{\theta,e,j,p}}\frac{\partial}{\partial A_{\zeta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[+\overline{T}_{l,i}\cos\alpha_i\nabla\zeta\cdot\overline{T}'_{p,j}\cos\alpha_j\,\mathbf{e}_\zeta-\overline{T}_{p,j}\cos\alpha_j\nabla\theta\cdot\overline{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\theta\right] \quad (144)$$

$$\frac{\partial}{\partial A_{\theta,o,j,p}}\frac{\partial}{\partial A_{\zeta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[+\overline{T}_{l,i}\cos\alpha_i\nabla\zeta\cdot\overline{T}'_{p,j}\sin\alpha_j\,\mathbf{e}_\zeta-\overline{T}_{p,j}\sin\alpha_j\nabla\theta\cdot\overline{T}'_{l,i}\cos\alpha_i\,\mathbf{e}_\theta\right] \quad (145)$$

$$\frac{\partial}{\partial A_{\zeta,e,j,p}}\frac{\partial}{\partial A_{\zeta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[-\overline{T}_{l,i}\cos\alpha_i\cancel{\nabla\zeta\cdot\overline{T}'_{p,j}}\cos\alpha_j\,\mathbf{e}_\theta-\overline{T}_{p,j}\cos\alpha_j\cancel{\nabla\zeta\cdot\overline{T}'_{l,i}}\cos\alpha_i\,\mathbf{e}_\theta\right] \quad (146)$$

$$\frac{\partial}{\partial A_{\zeta,o,j,p}}\frac{\partial}{\partial A_{\zeta,e,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[-\overline{T}_{l,i}\cos\alpha_i\cancel{\nabla\zeta\cdot\overline{T}'_{p,j}}\sin\alpha_j\,\mathbf{e}_\theta-\overline{T}_{p,j}\sin\alpha_j\cancel{\nabla\zeta\cdot\overline{T}'_{l,i}}\cos\alpha_i\,\mathbf{e}_\theta\right] \quad (147)$$

$$\frac{\partial}{\partial A_{\theta,e,j,p}}\frac{\partial}{\partial A_{\zeta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[+\overline{T}_{l,i}\sin\alpha_i\nabla\zeta\cdot\overline{T}'_{p,j}\cos\alpha_j\,\mathbf{e}_\zeta-\overline{T}_{p,j}\cos\alpha_j\nabla\theta\cdot\overline{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\theta\right] \quad (148)$$

$$\frac{\partial}{\partial A_{\theta,o,j,p}}\frac{\partial}{\partial A_{\zeta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[+\overline{T}_{l,i}\sin\alpha_i\nabla\zeta\cdot\overline{T}'_{p,j}\sin\alpha_j\,\mathbf{e}_\zeta-\overline{T}_{p,j}\sin\alpha_j\nabla\theta\cdot\overline{T}'_{l,i}\sin\alpha_i\,\mathbf{e}_\theta\right] \quad (149)$$

$$\frac{\partial}{\partial A_{\zeta,e,j,p}}\frac{\partial}{\partial A_{\zeta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[-\overline{T}_{l,i}\sin\alpha_i\cancel{\nabla\zeta\cdot\overline{T}'_{p,j}}\cos\alpha_j\,\mathbf{e}_\theta-\overline{T}_{p,j}\cos\alpha_j\cancel{\nabla\zeta\cdot\overline{T}'_{l,i}}\sin\alpha_i\,\mathbf{e}_\theta\right] \quad (150)$$

$$\frac{\partial}{\partial A_{\zeta,o,j,p}}\frac{\partial}{\partial A_{\zeta,o,i,l}}\int dv\ \mathbf{A}\cdot\mathbf{B} = \int dv\ \left[-\overline{T}_{l,i}\sin\alpha_i\cancel{\nabla\zeta\cdot\overline{T}'_{p,j}}\sin\alpha_j\,\mathbf{e}_\theta-\overline{T}_{p,j}\sin\alpha_j\cancel{\nabla\zeta\cdot\overline{T}'_{l,i}}\sin\alpha_i\,\mathbf{e}_\theta\right] \quad (151)$$

- 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

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

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

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

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

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

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

$$\tag{158}$$

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

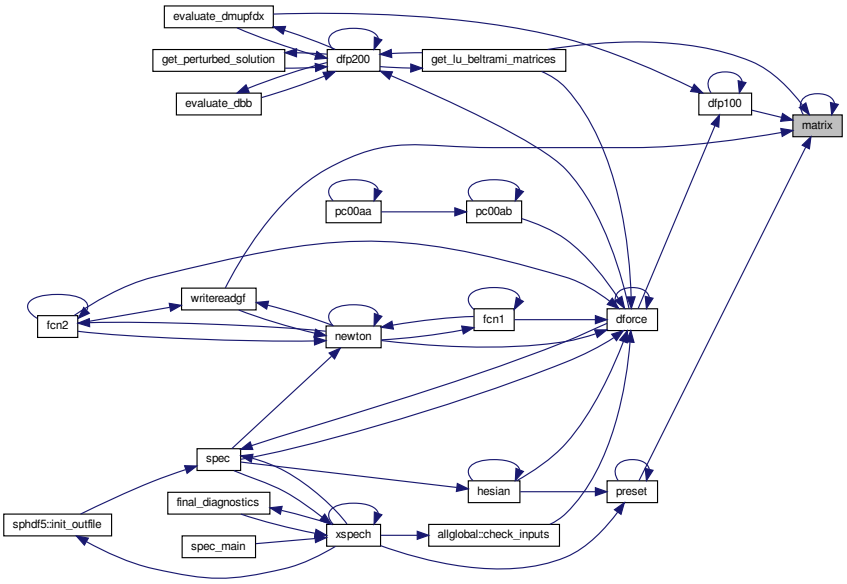
- The required geometric information is calculated in ma00aa().

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, matrix(), 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(), matrix(), preset(), and writereadgf().
Here is the call graph for this function:

Here is the caller graph for this function:



7.11.2.2 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 )
```

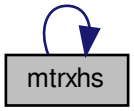
Constructs matrices that represent the Beltrami linear system, matrix-free.

Parameters

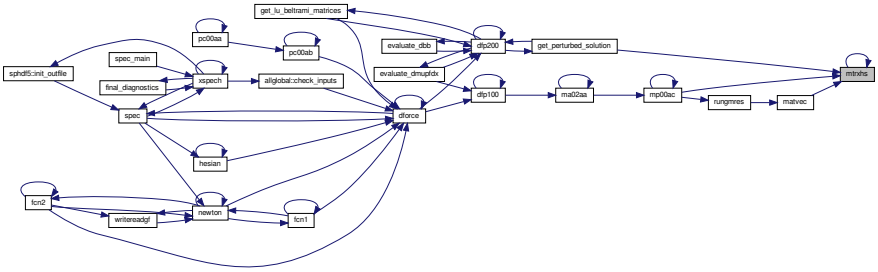
lvol	
mn	
lrad	
resultA	
resultD	
idx	

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, mtrxhs(), 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(), mp00ac(), and mtrxhs().

Here is the call graph for this function:



Here is the caller graph for this function:



7.11.2.3 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.

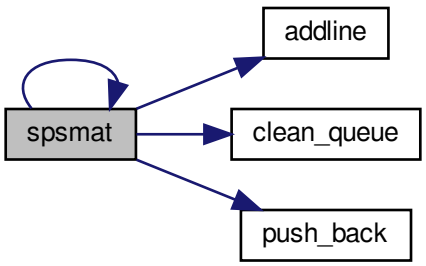
If the i-th and j-th unknowns in $\mathbf{a}$ correspond to A_{θ,m_i,n_i,l_i} and A_{θ,m_j,n_j,l_j}, respectively, then the matrix element $\hat{\mathcal{A}}_{i,j}$ describes the coupling strength between harmonics (m_i, n_i) and (m_j, n_j). Noting that if the Fourier series of the boundary $R_{m,n}$ 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)**.

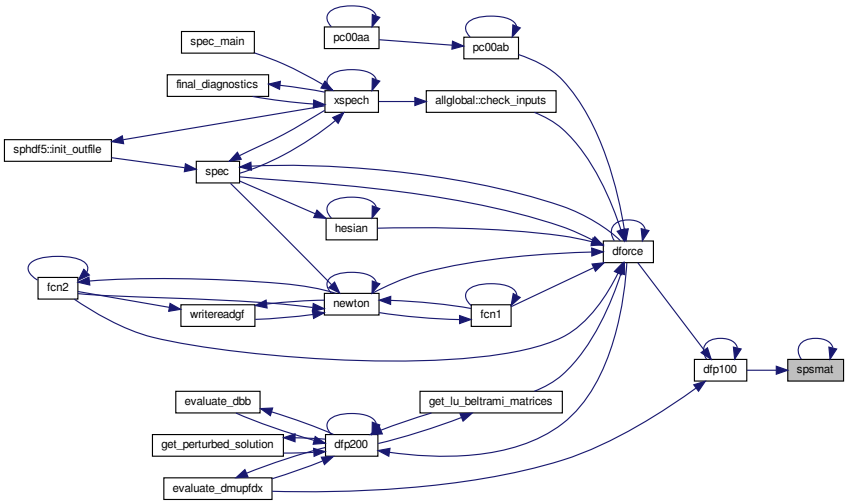
Parameters

lvol	
mn	
lrad	

References addline(), allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, clean_queue(), 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::dma, allglobal::dmas, allglobal::dmb, allglobal::dmd, allglobal::dmds, allglobal::dmg, allglobal::dtoocc, allglobal::dtoocs, allglobal::dtoosc, allglobal::dtooss, allglobal::ibnc, allglobal::ibns, allglobal::idmas, allglobal::im, allglobal::in, allglobal::ivnc, allglobal::ivns, allglobal::jdmas, allglobal::lcoordinatesingularity, allglobal::liluprecond, 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::ndmas, allglobal::ndmasmax, allglobal::notstellsym, constants::one, fileunits::ounit, push_back(), allglobal::rtm, allglobal::rtt, numerical::small, spsmat(), 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(), and spsmat().
Here is the call graph for this function:



Here is the caller graph for this function:



7.12 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.

7.12.1 Detailed Description

7.12.2 Function/Subroutine Documentation

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

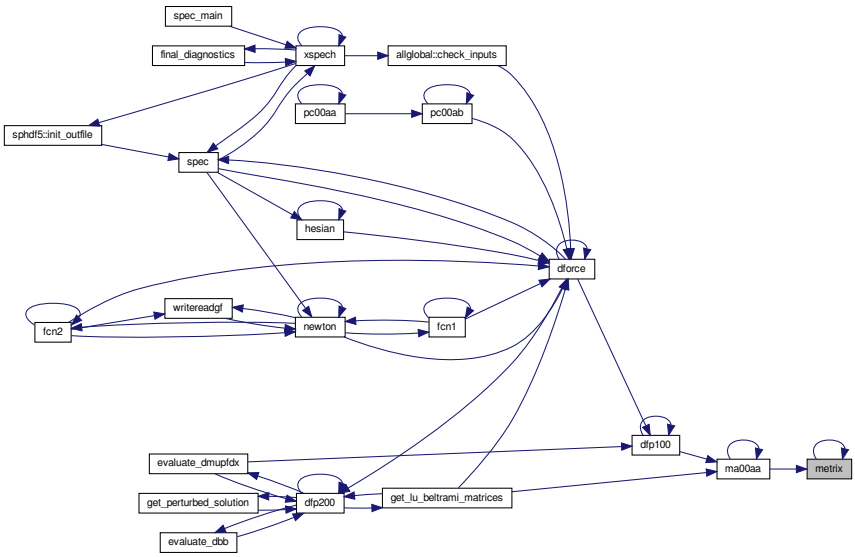
$$\begin{aligned}
\sqrt{g}\;g^{ss} &= \left(g_{\theta\theta}g_{\zeta\zeta} - g_{\theta\zeta}g_{\theta\zeta}\right)/\sqrt{g} \\
\sqrt{g}\;g^{s\theta} &= \left(g_{\theta\zeta}g_{s\zeta} - g_{s\theta}g_{\zeta\zeta}\right)/\sqrt{g} \\
\sqrt{g}\;g^{s\zeta} &= \left(g_{s\theta}g_{\theta\zeta} - g_{\theta\theta}g_{s\zeta}\right)/\sqrt{g} \\
\sqrt{g}\;g^{\theta\theta} &= \left(g_{\zeta\zeta}g_{ss} - g_{s\zeta}g_{s\zeta}\right)/\sqrt{g} \\
\sqrt{g}\;g^{\theta\zeta} &= \left(g_{s\zeta}g_{s\theta} - g_{\theta\zeta}g_{ss}\right)/\sqrt{g} \\
\sqrt{g}\;g^{\zeta\zeta} &= \left(g_{ss}g_{\theta\theta} - g_{s\theta}g_{s\theta}\right)/\sqrt{g}
\end{aligned} \tag{159}$$

FFTs

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

References allglobal::cfmn, allglobal::cpus, allglobal::dbdx, allglobal::efmn, allglobal::goomne, allglobal::goomno, allglobal::gssmne, allglobal::gssmno, allglobal::gstmne, allglobal::gstmno, allglobal::gszmne, allglobal::gszmno, allglobal::gttmne, allglobal::gttmno, allglobal::gtzmne, allglobal::gtzmno, allglobal::guvij, allglobal::guvijsave, allglobal::gvuij, allglobal::gzzmne, allglobal::gzzmno, allglobal::ijreal, allglobal::im, allglobal::ime, allglobal::in, allglobal::ine, metrix(), allglobal::mn, allglobal::mne, allglobal::myid, allglobal::ncpu, allglobal::nt, allglobal::ntz, allglobal::nz, allglobal::ofmn, constants::one, fileunits::ounit, allglobal::sfmn, allglobal::sg, numerical::small, and constants::zero.
Referenced by ma00aa(), and metrix().
Here is the call graph for this function:

Here is the caller graph for this function:



7.13 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

7.13.1 Detailed Description

7.13.2 Function/Subroutine Documentation

7.13.2.1 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,

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

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

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

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

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

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

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

  - if Lcoordinatesingularity=F and Lplasmaregion=T , then

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

  - if Lcoordinatesingularity=F and Lvacuumregion=T , then

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

  The quantities $\mathcal{B} \equiv$ dMB, $\mathcal{E} \equiv$ dME and $\mathcal{G} \equiv$ 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:

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

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

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

vacuum region

– For the vacuum region, the returned function is:

$$\mathbf{f}(\Delta\psi_t,\Delta\psi_p)\equiv\begin{cases}(\quad 0 \quad, & 0 &)^T, & \text{if } \texttt{Lconstraint} = -1\\ (\quad I-\texttt{curtor} \quad, & G-\texttt{curpol} &)^T, & \text{if } \texttt{Lconstraint} = 0\\ (\ \iota(-1)-\texttt{oita(lvol-1)}\ , & G-\texttt{curpol} &)^T, & \text{if } \texttt{Lconstraint} = 1\\ (\quad ? \quad, & ? &)^T, & \text{if } \texttt{Lconstraint} = 2\end{cases} \tag{167}$$

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

early termination

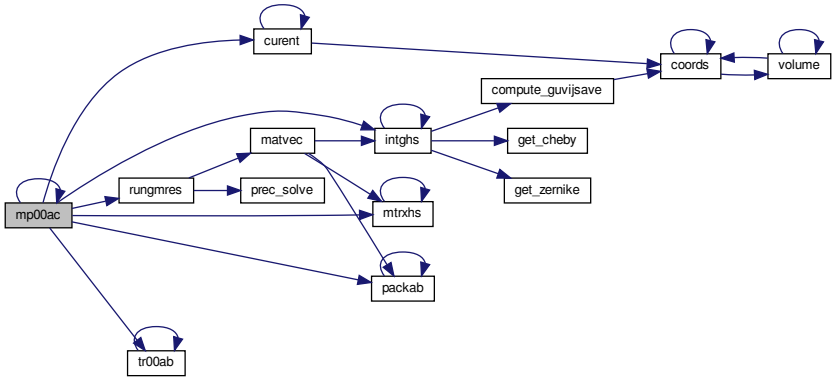
- If $|\mathbf{f}| < \texttt{mupftol}$, then early termination is enforced (i.e., `iflag` is set to a negative integer). (See ma02aa() for details of how mp00ac() is called iteratively.)

Parameters

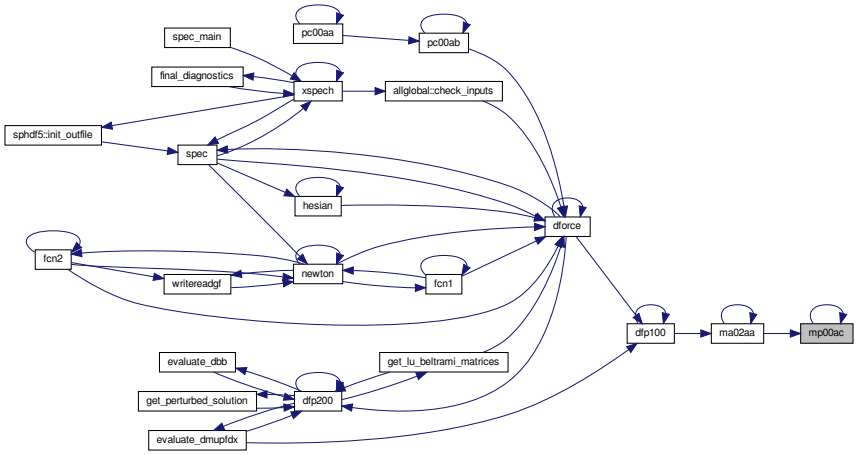
in	*Ndof*	
in	*Xdof*	
	Fdof	
	Ddof	
in	*Ldfjac*	
	iflag	indicates whether (i) iflag=1: "function" values are required; or (ii) iflag=2: "derivative" values are required

References allglobal::adotx, allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::cpus, curent(), inputlist::curpol, inputlist::curtor, allglobal::ddotx, allglobal::diotadxup, allglobal::ditgpdxtp, allglobal::dma, allglobal::dmas, allglobal::dmb, allglobal::dmd, allglobal::dmds, allglobal::dmg, allglobal::dpflux, allglobal::dtflux, inputlist::epsgmres, inputlist::epsilu, allglobal::gmreslastsolution, constants::half, inputlist::helicity, allglobal::idmas, allglobal::im, allglobal::imagneticok, allglobal::in, intghs(), inputlist::iota, allglobal::iquad, allglobal::ivol, allglobal::jdmas, allglobal::labintegral, allglobal::lbbintegral, inputlist::lconstraint, allglobal::lcoordinatesingularity, inputlist::lgmresprec, allglobal::liluprecond, inputlist::lmatsolver, allglobal::lplasmaregion, inputlist::lrad, allglobal::lvacuumregion, numerical::machprec, allglobal::mn, allglobal::mns, mp00ac(), allglobal::mpi_comm_spec, mtrxhs(), inputlist::mu, inputlist::mupftol, allglobal::myid, allglobal::nadof, allglobal::ncpu, allglobal::ndmas, allglobal::ndmasmax, inputlist::nitergmres, allglobal::notmatrixfree, allglobal::notstellsym, allglobal::nt, inputlist::ntor, allglobal::nz, inputlist::oita, constants::one, fileunits::ounit, packab(), rungmres(), numerical::small, allglobal::solution, tr00ab(), inputlist::wmacros, allglobal::xoffset, allglobal::yesstellsym, and constants::zero.

Referenced by ma02aa(), and mp00ac().
Here is the call graph for this function:



Here is the caller graph for this function:



7.14 Force-driver

Functions/Subroutines

- subroutine newton (NGdof, position, ihybrd)

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

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

  Objective to be given to the Newton solver, using only function values.
- subroutine fcn2 (NGdof, xx, fvec, fjac, Ldfjac, irevcm)

  Objective to be given to the Newton solver, using function values and derivatives.

7.14.1 Detailed Description

7.14.2 Function/Subroutine Documentation

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

logic, writing/reading from file

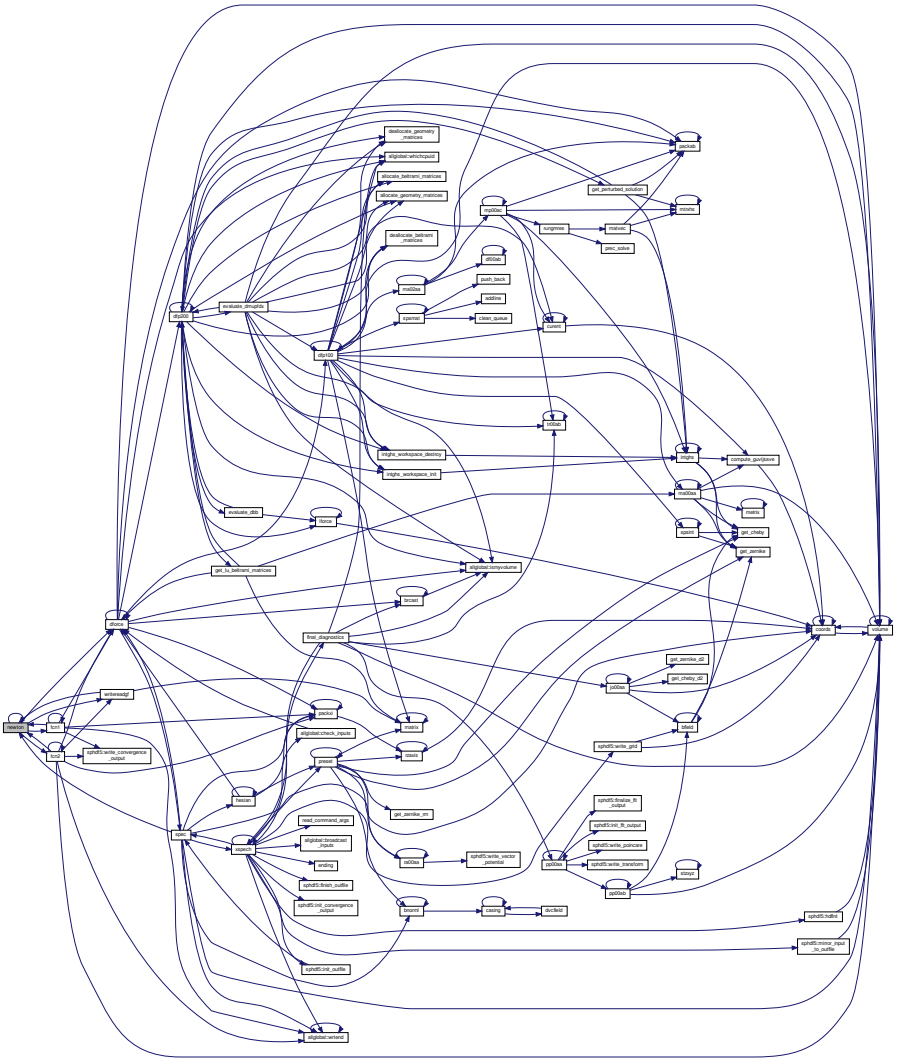
- Before proceeding with iterative search, dforce() is called to determine the magnitude of the initial force imbalance, and if this is less than forcetol then the iterative search will not be performed.
- As the iterations proceed, wrtend() will be called to save itermediate information (also see xspech()).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

Parameters

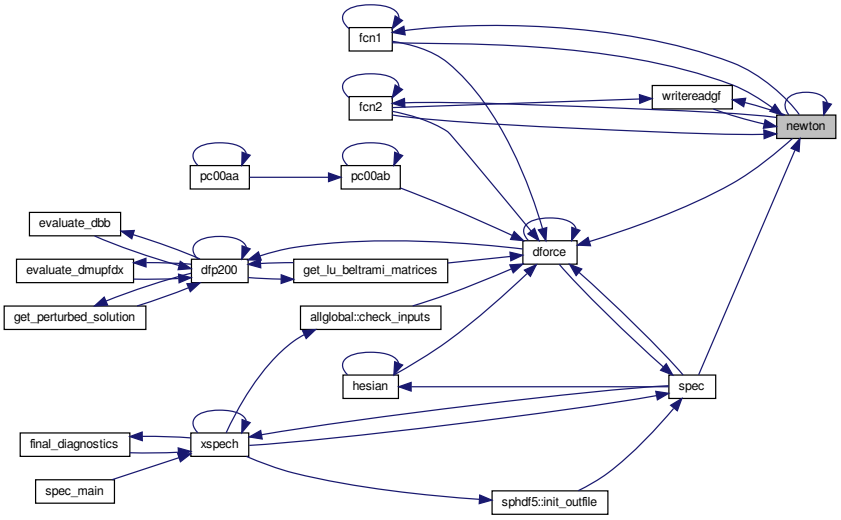
in	*NGdof*	
in,out	*position*	
out	*ihybrd*	

References allglobal::bbe, allglobal::bbo, inputlist::c05factor, inputlist::c05xmax, inputlist::c05xtol, allglobal::cpus, allglobal::dbbdmp, allglobal::dessian, allglobal::dffdrz, dforce(), allglobal::dmupfdx, allglobal::energy, fcn1(), fcn2(), allglobal::forceerr, inputlist::forcetol, allglobal::hessian, inputlist::igeometry, allglobal::iie, allglobal::iio, allglobal::im, allglobal::in, allglobal::irbc, allglobal::irbs, allglobal::izbc, allglobal::izbs, newtontime::lastcpu, inputlist::lcheck, inputlist::lfindzero, allglobal::lgdof, allglobal::lhessian2dallocated, allglobal::lhessian3dallocated, allglobal::lhessianallocated, allglobal::localconstraint, inputlist::lreadgf, allglobal::mn, allglobal::mpi_comm_spec, allglobal::myid, allglobal::ncpu, newtontime::ndcalls, newton(), newtontime::nfcalls, allglobal::nfreeboundaryiterations, allglobal::notstellsym, inputlist::nvol, constants::one, fileunits::ounit, numerical::sqrtmachprec, constants::ten, constants::two, inputlist::wmacros, writereadgf(), and constants::zero.
Referenced by fcn1(), fcn2(), newton(), spec(), and writereadgf().

Here is the call graph for this function:



Here is the caller graph for this function:



7.14.2.2 writereadgf() `subroutine writereadgf (`

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

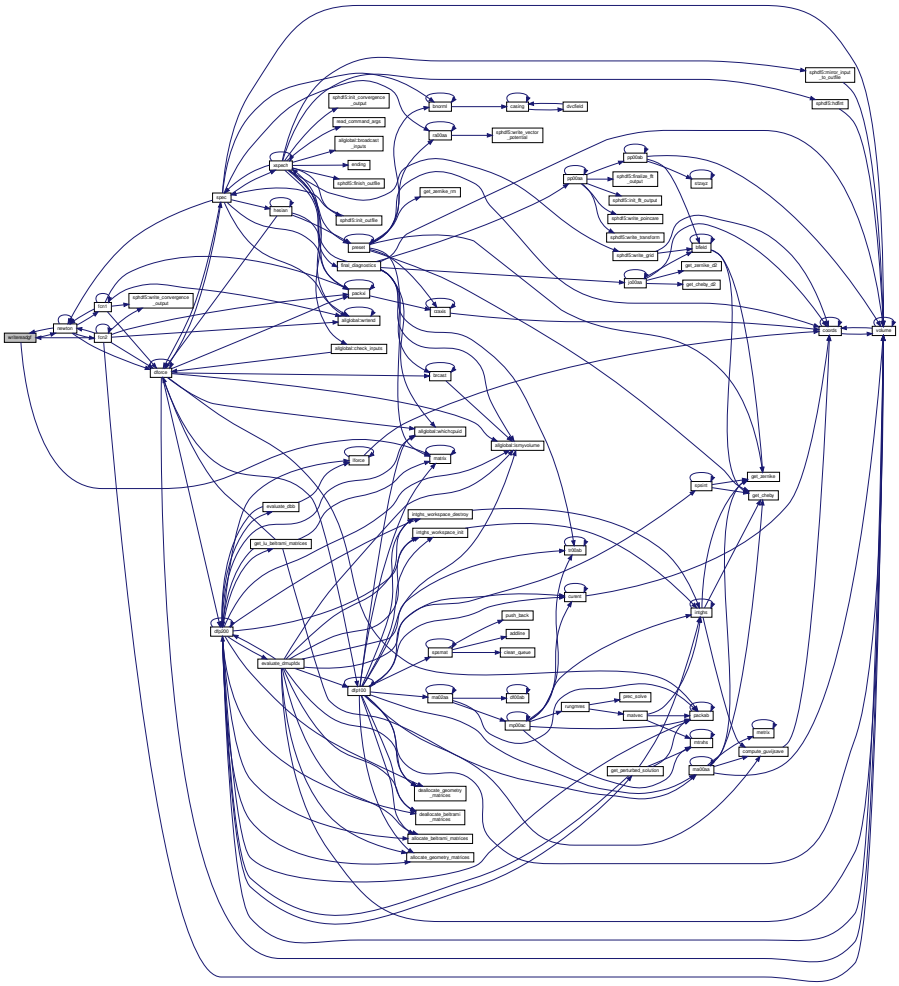
read or write force-derivative matrix

Parameters

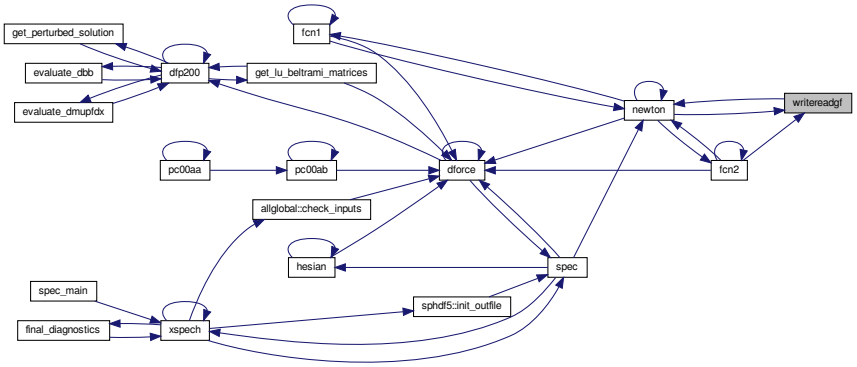
in	*readorwrite*	
in	*NGdof*	
out	*ireadhessian*	

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:



7.14.2.3 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 )
```

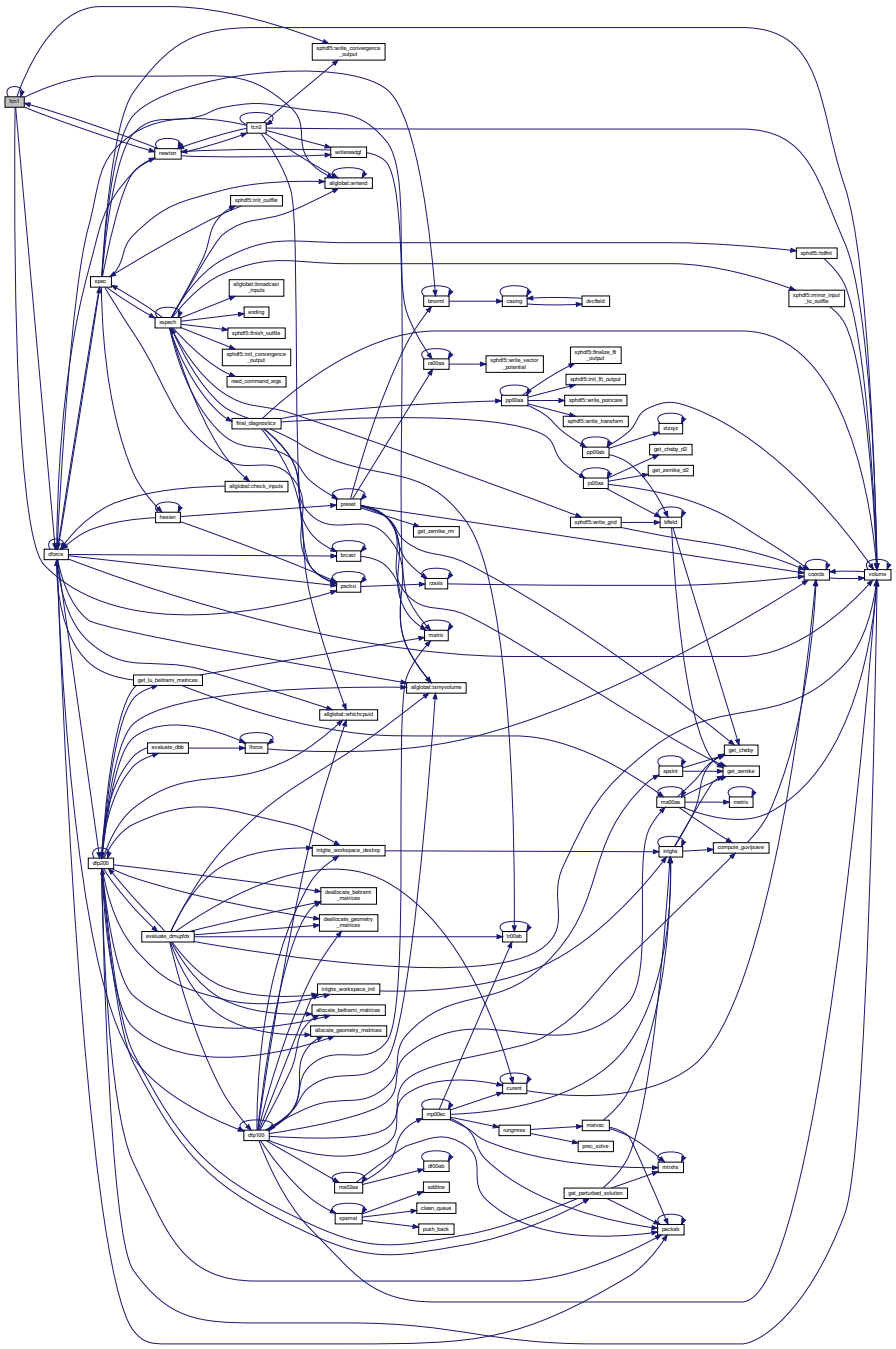
Objective to be given to the Newton solver, using only function values.

Parameters

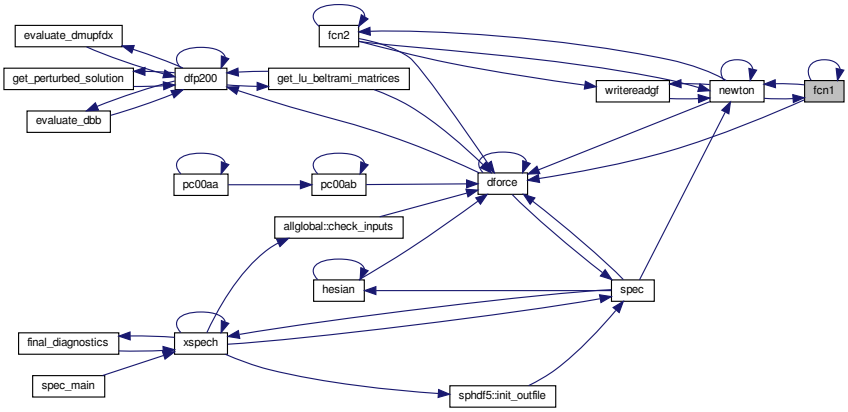
in	*NGdof*	
in	*xx*	
out	*fvec*	
in	*irevcm*	

References allglobal::bbe, allglobal::bbo, inputlist::c05factor, inputlist::c05xmax, inputlist::c05xtol, allglobal::cpus, allglobal::dbbdmp, allglobal::dessian, allglobal::dffdrz, dforce(), allglobal::dmupfdx, allglobal::energy, fcn1(), allglobal::forceerr, inputlist::forcetol, allglobal::hessian, inputlist::igeometry, allglobal::iie, allglobal::iio, allglobal::im, allglobal::in, allglobal::irbc, allglobal::irbs, allglobal::izbc, allglobal::izbs, newtontime::lastcpu, inputlist::lcheck, inputlist::lfindzero, allglobal::lgdof, allglobal::lhessianallocated, inputlist::lreadgf, allglobal::mn, allglobal::mpi_comm_spec, allglobal::myid, allglobal::ncpu, newtontime::ndcalls, newton(), newtontime::nfcalls, allglobal::nfreeboundaryiterations, allglobal::notstellsym, inputlist::nvol, constants::one, fileunits::ounit, packxi(), numerical::sqrtmachprec, constants::ten, constants::two, inputlist::wmacros, sphdf5::write_convergence_output(), allglobal::wrtend(), and constants::zero.
Referenced by fcn1(), and newton().

Here is the call graph for this function:



Here is the caller graph for this function:



7.14.2.4 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 )
```

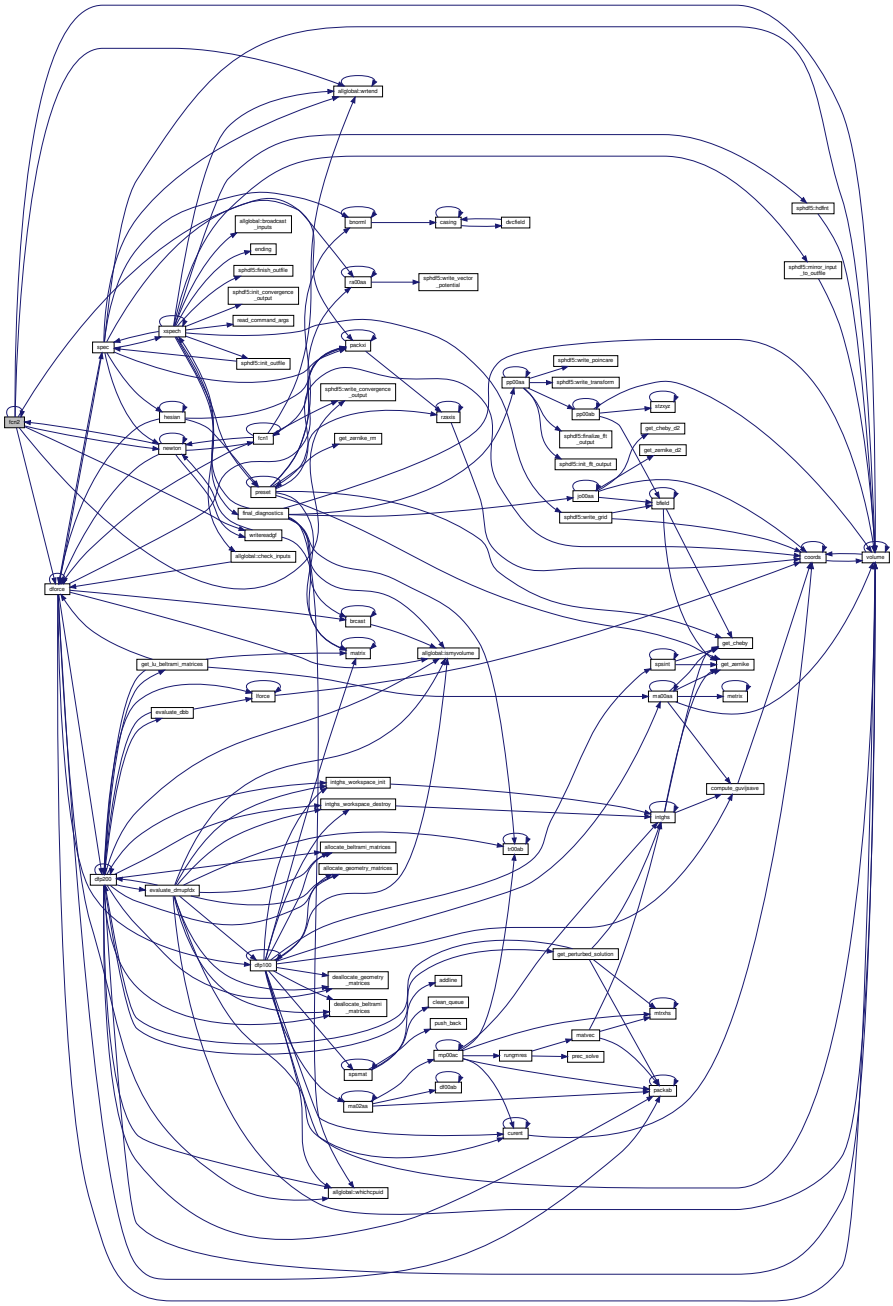
Objective to be given to the Newton solver, using function values and derivatives.

Parameters

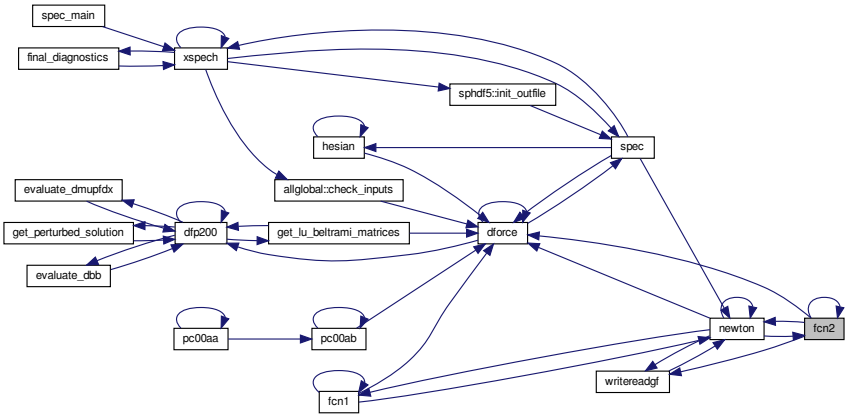
in	*NGdof*	
in	*xx*	
out	*fvec*	
out	*fjac*	
in	*Ldfjac*	
in	*irevcm*	indicator for reverse communication; provided by solver to tell this method what to compute

References allglobal::bbe, allglobal::bbo, inputlist::c05factor, inputlist::c05xmax, inputlist::c05xtol, allglobal::cpus, allglobal::dbbdmp, allglobal::dessian, allglobal::dffdrz, dforce(), allglobal::dmupfdx, allglobal::energy, fcn2(), allglobal::forceerr, inputlist::forcetol, allglobal::hessian, inputlist::igeometry, allglobal::iie, allglobal::iio, allglobal::im, allglobal::in, allglobal::irbc, allglobal::irbs, allglobal::izbc, allglobal::izbs, newtontime::lastcpu, inputlist::lcheck, inputlist::lfindzero, allglobal::lgdof, allglobal::lhessianallocated, inputlist::lreadgf, allglobal::mn, allglobal::mpi_comm_spec, allglobal::myid, allglobal::ncpu, newtontime::ndcalls, newton(), newtontime::nfcalls, allglobal::nfreeboundaryiterations, allglobal::notstellsym, inputlist::nvol, 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 fcn2(), and newton().

Here is the call graph for this function:



Here is the caller graph for this function:



7.15 "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.

7.15.1 Detailed Description

7.15.2 Function/Subroutine Documentation

7.15.2.1 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:

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

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

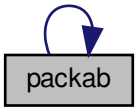
Parameters

packorunpack	

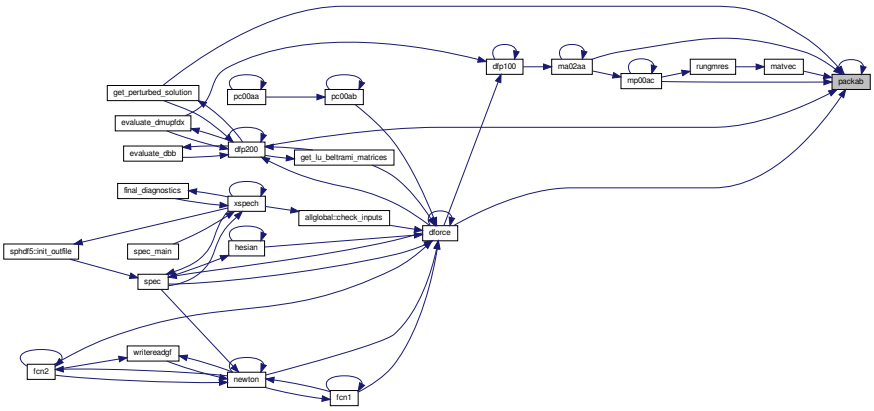
Parameters

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, packab(), numerical::small, allglobal::tt, allglobal::yesstellsym, and constants::zero.
Referenced by dforce(), dfp200(), get_perturbed_solution(), ma02aa(), matvec(), mp00ac(), and packab().
Here is the call graph for this function:



Here is the caller graph for this function:



7.15.2.2 packxi() `subroutine packxi (`

```
integer, intent(in) NGdof,
real, dimension(0:ngdof) position,
integer, intent(in) Mvol,
integer, intent(in) mn,
real, dimension(1:mn,0:mvol) iRbc,
real, dimension(1:mn,0:mvol) 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:

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

  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,

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

  where $L(\zeta) \equiv \int_0^{2\pi} dl$ and $dl \equiv \sqrt{\partial_\theta R_1(\theta,\zeta)^2 + \partial_\theta Z_1(\theta,\zeta)^2}\, d\theta$.
- Note that if dl does not depend on 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.

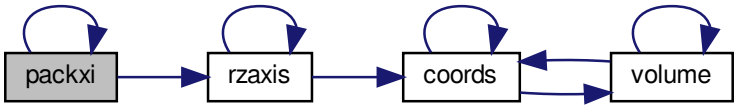
some numerical comments

- 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.

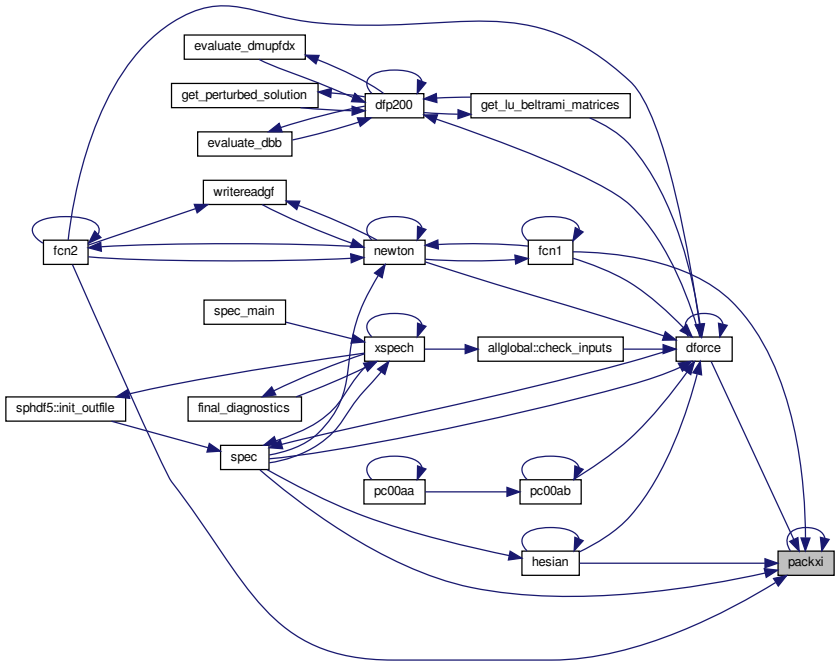
Parameters

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, packxi(), allglobal::psifactor, allglobal::rscale, rzaxis(), allglobal::sfmn, allglobal::simn, allglobal::trij, allglobal::tzij, allglobal::yesstellsym, and constants::zero.
Referenced by dforce(), fcn1(), fcn2(), hesian(), packxi(), and spec().
Here is the call graph for this function:



Here is the caller graph for this function:



7.16 Conjugate-Gradient method

Functions/Subroutines

- subroutine pc00aa (NGdof, position, Nvol, mn, ie04dgf)

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

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

7.16.1 Detailed Description

7.16.2 Function/Subroutine Documentation

7.16.2.1 pc00aa()

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

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

energy functional

The energy functional is described in pc00ab() .

relevant input variables

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

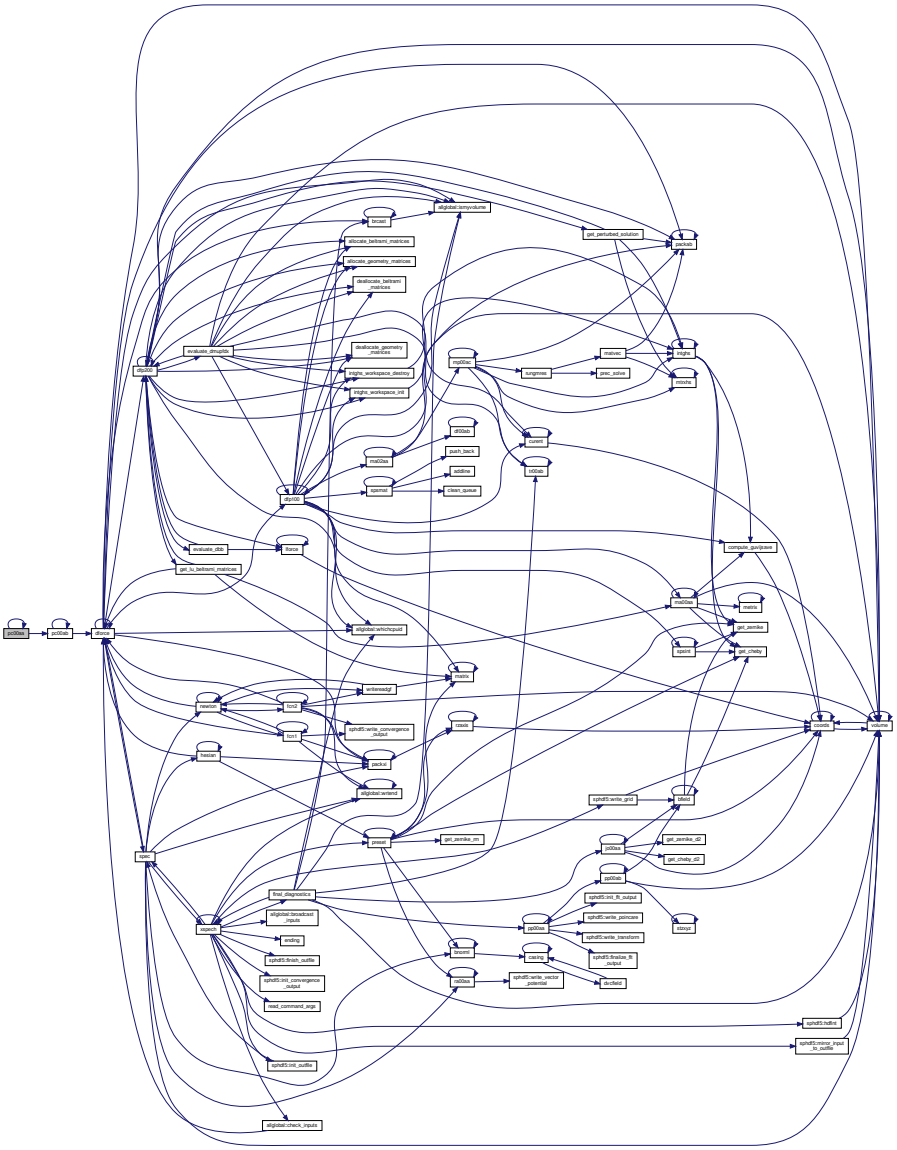
Parameters

in	*NGdof*	
in,out	*position*	
in	*Nvol*	
in	*mn*	
	ie04dgf	

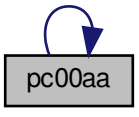
References allglobal::cpus, allglobal::energy, allglobal::forceerr, inputlist::forcetol, allglobal::myid, allglobal::ncpu, fileunits::ounit, pc00aa(), pc00ab(), constants::ten, and constants::zero.

Referenced by pc00aa().

Here is the call graph for this function:



Here is the caller graph for this function:



7.16.2.2 pc00ab() `subroutine pc00ab (`

```
integer mode,
```

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

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

Energy functional

- The energy functional is

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

  where $N \equiv$ `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, ι, 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

$$\begin{aligned} \frac{\partial R_j}{\partial t} &\equiv -\frac{\partial}{\partial R_j} \sum_{l=1}^{N} \int \left(\frac{p}{\gamma - 1} + \frac{B^2}{2} \right) dv, \\ \frac{\partial Z_j}{\partial t} &\equiv -\frac{\partial}{\partial Z_j} \sum_{l=1}^{N} \int \left(\frac{p}{\gamma - 1} + \frac{B^2}{2} \right) dv. \end{aligned} \tag{172}$$

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

Spectral energy minimization

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

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

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

  where u is a angle variation.

- The corresponding variation in each of the Fourier harmonics is

$$\delta R_j \equiv \oint\oint d\theta d\zeta \;\; R_\theta \; u \; \cos\alpha_j, \tag{175}$$

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

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

$$M \equiv \frac{\sum_j (m_j^p + n_j^q)(R_{l,j}^2 + Z_{l,j}^2)}{\sum_j (R_{l,j}^2 + Z_{l,j}^2)}, \tag{177}$$

- Using the notation

$$N \equiv \sum_j \lambda_j (R_{l,j}^2 + Z_{l,j}^2), \tag{178}$$

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

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

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

- For tangential variations,

$$\delta N = 2 \oint\oint d\theta d\zeta \quad u \left(R_\theta \sum_j \lambda_j R_j \cos\alpha_j + Z_\theta \sum_j \lambda_j Z_j \sin\alpha_j \right), \tag{181}$$

$$\delta D = 2 \oint\oint d\theta d\zeta \quad u \left(R_\theta \sum_j R_j \cos\alpha_j + Z_\theta \sum_j Z_j \sin\alpha_j \right). \tag{182}$$

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

$$\frac{\partial u}{\partial t} = -\left[R_\theta \sum_j (\lambda_j - M) R_j \cos\alpha_j / D + Z_\theta \sum_j (\lambda_j - M) Z_j \sin\alpha_j / D \right]. \tag{183}$$

- This suggests that position should be advanced according to

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

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

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

numerical implementation

- The spectral condensation terms,

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

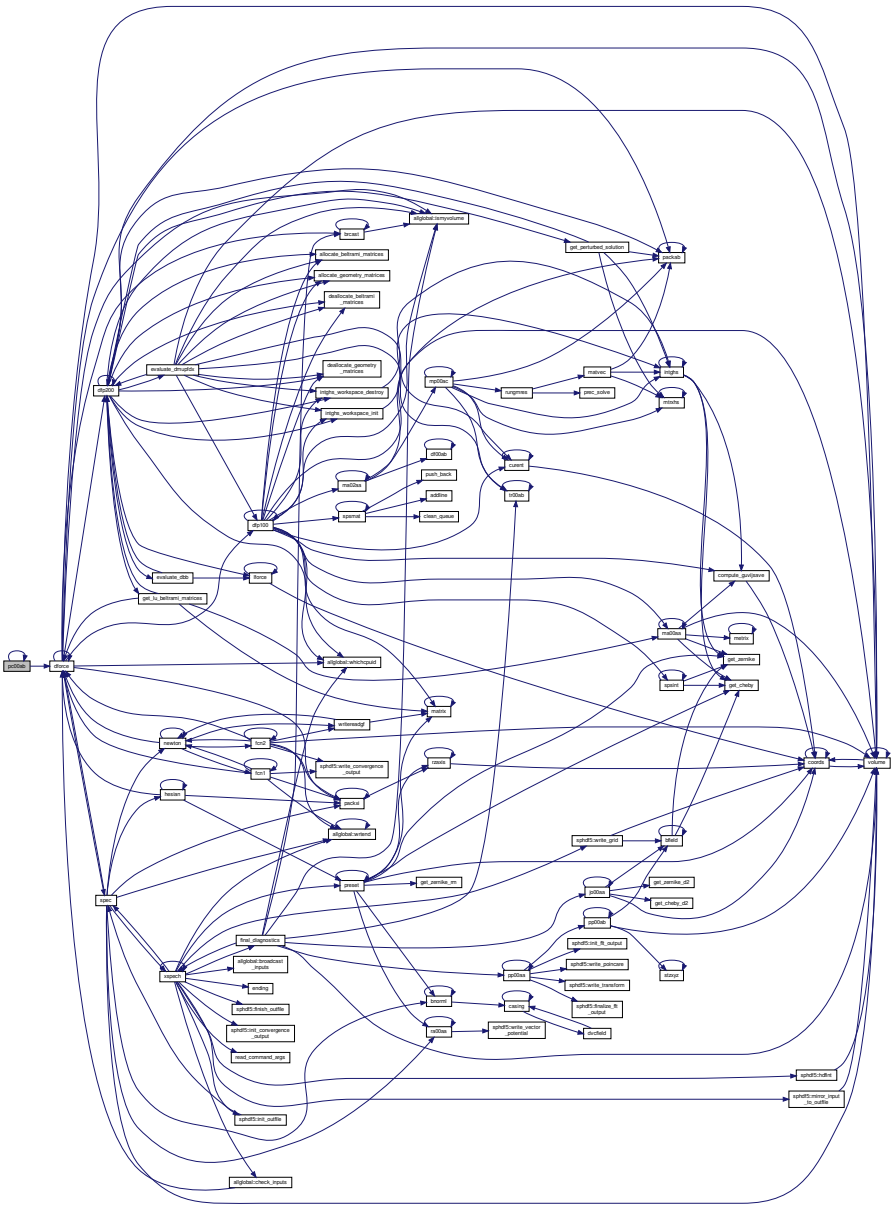
$$Z_\theta (R_\theta X + Z_\theta Y) = \sum_{j,k,l} m_j m_k (\lambda_l - M) Z_j (-R_k R_l \cos\alpha_j \sin\alpha_k \cos\alpha_l + Z_k Z_l \cos\alpha_j \cos\alpha_k \sin\alpha_l) \tag{187}$$

are calculated using triple angle expressions...

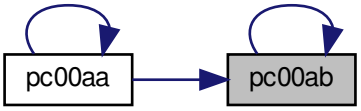
Todo IT IS VERY LIKELY THAT FFTs WOULD BE FASTER!!!

References allglobal::cpus, allglobal::dbbdrz, dforce(), allglobal::diidrz, inputlist::epsilon, allglobal::forceerr, inputlist::forcetol, constants::half, inputlist::igeometry, allglobal::lbbintegral, allglobal::mn, allglobal::myid, inputlist::nvol, constants::one, fileunits::ounit, pc00ab(), allglobal::yesstellsym, and constants::zero.
Referenced by pc00aa(), and pc00ab().

Here is the call graph for this function:



Here is the caller graph for this function:



7.17 Initialization of the code

Functions/Subroutines

- subroutine preset

  Allocates and initializes internal arrays.

7.17.1 Detailed Description

7.17.2 Function/Subroutine Documentation

7.17.2.1 preset() `subroutine preset`

Allocates and initializes internal arrays.

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

- `LGdof` ≡ the number of degrees-of-freedom in the geometry (i.e. Fourier harmonics) of each interface
- `NGdof` ≡ 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

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

  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

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

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

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

- `TT(0:Lrad,0:1,0:1)` gives the Chebyshev polynomials, and their first derivative, evaluated at $s = -1$ 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

$$T_l(-1) = \begin{cases} +1, & \text{if } l \text{ is even}, \\ -1, & \text{if } l \text{ is odd}; \end{cases} \qquad T_l(+1) = \begin{cases} +1, & \text{if } l \text{ is even}, \\ +1, & \text{if } l \text{ is odd}; \end{cases} \tag{190}$$

$$T_l'(-1) = \begin{cases} -l^2, & \text{if } l \text{ is even}, \\ +l^2, & \text{if } l \text{ is odd}; \end{cases} \qquad T_l'(+1) = \begin{cases} +l^2, & \text{if } l \text{ is even}, \\ +l^2, & \text{if } l \text{ is odd}. \end{cases} \tag{191}$$

- `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,

$$\sum_i f_i \cos(m_i\theta - n_i\zeta) \equiv \sum_{n=0}^{N_0} f_{0,n}\cos(-n\zeta) + \sum_{m=1}^{M_0}\sum_{n=-N_0}^{N_0} f_{m,n}\cos(m\theta - n\zeta), \tag{192}$$

  and the same representation but with enhanced resolution,

$$\sum_k \bar{f}_k \cos(\bar{m}_k\theta - \bar{n}_k\zeta) \equiv \sum_{n=0}^{N_1} f_{0,n}\cos(-n\zeta) + \sum_{m=1}^{M_1}\sum_{n=-N_1}^{N_1} f_{m,n}\cos(m\theta - n\zeta), \tag{193}$$

  with $M_1 \geq M_0$ and $N_1 \geq N_0$; then $k_i \equiv$ `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 $\bar{g}^{\mu\nu} = \sum_k \bar{g}^{\mu\nu}_k \cos\alpha_k$ for $\alpha_k \equiv m_k\theta - n_k\zeta$,

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

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

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

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

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

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

djkp
iotakki
cheby(0:Lrad,0:2): Chebyshev polynomial workspace

- `cheby(0:Lrad,0:2)` is global workspace for computing the Chebyshev polynomials, and their derivatives, using the recurrence relations $T_0(s) = 1, T_1(s) = s$ and $T_l(s) = 2\,s\,T_{l-1}(s) - T_{l-2}(s)$.
- 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.

lquad, gaussianweight, gaussianabscissae: Gauss-Legendre quadrature

- The volume integrals are computed using a "Fourier" integration over the angles and by Gauss-Legendre quadrature over the radial, i.e. $\int f(s)ds = \sum_k \omega_k f(s_k)$.
- The quadrature resolution in each volume is give by `Iquad(1:Mvol)` which is determined as follows:
  - if `Nquad.gt.0` , then `Iquad(vvol)=Nquad`
  - if `Nquad.le.0` and .not.Lcoordinatesingularity , then `Iquad(vvol)=2*Lrad`(vvol)-Nquad
  - if `Nquad.le.0` and `Lcoordinatesingularity` , then `Iquad(vvol)=2*Lrad`(vvol)-Nquad+Mpol
- The Gaussian weights and abscissae are given by `gaussianweight(1:maxIquad,1:Mvol)` and `gaussianabscissae(1:maxIquad,1:Mvol)`, which are computed using modified Numerical Recipes routine gauleg() .
- `Iquad` $_v$ is passed through to ma00aa() to compute the volume integrals of the metric elements; also see jo00aa(), where `Iquad` $_v$ is used to compute the volume integrals of $||\nabla \times \mathbf{B} - \mu\mathbf{B}||$.

LBsequad, LBnewton and LBlinear

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

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

- weight on force-imbalance harmonics;

$$\texttt{BBweight}_i \equiv \texttt{opsilon} \times \exp\left[-\texttt{escale} \times (m_i^2 + n_i^2)\right] \tag{198}$$

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

mmpp(1:mn): spectral condensation weight factors

- spectral condensation weight factors;

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

  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

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

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

  where $\overline{T}_{l,i}(s) \equiv \bar{s}^{m_i/2}\, T_l(s)$, $T_l(s)$ 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

$$A_{\theta,e,i,l} \equiv \texttt{Ate(v,0,j)\%s(l)}, \tag{202}$$
$$A_{\zeta,e,i,l} \equiv \texttt{Aze(v,0,j)\%s(l)}, \tag{203}$$
$$A_{\theta,o,i,l} \equiv \texttt{Ato(v,0,j)\%s(l)}, \text{and} \tag{204}$$
$$A_{\zeta,o,i,l} \equiv \texttt{Azo(v,0,j)\%s(l)}; \tag{205}$$

  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

$$\texttt{cosi}_{j,i} = \cos(m_i\theta_j - n_i\zeta_j), \tag{206}$$
$$\texttt{sini}_{j,i} = \sin(m_i\theta_j - n_i\zeta_j). \tag{207}$$

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

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

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

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

- `psifactor` is used in packxi(), dforce() and hesian().

- `inifactor` is similarly constructed, with

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

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

Bsupumn and Bsupvmn
diotadxup and glambda: transformation to straight fieldline angle

- Given the Beltrami fields in any volume, the rotational-transform on the adjacent interfaces may be determined (in tr00ab()) by constructing the straight fieldline angle on the interfaces.

- The rotational transform on the inner or outer interface of a given volume depends on the magnetic field in that volume, i.e. $\iota_\pm = \iota(\mathbf{B}_\pm)$, so that

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

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

$$\delta\mathbf{B}_\pm = \frac{\partial \mathbf{B}_\pm}{\partial x_j}\delta x_j + \frac{\partial \mathbf{B}_\pm}{\partial \mu}\delta\mu + \frac{\partial \mathbf{B}_\pm}{\partial \Delta\psi_p}\delta\Delta\psi_p. \tag{211}$$

- 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. $\frac{\partial \iota_\pm}{\partial x_j}$,
    - `0` : the rotational-transform itself,
    - `1`,2 : the derivatives with respec to μ and $\Delta\psi_p$, i.e. $\frac{\partial \iota_\pm}{\partial \mu}$ and $\frac{\partial \iota_\pm}{\partial \Delta\psi_p}$;
  - The third index labels volume.
- The values of `diotadxup` are assigned in mp00aa() after calling tr00ab().

vvolume, lBBintegral and lABintegral

- volume integrals

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

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

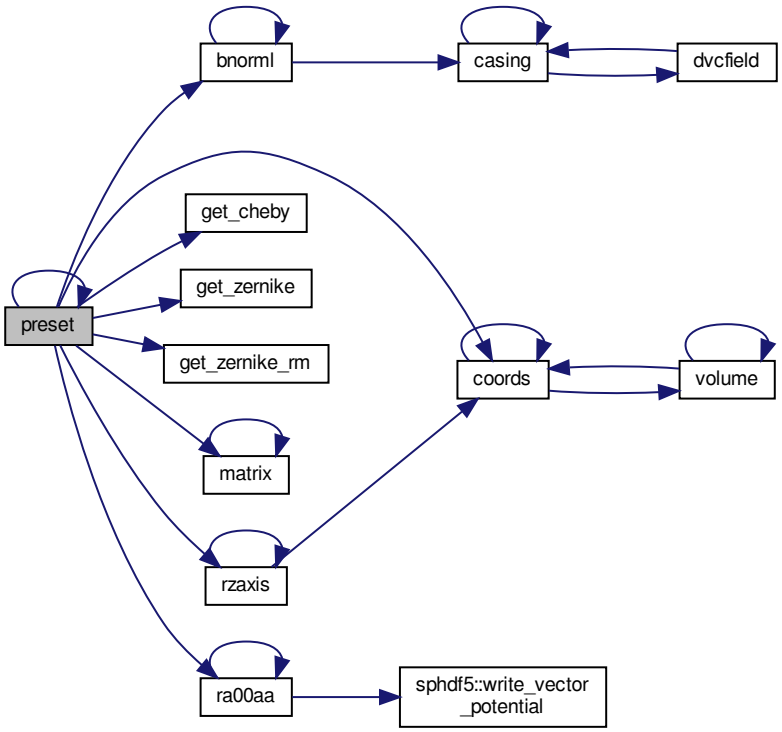
$$\texttt{lABintegral(i)} = \int_{\mathcal{V}_i} \mathbf{A}\cdot\mathbf{B}\, dv \tag{214}$$

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, allglobal::gaussianabscissae, allglobal::gaussianweight, get_cheby(), get_zernike(), get_zernike_rm(), allglobal::glambda, allglobal::gmreslastsolution, constants::goldenmean, 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, constants::half, allglobal::halfmm, inputlist::helicity, allglobal::hnt, allglobal::hnz, allglobal::ibnc, allglobal::ibns, allglobal::iemn, inputlist::igeometry, allglobal::iie, allglobal::iio, allglobal::ijimag, allglobal::ijreal, allglobal::im, allglobal::imagneticok, allglobal::ime, inputlist::impol, allglobal::ims, allglobal::in, allglobal::ine, allglobal::inifactor, allglobal::ins, inputlist::intor, allglobal::iomn, inputlist::iota, allglobal::iotakadd, allglobal::iotakkii, allglobal::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,

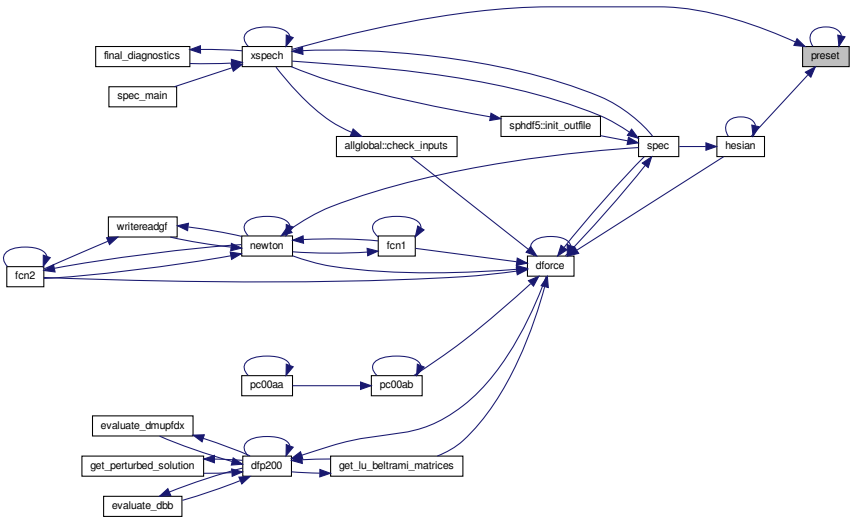
inputlist::lmatsolver, allglobal::lmavalue, allglobal::lmb, allglobal::lmbvalue, allglobal::lmc, allglobal::lmcvalue, allglobal::lmd, allglobal::lmdvalue, allglobal::lme, allglobal::lmevalue, allglobal::lmf, allglobal::lmfvalue, allglobal::lmg, allglobal::lmgvalue, allglobal::lmh, allglobal::lmhvalue, 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, constants::pi2, inputlist::pl, fftw_interface::planb, fftw_interface::planf, allglobal::pomn, inputlist::pr, preset(), allglobal::psifactor, inputlist::ql, inputlist::qr, constants::quart, 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, 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(), preset(), and xspech().

Here is the call graph for this function:



Here is the caller graph for this function:



7.18 Output file(s)

Modules

- module sphdf5

  writing the HDF5 output file

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.

7.18.1 Detailed Description

7.18.2 Function/Subroutine Documentation

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

Writes vector potential to .ext.sp.A .
representation of vector potential

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

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

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

  where $\overline{T}_{l,i}(s) \equiv \bar{s}^{m_i/2}\, T_l(s)$, $T_l(s)$ 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:

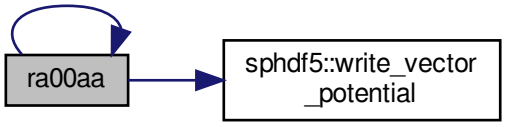
```
open(aunit, file="."//trim(ext)//".sp.A", status="replace", form="unformatted" )
write(aunit) mvol, mpol, ntor, mn, nfp ! integers;
write(aunit) im(1:mn) ! integers; poloidal modes;
write(aunit) in(1:mn) ! integers; toroidal modes;
do vvol = 1, mvol ! integers; loop over volumes;
write(aunit) lrad(vvol) ! 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

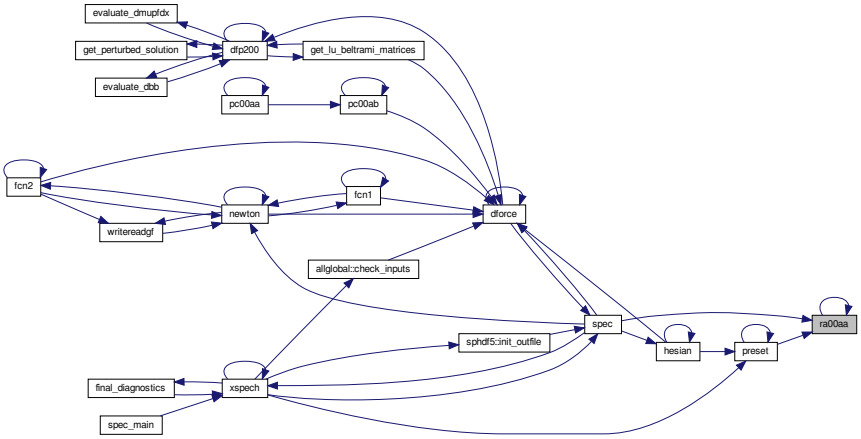
in	*writeorread*	'W' to write the vector potential; 'R' to read it

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, ra00aa(), inputlist::wmacros, sphdf5::write_vector_potential(), and constants::zero.
Referenced by preset(), ra00aa(), and spec().

Here is the call graph for this function:



Here is the caller graph for this function:



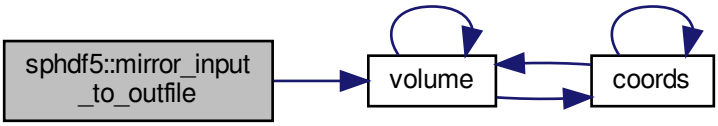
7.18.2.2 mirror_input_to_outfile() `subroutine sphdf5::mirror_input_to_outfile`

Mirror input variables into output file.

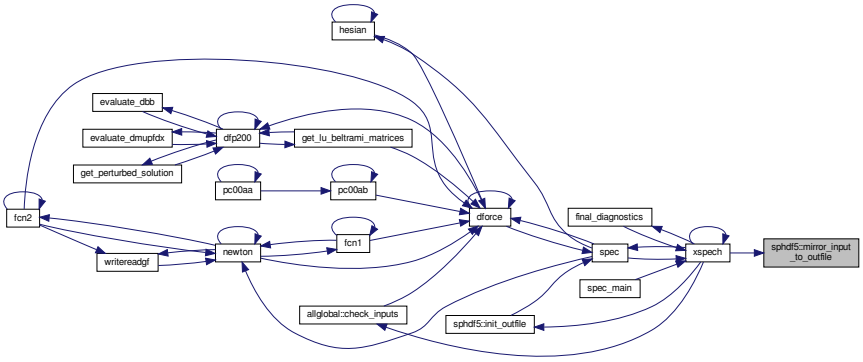
The goal of this routine is to have an exact copy of the input file contents that were used to parameterize a given SPEC run. This also serves to check after the run if SPEC correctly understood the text-based input file.

References inputlist::absacc, inputlist::absreq, inputlist::adiabatic, inputlist::bnc, inputlist::bns, inputlist::bnsblend, inputlist::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, allglobal::in, 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::ltransform, inputlist::lzerovac, inputlist::maxrndgues, inputlist::mcasingcal, inputlist::mfreeits, inputlist::mpol, inputlist::mregular, inputlist::mu, inputlist::mupfits, inputlist::mupftol, allglobal::myid, 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:



7.18.2.3 init_convergence_output() `subroutine sphdf5::init_convergence_output`

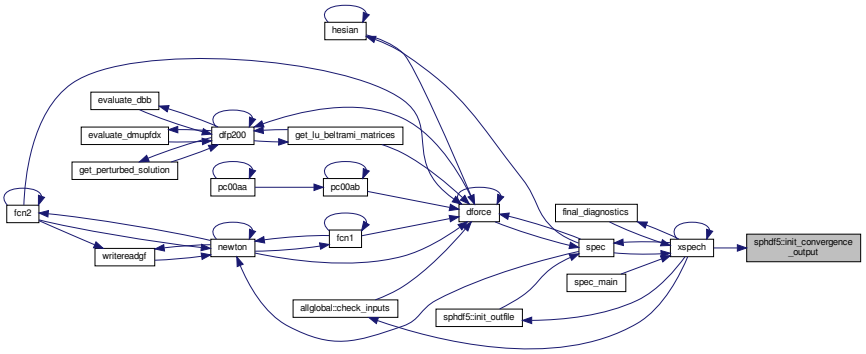
Prepare convergence evolution output.

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

```
DATATYPE  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, allglobal::myid, and sphdf5::plist_id.
Referenced by xspech().

Here is the caller graph for this function:



7.18.2.4 write_grid() `subroutine sphdf5::write_grid`

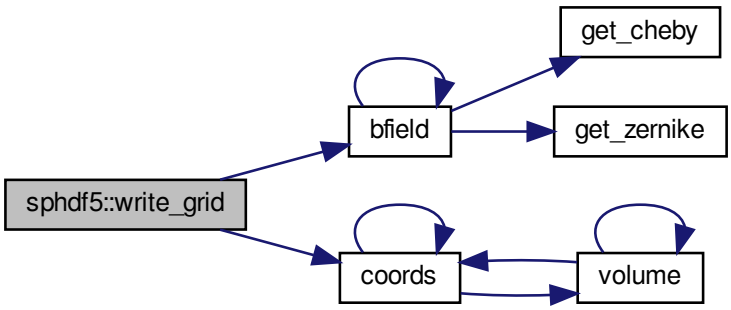
Write the magnetic field on a grid.

The magnetic field is evaluated on a regular grid in (s, 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.

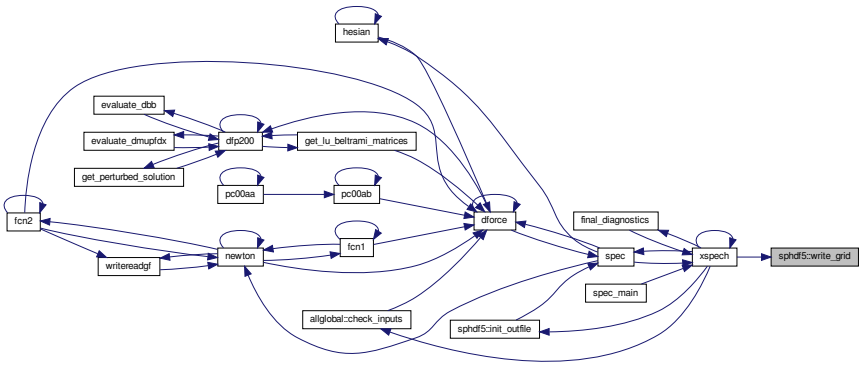
References bfield(), coords(), sphdf5::file_id, allglobal::gbzeta, inputlist::igeometry, allglobal::ijimag, allglobal::ijreal, allglobal::ivol, allglobal::jireal, allglobal::lcoordinatesingularity, allglobal::lplasmaregion, inputlist::lrad, allglobal::lvacuumregion, allglobal::mn, allglobal::myid, inputlist::ngrid,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



7.18.2.5 init_flt_output()

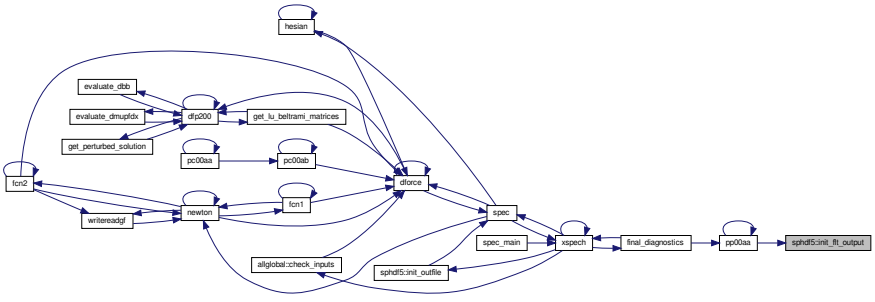
`subroutine sphdf5::init_flt_output (`
`integer, intent(in)` *numTrajTotal*)

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, allglobal::lmns, sphdf5::memspace_diotadxup, sphdf5::memspace_r, sphdf5::memspace_s, sphdf5::memspace_success, sphdf5::memspace_t, sphdf5::memspace_z, allglobal::myid, inputlist::nppts, allglobal::nz, sphdf5::rankp, and sphdf5::rankt.
Referenced by pp00aa().
Here is the caller graph for this function:



7.18.2.6 write_poincare()

`subroutine sphdf5::write_poincare (`
`integer, intent(in)` *offset,*

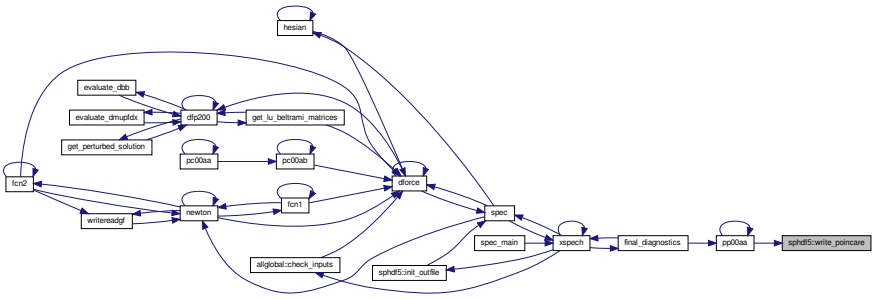
```
real, dimension(:,:,:), intent(in) data,
integer, dimension(:), intent(in) success )
```

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, allglobal::myid, inputlist::nppts, and allglobal::nz.
Referenced by pp00aa().
Here is the caller graph for this function:



7.18.2.7 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 )
```

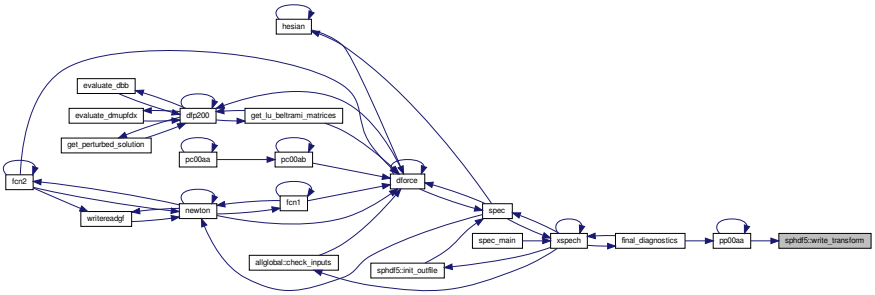
Write the rotational transform output from field line following.

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:



7.18.2.8 finalize_flt_output() `subroutine sphdf5::finalize_flt_output`

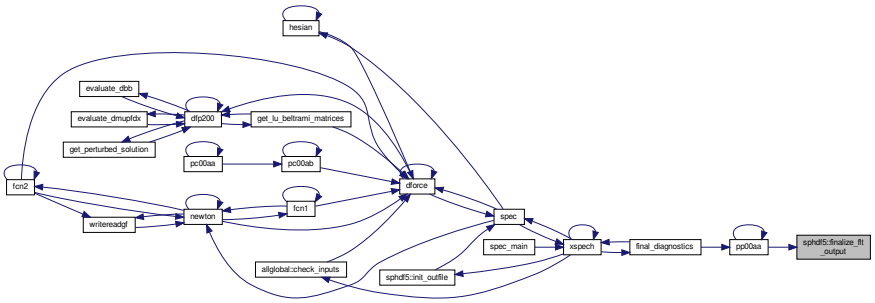
Finalize Poincare output.

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

References sphdf5::dset_id_diotadxup, sphdf5::dset_id_fiota, sphdf5::dset_id_r, sphdf5::dset_id_s, sphdf5::dset_id_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:



7.18.2.9 write_vector_potential() `subroutine sphdf5::write_vector_potential (`

```
integer, intent(in) sumLrad,
real, dimension(:,:), intent(in) allAte,
real, dimension(:,:), intent(in) allAze,
real, dimension(:,:), intent(in) allAto,
real, dimension(:,:), intent(in) allAzo )
```

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

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

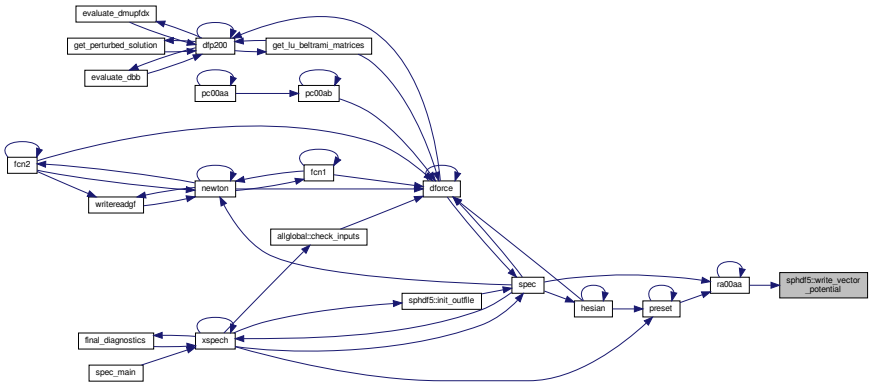
Parameters

sumLrad	total sum over `Lrad` in all nested volumes

Parameters

allAte	$A^{\theta}_{\mathrm{even}}$ for all nested volumes
allAze	$A^{\zeta}_{\mathrm{even}}$ for all nested volumes
allAto	$A^{\theta}_{\mathrm{odd}}$ for all nested volumes
allAzo	A^{ζ}_{odd} for all nested volumes

References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, sphdf5::file_id, allglobal::mn, and allglobal::myid.
Referenced by ra00aa().
Here is the caller graph for this function:



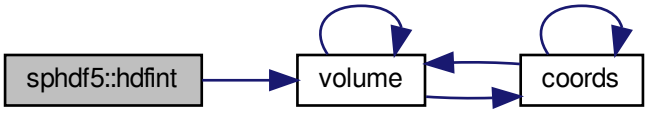
7.18.2.10 hdfint() `subroutine sphdf5::hdfint`

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

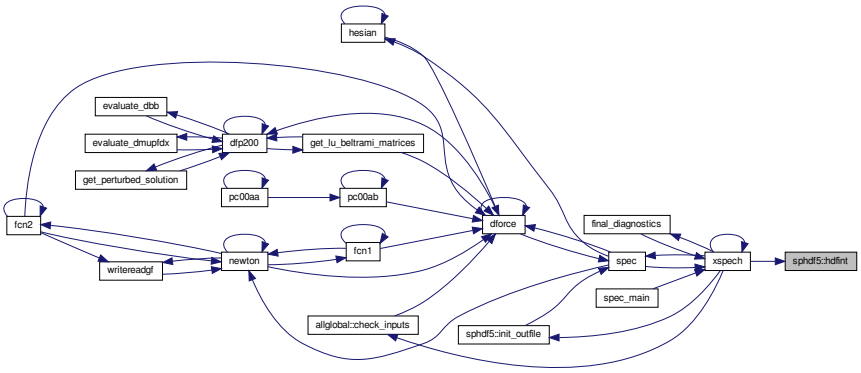
- In addition to the input variables, which are described in global(), the following quantities are written to `ext.↩ sp.h5`:
- All quantities marked as real should be treated as double precision.

References inputlist::adiabatic, allglobal::beltramierror, inputlist::bnc, inputlist::bns, allglobal::bsupumn, allglobal::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::ims, allglobal::in, allglobal::ins, allglobal::irbc, allglobal::irbs, allglobal::ivnc, allglobal::ivns, inputlist::ivolume, allglobal::izbc, allglobal::izbs, inputlist::lcheck, allglobal::lmns, inputlist::lperturbed, inputlist::lrad, allglobal::mn, allglobal::mns, inputlist::mu, allglobal::myid, 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:



7.19 Coordinate axis

Functions/Subroutines

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

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

7.19.1 Detailed Description

7.19.2 Function/Subroutine Documentation

7.19.2.1 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,

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

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

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

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

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

$$\frac{\partial R_0}{\partial Z^s_{i,j}} = \int \left(+\Delta R_i Z_{i,\theta}\, m_j \cos\alpha_j / \dot{l}\right) d\theta/L \tag{221}$$

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

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

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

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

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

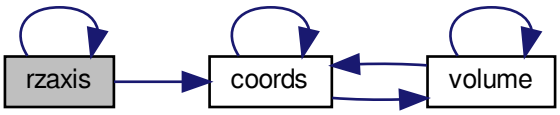
some numerical comments

- First, the differential poloidal length, $\dot{l} \equiv \sqrt{R_\theta^2 + Z_\theta^2}$, is computed in real space using an inverse FFT from the Fourier harmonics of R and Z.
- Second, the Fourier harmonics of dl are computed using an FFT. The integration over 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.

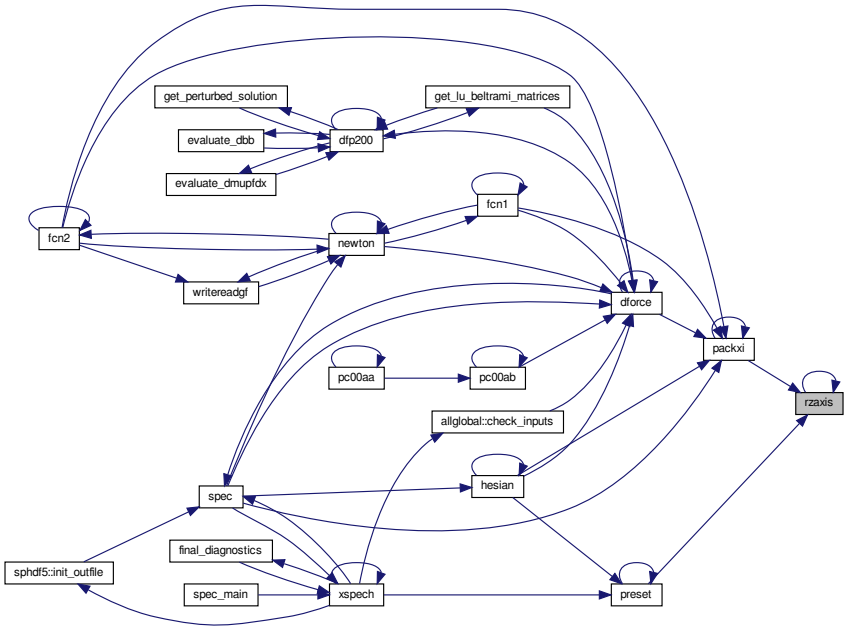
Parameters

in	*Mvol*	
in	*mn*	
	inRbc	
	inZbs	
	inRbs	
	inZbc	
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, 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::lfreebound, inputlist::linitialize, 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, rzaxis(), allglobal::sfmn, allglobal::sg, allglobal::simn, allglobal::sini, constants::two, numerical::vsmall, inputlist::wmacros, allglobal::yesstellsym, constants::zero, and allglobal::zij.
Referenced by packxi(), preset(), and rzaxis().
Here is the call graph for this function:



Here is the caller graph for this function:



7.20 Rotational Transform

Functions/Subroutines

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

  Calculates rotational transform given an arbitrary tangential field.

7.20.1 Detailed Description

7.20.2 Function/Subroutine Documentation

7.20.2.1 tr00ab()

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

Calculates rotational transform given an arbitrary tangential field.
Calculates transform, $\iota = \dot{\theta}(1+\lambda_\theta) + \lambda_\zeta$, given $\mathbf{B}|_{\mathcal{I}}$.
constructing straight field line angle on interfaces

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

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

  and insisting that

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

where ι is a constant that is to be determined.

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

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

- Expanding this equation we obtain

$$\begin{aligned} & \left(A'_{\theta,e,k} \cos\alpha_k + A'_{\theta,o,k} \sin\alpha_k\right) \, \iota \\ + & \left(A'_{\zeta,e,k} \cos\alpha_k + A'_{\zeta,o,k} \sin\alpha_k\right) \, \left(+m_j \lambda_{o,j} \cos\alpha_j - m_j \lambda_{e,j} \sin\alpha_j\right) \\ - & \left(A'_{\theta,e,k} \cos\alpha_k + A'_{\theta,o,k} \sin\alpha_k\right) \, \left(-n_j \lambda_{o,j} \cos\alpha_j + n_j \lambda_{e,j} \sin\alpha_j\right) \\ = & - \left(A'_{\zeta,e,k} \cos\alpha_k + A'_{\zeta,o,k} \sin\alpha_k\right), \end{aligned} \tag{229}$$

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

- After applying double angle formulae,

$$\begin{aligned} & \left(A'_{\theta,e,k} \cos\alpha_k + A'_{\theta,o,k} \sin\alpha_k\right) \, \iota \\ + & \lambda_{o,j} \left(+m_j A'_{\zeta,e,k} + n_j A'_{\theta,e,k}\right) \left[+\cos(\alpha_k + \alpha_j) + \cos(\alpha_k - \alpha_j)\right]/2 \\ + & \lambda_{e,j} \left(-m_j A'_{\zeta,e,k} - n_j A'_{\theta,e,k}\right) \left[+\sin(\alpha_k + \alpha_j) - \sin(\alpha_k - \alpha_j)\right]/2 \\ + & \lambda_{o,j} \left(+m_j A'_{\zeta,o,k} + n_j A'_{\theta,o,k}\right) \left[+\sin(\alpha_k + \alpha_j) + \sin(\alpha_k - \alpha_j)\right]/2 \\ + & \lambda_{e,j} \left(-m_j A'_{\zeta,o,k} - n_j A'_{\theta,o,k}\right) \left[-\cos(\alpha_k + \alpha_j) + \cos(\alpha_k - \alpha_j)\right]/2 \\ = & - \left(A'_{\zeta,e,k} \cos\alpha_k + A'_{\zeta,o,k} \sin\alpha_k\right), \end{aligned} \tag{230}$$

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

$$\mathbf{x} = (\underbrace{\iota}_{\mathtt{x[1]}}, \underbrace{\lambda_{o,2}, \lambda_{o,3}, \ldots}_{\mathtt{x[\ 2:\ N\ ]}}, \underbrace{\lambda_{e,2}, \lambda_{e,3}, \ldots}_{\mathtt{x[N+1:2N-1]}})^T. \tag{231}$$

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

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

where i labels the grid point.

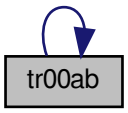
- This is a matrix equation...

Parameters

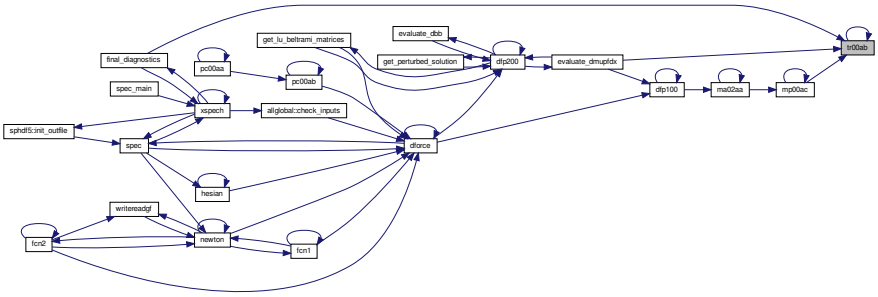
lvol	
mn	
NN	
Nt	
Nz	
iflag	
ldiota	

References allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::cpus, allglobal::glambda, constants::goldenmean, constants::half, allglobal::hnt, allglobal::hnz, allglobal::im, inputlist::imethod, allglobal::ims, allglobal::in, allglobal::ins, inputlist::iorder, allglobal::iotakadd, allglobal::iotakkii, allglobal::iotaksgn, allglobal::iotaksub, inputlist::iotatol, inputlist::iprecon, allglobal::lcoordinatesingularity, inputlist::lrad, inputlist::lsparse, inputlist::lsvdiota, allglobal::lvacuumregion, numerical::machprec, allglobal::mns, allglobal::mpi_comm_spec, inputlist::mpol, allglobal::myid, allglobal::ncpu, allglobal::notstellsym, inputlist::ntor, allglobal::ntz, inputlist::nvol, constants::one,

fileunits::ounit, constants::pi2, allglobal::regumm, allglobal::rtt, numerical::small, numerical::sqrtmachprec, constants::third, tr00ab(), allglobal::tt, constants::two, numerical::vsmall, inputlist::wmacros, allglobal::yesstellsym, and constants::zero.
Referenced by evaluate_dmupfdx(), final_diagnostics(), mp00ac(), and tr00ab().
Here is the call graph for this function:



Here is the caller graph for this function:



7.21 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.

7.21.1 Detailed Description

7.21.2 Function/Subroutine Documentation

7.21.2.1 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

$$V = \int_{\mathcal{V}} dv = \frac{1}{3}\int_{\mathcal{V}} \nabla\cdot\mathbf{x}\, dv = \frac{1}{3}\int_{\mathcal{S}} \mathbf{x}\cdot d\mathbf{s} = \frac{1}{3}\int_0^{2\pi} d\theta \int_0^{2\pi/N} d\zeta \quad \mathbf{x}\cdot\mathbf{x}_\theta\times\mathbf{x}_\zeta\big|^s \tag{233}$$

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

representation of surfaces

- The coordinate functions are

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

$$Z(\theta,\zeta) = \sum_i Z_{e,i}\ \cos\alpha_i + \sum_i Z_{o,i}\ \sin\alpha_i, \tag{235}$$

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 : $\sqrt{g} = R_s$

$$\begin{aligned} V &= \int_0^{2\pi} d\theta \int_0^{2\pi/N} d\zeta\ R \\ &= 2\pi\ \frac{2\pi}{N}\ R_{e,1} \end{aligned} \tag{236}$$

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

$$\begin{aligned} V &= \frac{1}{2}\int_0^{2\pi} d\theta \int_0^{2\pi/N} d\zeta\ R^2 \\ &= \frac{1}{2}\ 2\pi\ \frac{2\pi}{N}\ \frac{1}{2}\ \sum_i\sum_j R_{e,i}R_{e,j}\left[\cos(\alpha_i-\alpha_j)+\cos(\alpha_i+\alpha_j)\right] \\ &+ \frac{1}{2}\ 2\pi\ \frac{2\pi}{N}\ \frac{1}{2}\ \sum_i\sum_j R_{o,i}R_{o,j}\left[\cos(\alpha_i-\alpha_j)-\cos(\alpha_i+\alpha_j)\right] \end{aligned} \tag{237}$$

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

$$\begin{aligned} V &= \frac{1}{3}\int_0^{2\pi} d\theta \int_0^{2\pi/N} d\zeta\ R\left(ZR_\theta - RZ_\theta\right) \\ &= \frac{1}{3}\sum_i\sum_j\sum_k R_{e,i}\left(Z_{e,j}R_{o,k} - R_{e,j}Z_{o,k}\right)(+m_k)\iint d\theta d\zeta\ \cos\alpha_i\cos\alpha_j\cos\alpha_k \\ &+ \frac{1}{3}\sum_i\sum_j\sum_k R_{e,i}\left(Z_{o,j}R_{e,k} - R_{o,j}Z_{e,k}\right)(-m_k)\iint d\theta d\zeta\ \cos\alpha_i\sin\alpha_j\sin\alpha_k \\ &+ \frac{1}{3}\sum_i\sum_j\sum_k R_{o,i}\left(Z_{e,j}R_{e,k} - R_{e,j}Z_{e,k}\right)(-m_k)\iint d\theta d\zeta\ \sin\alpha_i\cos\alpha_j\sin\alpha_k \\ &+ \frac{1}{3}\sum_i\sum_j\sum_k R_{o,i}\left(Z_{o,j}R_{o,k} - R_{o,j}Z_{o,k}\right)(+m_k)\iint d\theta d\zeta\ \sin\alpha_i\sin\alpha_j\cos\alpha_k \end{aligned} \tag{238}$$

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

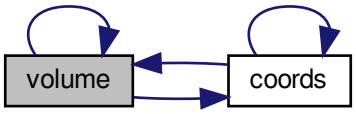
$$\begin{aligned} 4\ \cos\alpha_i\cos\alpha_j\cos\alpha_k &= +\ \cos(\alpha_i+\alpha_j+\alpha_k) + \cos(\alpha_i+\alpha_j-\alpha_k) + \cos(\alpha_i-\alpha_j+\alpha_k) + \cos(\alpha_i-\alpha_j-\alpha_k) \\ 4\ \cos\alpha_i\sin\alpha_j\sin\alpha_k &= -\ \cos(\alpha_i+\alpha_j+\alpha_k) + \cos(\alpha_i+\alpha_j-\alpha_k) + \cos(\alpha_i-\alpha_j+\alpha_k) - \cos(\alpha_i-\alpha_j-\alpha_k) \\ 4\ \sin\alpha_i\cos\alpha_j\sin\alpha_k &= -\ \cos(\alpha_i+\alpha_j+\alpha_k) + \cos(\alpha_i+\alpha_j-\alpha_k) - \cos(\alpha_i-\alpha_j+\alpha_k) + \cos(\alpha_i-\alpha_j-\alpha_k) \\ 4\ \sin\alpha_i\sin\alpha_j\cos\alpha_k &= -\ \cos(\alpha_i+\alpha_j+\alpha_k) - \cos(\alpha_i+\alpha_j-\alpha_k) + \cos(\alpha_i-\alpha_j+\alpha_k) + \cos(\alpha_i-\alpha_j-\alpha_k) \end{aligned} \tag{239}$$

- The required derivatives are

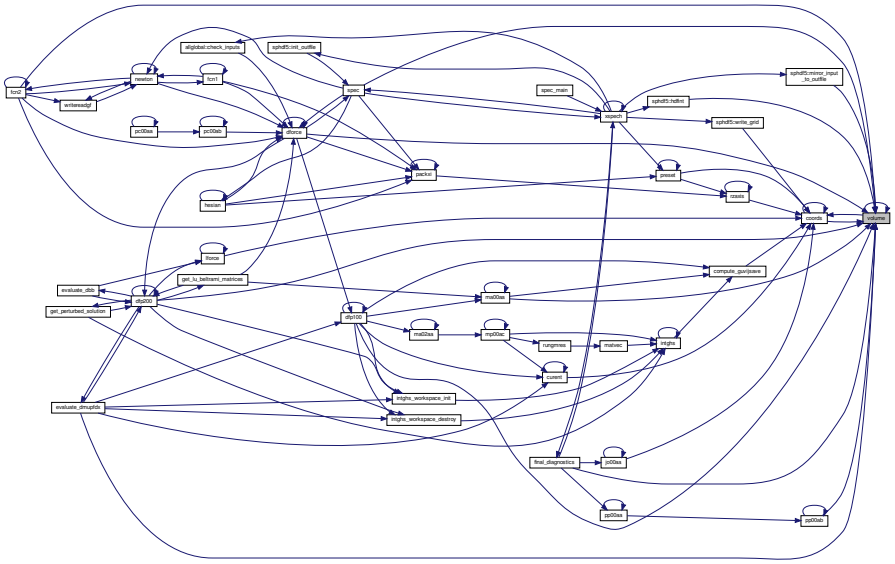
$$\begin{aligned} 3\frac{\partial V}{\partial R_{e,i}} &= (+Z_{e,j}R_{o,k}m_k - R_{e,j}Z_{o,k}m_k - R_{e,j}Z_{o.k}m_k) && \iint d\theta d\zeta\ \cos\alpha_i \cos\alpha_j \cos\alpha_k \\ &+ (-Z_{o,j}R_{e,k}m_k + R_{o,j}Z_{e,k}m_k + R_{o,j}Z_{e,k}m_k) && \iint d\theta d\zeta\ \cos\alpha_i \sin\alpha_j \sin\alpha_k \\ &+ (-R_{o,k}Z_{e,j}m_i) && \iint d\theta d\zeta\ \sin\alpha_i \cos\alpha_j \sin\alpha_k \\ &+ (-R_{e,k}Z_{o,j}m_i) && \iint d\theta d\zeta\ \sin\alpha_i \sin\alpha_j \cos\alpha_k \end{aligned} \tag{240}$$

$$\begin{aligned} 3\frac{\partial V}{\partial Z_{o,i}} &= (-R_{e,k}R_{e,j}m_i) && \iint d\theta d\zeta\ \cos\alpha_i \cos\alpha_j \cos\alpha_k \\ &+ (-R_{o,k}R_{o,j}m_i) && \iint d\theta d\zeta\ \cos\alpha_i \sin\alpha_j \sin\alpha_k \\ &+ (-R_{e,j}R_{e,k}m_k) && \iint d\theta d\zeta\ \sin\alpha_i \cos\alpha_j \sin\alpha_k \\ &+ (+R_{o,j}R_{o,k}m_k) && \iint d\theta d\zeta\ \sin\alpha_i \sin\alpha_j \cos\alpha_k \end{aligned} \tag{241}$$

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, volume(), numerical::vsmall, allglobal::vvolume, allglobal::yesstellsym, constants::zero, and allglobal::zij.
Referenced by coords(), dforce(), dfp100(), dfp200(), evaluate_dmupfdx(), fcn2(), final_diagnostics(), sphdf5::hdfint(), ma00aa(), sphdf5::mirror_input_to_outfile(), pp00ab(), spec(), and volume().
Here is the call graph for this function:



Here is the caller graph for this function:



7.22 Smooth boundary

Functions/Subroutines

- subroutine wa00aa (iwa00aa)

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

  Compute vacuum magnetic scalar potential (?)

7.22.1 Detailed Description

7.22.2 Function/Subroutine Documentation

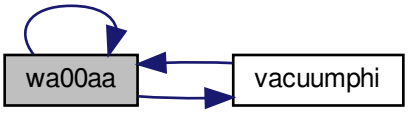
7.22.2.1 wa00aa() `subroutine wa00aa (`
`integer` *`iwa00aa`* `)`

Constructs smooth approximation to wall.
solution of Laplace's equation in two-dimensions

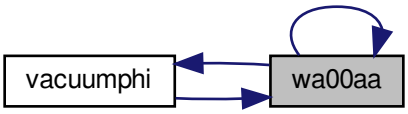
- The wall is given by a discrete set of points.
- The points must go anti-clockwise.

References laplaces::alpha, laplaces::cc, allglobal::cpus, laplaces::dorm, laplaces::exterior, fileunits::gunit, constants::half, laplaces::iangle, laplaces::ic, laplaces::icint, allglobal::im, allglobal::in, allglobal::irbc, allglobal::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, vacuumphi(), numerical::vsmall, wa00aa(), inputlist::wmacros, laplaces::xpoly, allglobal::yesstellsym, laplaces::ypoly, constants::zero, and allglobal::zij.
Referenced by vacuumphi(), and wa00aa().

Here is the call graph for this function:



Here is the caller graph for this function:



7.22.2.2 vacuumphi()

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

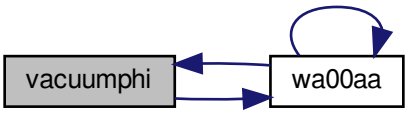
Compute vacuum magnetic scalar potential (?)

Parameters

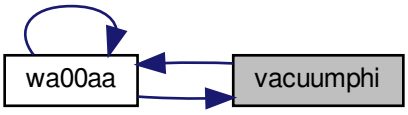
Nconstraints	
rho	
fvec	
iflag	

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:



7.23 Enhanced resolution for metric elements

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

7.23.1 Detailed Description

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

7.24 Enhanced resolution for transformation to straight-field line angle

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

Variables

- integer **allglobal::mns**

  enhanced resolution for straight field line transformation
- integer, dimension(:), allocatable **allglobal::ims**

  enhanced poloidal mode numbers for straight field line transformation

- integer, dimension(:), allocatable **allglobal::ins**

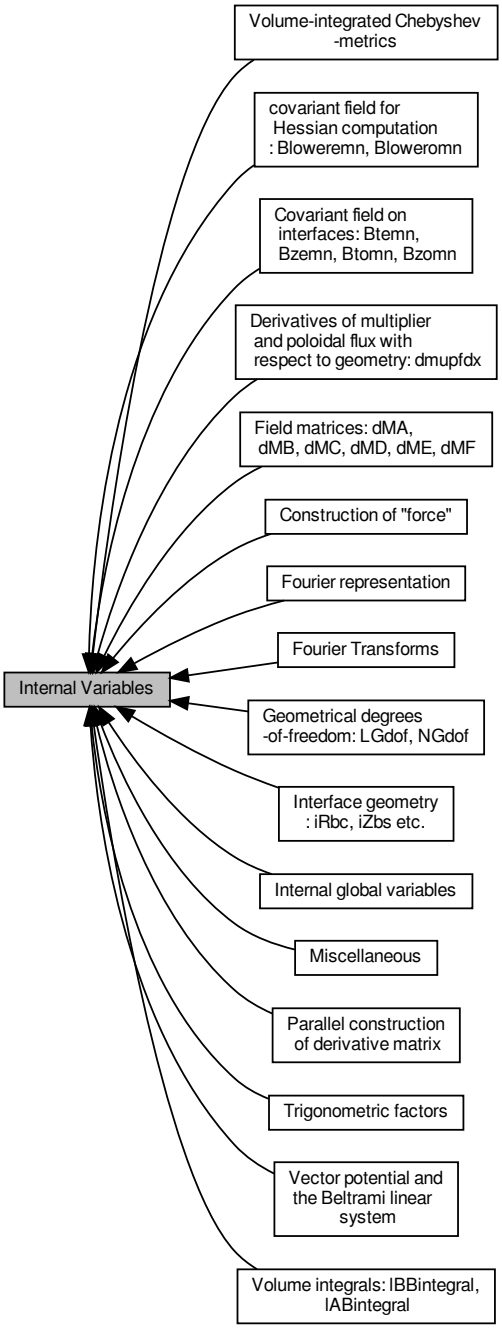
  enhanced toroidal mode numbers for straight field line transformation

7.24.1 Detailed Description

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

7.25 Internal Variables

Collaboration diagram for Internal Variables:



Modules

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

  The Fourier harmonics of the interfaces are contained in `iRbc(1:mn,0:Mvol)` *and* `iZbs(1:mn,0:Mvol)`*, where* `iRbc(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

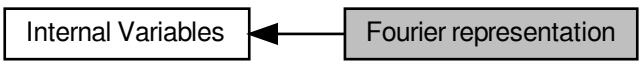
- type(derivative) **allglobal::dbdx**

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

7.25.1 Detailed Description

7.26 Fourier representation

Collaboration diagram for Fourier representation:



Variables

- integer **allglobal::mn**

  total number of Fourier harmonics for coordinates/fields; calculated from Mpol, Ntor in readin()
- integer, dimension(:), allocatable **allglobal::im**

  poloidal mode numbers for Fourier representation
- integer, dimension(:), allocatable **allglobal::in**

  toroidal mode numbers for Fourier representation
- real, dimension(:), allocatable **allglobal::halfmm**

  I saw this already somewhere...
- real, dimension(:), allocatable **allglobal::regumm**

  I saw this already somewhere...
- real **allglobal::rscale**

  no idea
- real, dimension(:,:), allocatable **allglobal::psifactor**

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

  no idea
- real, dimension(:), allocatable **allglobal::bbweight**

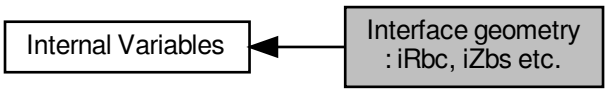
  weight on force-imbalance harmonics; used in dforce()
- real, dimension(:), allocatable **allglobal::mmpp**

  spectral condensation factors

7.26.1 Detailed Description

7.27 Interface geometry: iRbc, iZbs etc.

The Fourier harmonics of the interfaces are contained in `iRbc(1:mn,0:Mvol)` and `iZbs(1:mn,0:Mvol)`, where `iRbc(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**

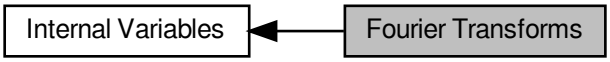
7.27.1 Detailed Description

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

7.28 Fourier Transforms

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

Collaboration diagram for Fourier Transforms:



Variables

- integer **allglobal::nt**
  discrete resolution along 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**

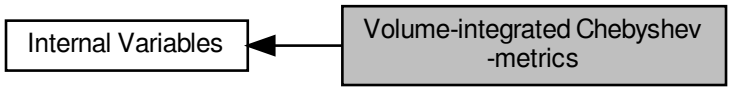
  described in preset()

7.28.1 Detailed Description

The coordinate geometry and fields are mapped to/from Fourier space and real space using FFTW3. The resolution of the real space grid is given by `Nt=Ndiscrete*4*Mpol` and `Nz=Ndiscrete*4*Ntor`.
Various workspace arrays are allocated. These include `Rij(1:Ntz,0:3,0:3)` and `Zij(1:Ntz,0:3,0:3)`, which contain the coordinates in real space and their derivatives; `sg(0:3,Ntz)`, which contains the Jacobian and its derivatives; and `guv(0:6,0:3,1:Ntz)`, which contains the metric elements and their derivatives.

7.29 Volume-integrated Chebyshev-metrics

These are allocated in dforce(), defined in ma00aa(), and are used in matrix() to construct the matrices.
Collaboration diagram for Volume-integrated Chebyshev-metrics:



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**

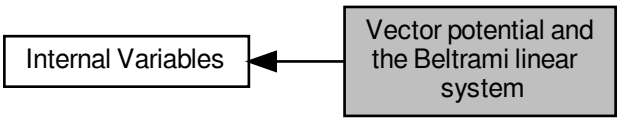
  minimum poloidal length constraint weight

7.29.1 Detailed Description

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

7.30 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?

7.30.1 Detailed Description

- In each volume, the total degrees of freedom in the Beltrami linear system is `NAdof(1:Nvol)`. This depends on `Mpol`, `Ntor` and `Lrad(vvol)`.
- The covariant components of the vector potential are written as

$$A_\theta = \sum_i \sum_{l=0}^{L} A_{\theta,e,i,l}\, T_l(s) \cos\alpha_i + \sum_i \sum_{l=0}^{L} A_{\theta,o,i,l}\, T_l(s) \sin\alpha_i \tag{242}$$

$$A_\zeta = \sum_i \sum_{l=0}^{L} A_{\zeta,e,i,l}\, T_l(s) \cos\alpha_i + \sum_i \sum_{l=0}^{L} A_{\zeta,o,i,l}\, T_l(s) \sin\alpha_i, \tag{243}$$

  where $T_l(s)$ are the Chebyshev polynomials and $\alpha_i \equiv m_i\theta - n_i\zeta$.

- The following internal arrays are declared in preset() :

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

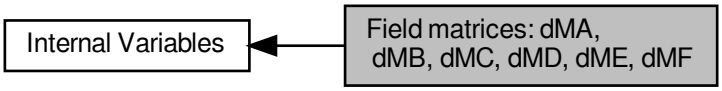
  `dAze(0,i)%s(l)` $\equiv A_{\zeta,e,i,l}$

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

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

7.31 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**

  number of independent degrees of freedom in angle transformation;
- real, dimension(:,:,:), allocatable **allglobal::dlambdaout**

7.31.1 Detailed Description

- The energy, $W \equiv \int dv\ \mathbf{B}\cdot\mathbf{B}$, and helicity, $K \equiv \int dv\ \mathbf{A}\cdot\mathbf{B}$, functionals may be written

$$W = \frac{1}{2}\, a_i\, A_{i,j}\, a_j + a_i\, B_{i,j}\, \psi_j + \frac{1}{2}\, \psi_i\, C_{i,j}\, \psi_j \tag{244}$$

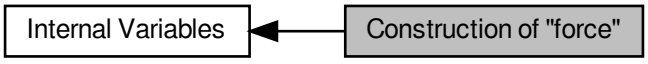
$$K = \frac{1}{2}\, a_i\, D_{i,j}\, a_j + a_i\, E_{i,j}\, \psi_j + \frac{1}{2}\, \psi_i\, F_{i,j}\, \psi_j \tag{245}$$

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

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

7.32 Construction of "force"

The force vector is comprised of `Bomn` and `Iomn`.
Collaboration diagram for Construction of "force":



Variables

- real, dimension(:,:,:), allocatable **allglobal::bemn**

  force vector; stellarator-symmetric (?)
- real, dimension(:,:), allocatable **allglobal::iomn**

  force vector; stellarator-symmetric (?)
- real, dimension(:,:,:), allocatable **allglobal::somn**

  force vector; non-stellarator-symmetric (?)
- real, dimension(:,:,:), allocatable **allglobal::pomn**

  force vector; non-stellarator-symmetric (?)
- real, dimension(:,:,:), allocatable **allglobal::bomn**

  force vector; stellarator-symmetric (?)
- real, dimension(:,:), allocatable **allglobal::iemn**

  force vector; stellarator-symmetric (?)
- real, dimension(:,:,:), allocatable **allglobal::semn**

  force vector; non-stellarator-symmetric (?)
- real, dimension(:,:,:), allocatable **allglobal::pemn**

  force vector; non-stellarator-symmetric (?)
- real, dimension(:), allocatable **allglobal::bbe**

  force vector (?); stellarator-symmetric (?)
- real, dimension(:), allocatable **allglobal::iio**

  force vector (?); stellarator-symmetric (?)
- real, dimension(:), allocatable **allglobal::bbo**

  force vector (?); non-stellarator-symmetric (?)
- real, dimension(:), allocatable **allglobal::iie**

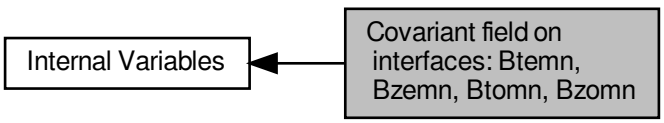
  force vector (?); non-stellarator-symmetric (?)

7.32.1 Detailed Description

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

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

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



Variables

- real, dimension(:,:,:), allocatable **allglobal::btemn**

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

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

covariant θ sine component of the tangential field on interfaces; non-stellarator-symmetric

- real, dimension(:,:,:), allocatable **allglobal::bzomn**

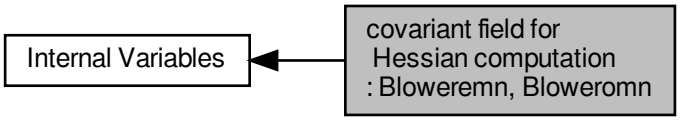
  covariant ζ sine component of the tangential field on interfaces; non-stellarator-symmetric

7.33.1 Detailed Description

The covariant field.

7.34 covariant field for Hessian computation: Bloweremn, Bloweromn

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



Variables

- real, dimension(:,:), allocatable **allglobal::bloweremn**

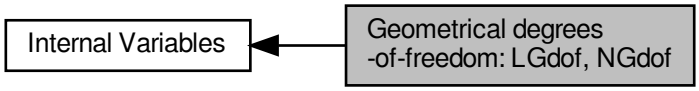
  covariant field for Hessian computation
- real, dimension(:,:), allocatable **allglobal::bloweromn**

  covariant field for Hessian computation

7.34.1 Detailed Description

7.35 Geometrical degrees-of-freedom: LGdof, NGdof

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



Variables

- integer **allglobal::lgdof**

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

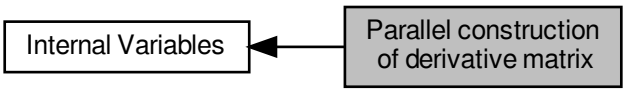
  total geometrical degrees of freedom

7.35.1 Detailed Description

The geometrical degrees-of-freedom.

7.36 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
- real, dimension(:,:,:,:,:), allocatable **allglobal::hdffdrz**

  derivatives of B^2 at the interfaces wrt geometry 2D Hessian;
- real, dimension(:,:,:,:,:), allocatable **allglobal::denergydrr**

  derivatives of energy at the interfaces wrt geometry 3D Hessian;
- real, dimension(:,:,:,:,:), allocatable **allglobal::denergydrz**

  derivatives of energy at the interfaces wrt geometry 3D Hessian;
- real, dimension(:,:,:,:,:), allocatable **allglobal::denergydzr**

  derivatives of energy at the interfaces wrt geometry 3D Hessian;
- real, dimension(:,:,:,:,:), allocatable **allglobal::denergydzz**

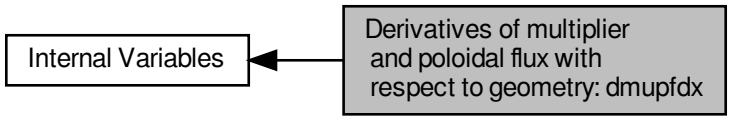
  derivatives of energy at the interfaces wrt geometry 3D Hessian;

7.36.1 Detailed Description

- The derivatives of force-balance, $[[p + B^2/2]]$, and the spectral constraints (see sw03aa()), with respect to the interface geometry is constructed in parallel by dforce().
- force-balance across the l-th interface depends on the fields in the adjacent interfaces.

7.37 Derivatives of multiplier and poloidal flux with respect to geometry: dmupfdx

Collaboration diagram for Derivatives of multiplier and poloidal flux with respect to geometry: dmupfdx:



Variables

- real, dimension(:,:,:,:,:), allocatable **allglobal::dmupfdx**
  derivatives of mu and dpflux wrt geometry at constant interface transform
- logical **allglobal::lhessianallocated**
  flag to indicate that force gradient matrix is allocated (?)
- real, dimension(:,:), allocatable **allglobal::hessian**
  force gradient matrix (?)
- real, dimension(:,:), allocatable **allglobal::dessian**
  derivative of force gradient matrix (?)
- logical **allglobal::lhessian2dallocated**
  flag to indicate that 2D Hessian matrix is allocated (?)
- real, dimension(:,:), allocatable **allglobal::hessian2d**
  Hessian 2D.
- real, dimension(:,:), allocatable **allglobal::dessian2d**
  derivative Hessian 2D
- logical **allglobal::lhessian3dallocated**
  flag to indicate that 2D Hessian matrix is allocated (?)
- real, dimension(:,:), allocatable **allglobal::hessian3d**
  Hessian 3D.
- real, dimension(:,:), allocatable **allglobal::dessian3d**
  derivative Hessian 3D

7.37.1 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

$$\delta\mathbf{B}_\pm = \frac{\partial \mathbf{B}_\pm}{\partial x_j}\delta x_j + \frac{\partial \mathbf{B}_\pm}{\partial \mu}\delta\mu + \frac{\partial \mathbf{B}_\pm}{\partial \Delta\psi_p}\delta\Delta\psi_p. \tag{246}$$

- This information is used to adjust the calculation of how force-balance, i.e. B^2 at the interfaces, varies with geometry at fixed interface rotational transform. Given

$$B^2_\pm = B^2_\pm(x_j, \mu, \Delta\psi_p), \tag{247}$$

we may derive

$$\frac{\partial B_{\pm}^2}{\partial x_j} = \frac{\partial B_{\pm}^2}{\partial x_j} + \frac{\partial B_{\pm}^2}{\partial \mu}\frac{\partial \mu}{\partial x_j} + \frac{\partial B_{\pm}^2}{\partial \Delta\psi_p}\frac{\partial \Delta\psi_p}{\partial x_j} \tag{248}$$

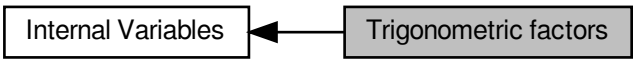
- The constraint to be enforced is that μ and $\Delta\psi_p$ must generally vary as the geometry is varied if the value of the rotational-transform constraint on the inner/outer interface is to be preserved, i.e.

$$\begin{pmatrix} \frac{\partial \iota_-}{\partial \mathbf{B}_-}\cdot\frac{\partial \mathbf{B}_-}{\partial \mu} & , & \frac{\partial \iota_-}{\partial \mathbf{B}_-}\cdot\frac{\partial \mathbf{B}_-}{\partial \Delta\psi_p} \\ \frac{\partial \iota_+}{\partial \mathbf{B}_+}\cdot\frac{\partial \mathbf{B}_+}{\partial \mu} & , & \frac{\partial \iota_+}{\partial \mathbf{B}_+}\cdot\frac{\partial \mathbf{B}_+}{\partial \Delta\psi_p} \end{pmatrix} \begin{pmatrix} \frac{\partial \mu}{\partial x_j} \\ \frac{\partial \Delta\psi_p}{\partial x_j} \end{pmatrix} = - \begin{pmatrix} \frac{\partial \iota_-}{\partial \mathbf{B}_-}\cdot\frac{\partial \mathbf{B}_-}{\partial x_j} \\ \frac{\partial \iota_+}{\partial \mathbf{B}_+}\cdot\frac{\partial \mathbf{B}_+}{\partial x_j} \end{pmatrix}. \tag{249}$$

- 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`.

7.38 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

7.38.1 Detailed Description

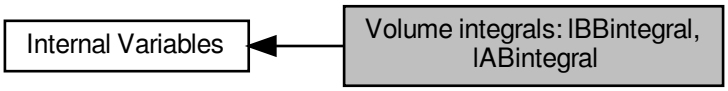
- To facilitate construction of the metric integrals, various trigonometric identities are exploited.
- The following are used for volume integrals (see volume()):

$$a_{i,j,k} = 4\, m_k \oint\!\!\oint d\theta d\zeta \;\; \cos(\alpha_i)\cos(\alpha_j)\cos(\alpha_k)/(2\pi)^2, \tag{250}$$

$$b_{i,j,k} = 4\, m_j \oint\!\!\oint d\theta d\zeta \;\; \cos(\alpha_i)\sin(\alpha_j)\sin(\alpha_k)/(2\pi)^2, \tag{251}$$

7.39 Volume integrals: lBBintegral, lABintegral

Collaboration diagram for Volume integrals: lBBintegral, lABintegral:



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

7.39.1 Detailed Description

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

$$F_l \equiv \left(\int_{\mathcal{V}_l} \frac{p_l}{\gamma - 1} + \frac{B_l^2}{2} dv \right) = \frac{P_l}{\gamma - 1} V_l^{1-\gamma} + \int_{\mathcal{V}_l} \frac{B_l^2}{2} dv, \tag{252}$$

  where the second expression is derived using $p_l V_l^\gamma = P_l$, where P_l is the adiabatic-constant. In Eqn. (252), it is implicit that $\mathbf{B}$ 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)

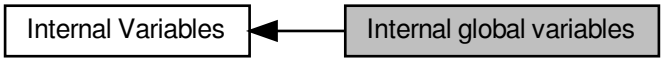
  $\partial F_l/\partial R_{l,j} \equiv$ dFF(ll,1, j)

  $\partial F_l/\partial Z_{l,j} \equiv$ 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).

7.40 Internal global variables

internal global variables; internal logical variables; default values are provided here; these may be changed according to input values
Collaboration diagram for Internal global variables:



Variables

- integer **allglobal::ivol**

  labels volume; some subroutines (called by NAG) are fixed argument list but require the volume label
- real **allglobal::gbzeta**

  toroidal (contravariant) field; calculated in bfield; required to convert $\dot{\theta}$ to B^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**

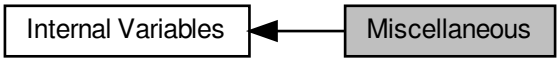
  used in mg00aa() to determine (s,θ,ζ) given (R,Z,φ)

7.40.1 Detailed Description

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

7.41 Miscellaneous

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



Variables

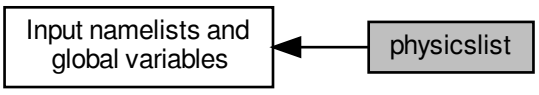
- integer **allglobal::globaljk**
  labels position
- real, dimension(:,:), allocatable **allglobal::dxyz**
  computational boundary; position
- real, dimension(:,:), allocatable **allglobal::nxyz**
  computational boundary; normal
- real, dimension(:,:), allocatable **allglobal::jxyz**
  plasma boundary; surface current
- real, dimension(1:2) **allglobal::tetazeta**
  what is this?
- real **allglobal::virtualcasingfactor** = -one / (four∗pi)
  this agrees with diagno
- integer **allglobal::iberror**
  for computing error in magnetic field
- integer **allglobal::nfreeboundaryiterations**
  number of free-boundary iterations already performed
- integer, parameter **allglobal::node** = 2
  best to make this global for consistency between calling and called routines
- logical **allglobal::first_free_bound** = .false.
  flag to indicate that this is the first free-boundary iteration

7.41.1 Detailed Description

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

7.42 physicslist

The namelist `physicslist` controls the geometry, profiles, and numerical resolution.
Collaboration diagram for physicslist:



Variables

- integer inputlist::igeometry = 3

  selects Cartesian, cylindrical or toroidal geometry;
- integer **inputlist::istellsym** = 1

  stellarator symmetry is enforced if `Istellsym==1`
- integer **inputlist::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;

7.42.1 Detailed Description

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

7.42.2 Variable Documentation

7.42.2.1 igeometry `integer inputlist::igeometry = 3`

selects Cartesian, cylindrical or toroidal geometry;

- `Igeometry=1` : Cartesian; geometry determined by R;
- `Igeometry=2` : cylindrical; geometry determined by R;
- `Igeometry=3` : toroidal; geometry determined by R *and* Z;

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

7.42.2.2 nfp `integer inputlist::nfp = 1`

field periodicity

- all Fourier representations are of the form $\cos(m\theta - nN\zeta)$, $\sin(m\theta - nN\zeta)$, where $N \equiv$`Nfp`
- constraint: `Nfp` >= 1

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

7.42.2.3 nvol `integer inputlist::nvol = 1`

number of volumes

- each volume $\mathcal{V}_l$ is bounded by the $\mathcal{I}_{l-1}$ and $\mathcal{I}_l$ interfaces
- note that in cylindrical or toroidal geometry, $\mathcal{I}_0$ is the degenerate coordinate axis
- constraint: `Nvol`<=`MNvol`

Referenced by brcast(), allglobal::broadcast_inputs(), allglobal::check_inputs(), df00ab(), dforce(), dfp100(), dfp200(), dvcfield(), evaluate_dbb(), evaluate_dmupfdx(), fcn1(), fcn2(), final_diagnostics(), sphdf5::hdfint(), hesian(), jo00aa(), lforce(), sphdf5::mirror_input_to_outfile(), newton(), packxi(), pc00ab(), pp00aa(), pp00ab(), preset(), spec(), stzxyz(), tr00ab(), volume(), wa00aa(), sphdf5::write_grid(), writereadgf(), and allglobal::wrtend().

7.42.2.4 mpol `integer inputlist::mpol = 0`

number of poloidal Fourier harmonics

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

$$f(\theta,\zeta) \quad = \quad \sum_{n=0}^{\mathtt{Ntor}} f_{0,n}\cos(-n\,\mathtt{Nfp}\,\zeta) + \sum_{m=1}^{\mathtt{Mpol}}\sum_{n=-\mathtt{Ntor}}^{\mathtt{Ntor}} f_{m,n}\cos(m\theta - n\,\mathtt{Nfp}\,\zeta), \tag{253}$$

  Internally these "double" summations are written as a "single" summation, e.g. $f(\theta,\zeta) = \sum_j f_j \cos(m_j\theta - n_j\zeta)$.

Referenced by allocate_geometry_matrices(), bfield(), bfield_tangent(), allglobal::broadcast_inputs(), allglobal::check_inputs(), dfp200(), intghs(), intghs_workspace_init(), jo00aa(), ma00aa(), matrix(), sphdf5::mirror_input_to_outfile(), mtrxhs(), preset(), ra00aa(), spsint(), spsmat(), tr00ab(), wa00aa(), writereadgf(), and allglobal::wrtend().

7.42.2.5 ntor `integer inputlist::ntor = 0`

number of toroidal Fourier harmonics

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

$$f(\theta,\zeta) \quad = \quad \sum_{n=0}^{\mathtt{Ntor}} f_{0,n}\cos(-n\,\mathtt{Nfp}\,\zeta) + \sum_{m=1}^{\mathtt{Mpol}}\sum_{n=-\mathtt{Ntor}}^{\mathtt{Ntor}} f_{m,n}\cos(m\theta - n\,\mathtt{Nfp}\,\zeta), \tag{254}$$

  Internally these "double" summations are written as a "single" summation, e.g. $f(\theta,\zeta) = \sum_j f_j \cos(m_j\theta - n_j\zeta)$.

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), coords(), dforce(), dfp200(), evaluate_dbb(), sphdf5::mirror_input_to_outfile(), mp00ac(), packxi(), preset(), ra00aa(), rzaxis(), stzxyz(), tr00ab(), wa00aa(), writereadgf(), and allglobal::wrtend().

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

7.42.2.7 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 mp00ac(), pp00aa(), preset(), spec(), and allglobal::wrtend().

7.42.2.8 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().

7.42.2.9 helicity `real, dimension(1:mnvol) inputlist::helicity = 0.0`

helicity, $\mathcal{K}$, in each volume, $\mathcal{V}_i$

- on exit, `helicity` is set to the computed values of $\mathcal{K} \equiv \int \mathbf{A} \cdot \mathbf{B} \, dv$

Referenced by brcast(), allglobal::broadcast_inputs(), allglobal::check_inputs(), df00ab(), sphdf5::hdfint(), hesian(), ma02aa(), sphdf5::mirror_input_to_outfile(), mp00ac(), preset(), spec(), and allglobal::wrtend().

7.42.2.10 pscale `real inputlist::pscale = 0.0`

pressure scale factor

- the initial pressure profile is given by `pscale` $*$ `pressure`

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), dfp200(), evaluate_dbb(), lforce(), sphdf5::mirror_input_to_outfile(), spec(), volume(), and allglobal::wrtend().

7.42.2.11 pressure `real, dimension(1:mnvol+1) inputlist::pressure = 0.0`

pressure in each volume

- The pressure is *not* held constant, but $p_l V_l^\gamma = P_l$ *is* held constant, where P_l is determined by the initial pressures and the initial volumes, V_l.
- Note that if `gamma==0.0`, then $p_l \equiv P_l$.
- On output, the pressure is given by $p_l = P_l / V_l^\gamma$, where V_l is the final volume.
- `pressure` is only used in calculation of interface force-balance.

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

7.42.2.12 ladiabatic `integer inputlist::ladiabatic = 0`

logical flag

- If `Ladiabatic==0`, the adiabatic constants are determined by the initial pressure and volume.
- If `Ladiabatic==1`, the adiabatic constants are determined by the given input `adiabatic`.

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

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

adiabatic constants in each volume

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

7.42.2.14 pl `integer, dimension(0:mnvol) inputlist::pl = 0`

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

7.42.2.15 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().

7.42.2.16 pr `integer, dimension(0:mnvol) inputlist::pr = 0`

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

7.42.2.17 qr `integer, dimension(0:mnvol) inputlist::qr = 0`

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

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

rotational-transform, ι, 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().

7.42.2.19 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().

7.42.2.20 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().

7.42.2.21 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().

7.42.2.22 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().

7.42.2.23 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().

7.42.2.24 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(), mp00ac(), and allglobal::wrtend().

7.42.2.25 mupfits `integer inputlist::mupfits = 8`

an upper limit on the transform/helicity constraint iterations;

- only relevant if constraints on transform, enclosed currents etc. are to be satisfied iteratively, see `Lconstraint`
- constraint: `mupfits` > 0

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), ma02aa(), sphdf5::mirror_input_to_outfile(), and allglobal::wrtend().

7.42.2.26 rpol `real inputlist::rpol = 1.0`

poloidal extent of slab (effective radius)

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

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

7.42.2.27 rtor `real inputlist::rtor = 1.0`

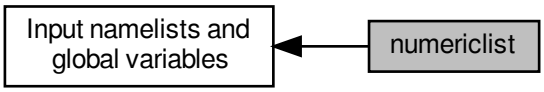
toroidal extent of slab (effective radius)

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

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

7.43 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` *.*

7.43.1 Detailed Description

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

7.43.2 Variable Documentation

7.43.2.1 linitialize `integer inputlist::linitialize = 0`

Used to initialize geometry using a regularization / extrapolation method.

- if `Linitialize` = $-I$, where I is a positive integer, the geometry of the $i = 1, N_V - I$ surfaces constructed by an extrapolation
- if `Linitialize` = 0, the geometry of the interior surfaces is provided after the namelists in the input file
- if `Linitialize` = 1, the interior surfaces will be intialized as $R_{l,m,n} = R_{N,m,n}\psi_{t,l}^{m/2}$, where $R_{N,m,n}$ is the plasma boundary and $\psi_{t,l}$ is the given toroidal flux enclosed by the l-th interface, normalized to the total enclosed toroidal flux; a similar extrapolation is used for $Z_{l,m,n}$
- Note that the Fourier harmonics of the boundary is *always* given by the `Rbc` and `Zbs` given in `physicslist`.
- if `Linitialize` = 2, the interior surfaces *and the plasma boundary* will be intialized as $R_{l,m,n} = R_{W,m,n}\psi_{t,l}^{m/2}$, where $R_{W,m,n}$ is the computational boundary and $\psi_{t,l}$ is the given toroidal flux enclosed by the l-th interface, normalized to the total enclosed toroidal flux; a similar extrapolation is used for $Z_{l,m,n}$
- Note that, for free-boundary calculations, the Fourier harmonics of the computational boundary are *always* given by the `Rwc` and `Zws` given in `physicslist`.
- if `Linitialize` = 1, 2, it is not required to provide the geometry of the interfaces after the namelists

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

7.43.2.2 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().

7.43.2.3 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().

7.43.2.4 ndiscrete `integer inputlist::ndiscrete = 2`

resolution of the real space grid on which fast Fourier transforms are performed is given by `Ndiscrete*Mpol*4`

- constraint `Ndiscrete>0`

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

7.43.2.5 nquad `integer inputlist::nquad = -1`

Resolution of the Gaussian quadrature.

- The resolution of the Gaussian quadrature, $\int f(s)ds = \sum_k \omega_k f(s_k)$, in each volume is given by `Iquad` $_v$,
- `Iquad` $_v$ is set in preset()

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

7.43.2.6 impol `integer inputlist::impol = -4`

Fourier resolution of straight-fieldline angle on interfaces.

- the rotational-transform on the interfaces is determined by a transformation to the straight-fieldline angle, with poloidal resolution given by `iMpol`
- if `iMpol<=0`, then `iMpol` = Mpol - iMpol

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

7.43.2.7 intor `integer inputlist::intor = -4`

Fourier resolution of straight-fieldline angle on interfaces;.

- the rotational-transform on the interfaces is determined by a transformation to the straight-fieldline angle, with toroidal resolution given by `iNtor`
- if `iNtor<=0` then `iNtor` = Ntor - iNtor
- if `Ntor==0`, then the toroidal resolution of the angle transformation is set `lNtor` = 0

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

7.43.2.8 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().

7.43.2.9 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(), final_diagnostics(), sphdf5::mirror_input_to_outfile(), tr00ab(), and allglobal::wrtend().

7.43.2.10 imethod `integer inputlist::imethod = 3`

controls iterative solution to sparse matrix arising in real-space transformation to the straight-fieldline angle; only relevant if `Lsparse.eq.2`;

See also

tr00ab() for details

- if `imethod` = 1, the method is `RGMRES`
- if `imethod` = 2, the method is `CGS`
- if `imethod` = 3, the method is `BICGSTAB`

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), sphdf5::mirror_input_to_outfile(), tr00ab(), and allglobal::wrtend().

7.43.2.11 iorder `integer inputlist::iorder = 2`

controls real-space grid resolution for constructing the straight-fieldline angle; only relevant if `Lsparse>0`
determines order of finite-difference approximation to the derivatives

- if `iorder` = 2,
- if `iorder` = 4,
- if `iorder` = 6,

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), sphdf5::mirror_input_to_outfile(), tr00ab(), and allglobal::wrtend().

7.43.2.12 iprecon `integer inputlist::iprecon = 0`

controls iterative solution to sparse matrix arising in real-space transformation to the straight-fieldline angle; only relevant if `Lsparse.eq.2`;

See also

tr00ab() for details

- if `iprecon` = 0, the preconditioner is 'N'
- if `iprecon` = 1, the preconditioner is 'J'
- if `iprecon` = 2, the preconditioner is 'S'

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), sphdf5::mirror_input_to_outfile(), tr00ab(), and allglobal::wrtend().

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

maximum regularization factor

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

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

7.43.2.14 lrzaxis `integer inputlist::lrzaxis = 1`

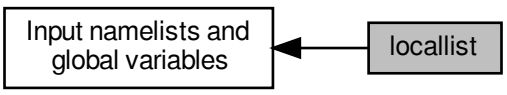
controls the guess of geometry axis in the innermost volume or initialization of interfaces

- 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().

7.44 locallist

The namelist `locallist` controls the construction of the Beltrami fields in each volume.
Collaboration diagram for locallist:



Variables

- integer inputlist::lbeltrami = 4

  Control flag for solution of Beltrami equation.
- integer inputlist::linitgues = 1

  controls how initial guess for Beltrami field is constructed
- integer **inputlist::lposdef** = 0

  redundant;

- real **inputlist::maxrndgues** = 1.0

  the maximum random number of the Beltrami field if `Linitgues` *= 3*
- integer **inputlist::lmatsolver** = 3

  1 for LU factorization, 2 for GMRES, 3 for GMRES matrix-free
- integer **inputlist::nitergmres** = 200

  number of max iteration for GMRES
- real **inputlist::epsgmres** = 1e-14

  the precision of GMRES
- integer **inputlist::lgmresprec** = 1

  type of preconditioner for GMRES, 1 for ILU sparse matrix
- real **inputlist::epsilu** = 1e-12

  the precision of incomplete LU factorization for preconditioning

7.44.1 Detailed Description

The namelist `locallist` controls the construction of the Beltrami fields in each volume.
The transformation to straight-fieldline coordinates is singular when the rotational-transform of the interfaces is rational; however, the rotational-transform is still well defined.

7.44.2 Variable Documentation

7.44.2.1 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().

7.44.2.2 linitgues `integer inputlist::linitgues = 1`

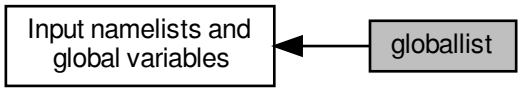
controls how initial guess for Beltrami field is constructed

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

7.45 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;

7.45.1 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,

$$F_{i,v} \equiv [[p + B^2/2]]_{i,v} \times \exp\left[-\mathtt{escale}(m_i^2 + n_i^2)\right] \times \mathtt{opsilon}, \tag{255}$$

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

$$F_{i,v} \equiv \mathtt{epsilon} \times I_{i,v} + \mathtt{upsilon} \times \left(\psi_v^\omega S_{i,v,1} - \psi_{v+1}^\omega S_{i,v+1,0}\right), \tag{256}$$

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

7.45.2 Variable Documentation

7.45.2.1 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(), fcn1(), fcn2(), hesian(), sphdf5::mirror_input_to_outfile(), newton(), packxi(), preset(), spec(), and allglobal::wrtend().

7.45.2.2 escale `real inputlist::escale = 0.0`

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

- `BBweight(i)` $\equiv$ `opsilon` $\times \exp\left[-\texttt{escale} \times (m_i^2 + n_i^2)\right]$
- defined in preset() ; used in dforce()
- also see Eqn. (255)

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

7.45.2.3 opsilon `real inputlist::opsilon = 1.0`

weighting of force-imbalance

- used in dforce(); also see Eqn. (255)

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

7.45.2.4 pcondense `real inputlist::pcondense = 2.0`

spectral condensation parameter

- used in preset() to define `mmpp(i)` $\equiv m_i^p$, where $p \equiv$ `pcondense`
- the angle freedom is exploited to minimize `epsilon` $\sum_i m_i^p (R_i^2 + Z_i^2)$ with respect to tangential variations in the interface geometry
- also see Eqn. (256)

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

7.45.2.5 epsilon `real inputlist::epsilon = 0.0`

weighting of spectral-width constraint

- used in dforce(); also see Eqn. (256)

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

7.45.2.6 forcetol `real inputlist::forcetol = 1.0e-10`

required tolerance in force-balance error; only used as an initial check

- if the initially supplied interfaces are consistent with force-balance to within `forcetol` then the geometry of the interfaces is not altered
- if not, then the geometry of the interfaces is changed in order to bring the configuration into force balance so that the geometry of interfaces is within `c05xtol`, defined below, of the true solution
- to force execution of either `C05NDF` or `C05PDF`, regardless of the initial force imbalance, set `forcetol` $<$ 0

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), fcn1(), fcn2(), sphdf5::mirror_input_to_outfile(), newton(), pc00aa(), pc00ab(), preset(), and allglobal::wrtend().

7.45.2.7 c05xtol `real inputlist::c05xtol = 1.0e-12`

required tolerance in position, $\mathbf{x} \equiv \{R_{i,v}, Z_{i,v}\}$

- used by both `C05NDF` and `C05PDF`; see the NAG documents for further details on how the error is defined
- constraint `c05xtol` $>$ 0.0

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), fcn1(), fcn2(), sphdf5::mirror_input_to_outfile(), newton(), and allglobal::wrtend().

7.45.2.8 c05factor `real inputlist::c05factor = 1.0e-02`

used to control initial step size in `C05NDF` and `C05PDF`

- constraint `c05factor` $>$ 0.0
- only relevant if `Lfindzero` $>$ 0

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), fcn1(), fcn2(), sphdf5::mirror_input_to_outfile(), newton(), and allglobal::wrtend().

7.45.2.9 lreadgf `logical inputlist::lreadgf = .true.`

read $\nabla_{\mathbf{x}}\mathbf{F}$ from file `ext.GF`

- only used if `Lfindzero` = 2
- only used in newton()

Referenced by allglobal::broadcast_inputs(), allglobal::check_inputs(), fcn1(), fcn2(), sphdf5::mirror_input_to_outfile(), newton(), and allglobal::wrtend().

7.45.2.10 mfreeits `integer inputlist::mfreeits = 0`

maximum allowed free-boundary iterations

- only used if `Lfreebound` = 1
- only used in xspech()

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

7.45.2.11 gbntol `real inputlist::gbntol = 1.0e-06`

required tolerance in free-boundary iterations

- only used if `Lfreebound` = 1
- only used in xspech()

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

7.45.2.12 gbnbld `real inputlist::gbnbld = 0.666`

normal blend

- The "new" magnetic field at the computational boundary produced by the plasma currents is updated using a Picard scheme:

$$(\mathbf{B}\cdot\mathbf{n})^{j+1} = \texttt{gBnbld}\times(\mathbf{B}\cdot\mathbf{n})^{j} + (1-\texttt{gBnbld})\times(\mathbf{B}\cdot\mathbf{n})^{*}, \tag{257}$$

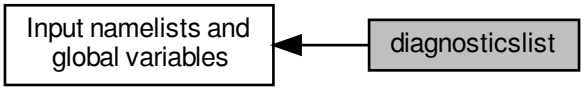
  where j labels free-boundary iterations, and $(\mathbf{B}\cdot\mathbf{n})^{*}$ is computed by virtual casing.

- only used if `Lfreebound` = 1
- only used in xspech()

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

7.46 diagnosticslist

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



Variables

- real **inputlist::odetol** = 1.0e-07

  o.d.e. integration tolerance for all field line tracing routines
- real **inputlist::absreq** = 1.0e-08

  redundant
- real **inputlist::relreq** = 1.0e-08

  redundant
- real **inputlist::absacc** = 1.0e-04

  redundant
- real **inputlist::epsr** = 1.0e-08

  redundant
- integer **inputlist::nppts** = 0

  number of toroidal transits used (per trajectory) in following field lines for constructing Poincaré plots; if `nPpts<1`, no Poincaré plot is constructed;
- real **inputlist::ppts** = 0.0

  stands for Poincare plot theta start. Chose at which angle (normalized over 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
- logical **inputlist::ltransform** = .false.

  to evaluate iota and straight field line coordinates
- real **inputlist::fudge** = 1.0e-00

  redundant
- real **inputlist::scaling** = 1.0e-00

  redundant

7.46.1 Detailed Description

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

7.46.2 Variable Documentation

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

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

- if `nPtrj(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().

7.46.2.2 lcheck `integer inputlist::lcheck = 0`

implement various checks

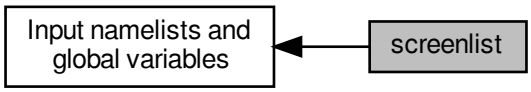
- if `Lcheck` = 0, no additional check on the calculation is performed
- if `Lcheck` = 1, the error in the current, i.e. $\nabla \times \mathbf{B} - \mu \mathbf{B}$ is computed as a post-diagnostic
- if `Lcheck` = 2, the analytic derivatives of the interface transform w.r.t. the helicity multiplier, 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 [6])
  - the input file for xdiagno is written by bnorml()
  - this provides the Cartesian coordinates on the computational boundary where the virtual casing routine casing() computes the magnetic field, with the values of the magnetic field being written to the screen for comparison
  - must set Freebound=1, Lfindzero>0, mfreeits!=0
  - xdiagno must be executed manually

Referenced by bnorml(), allglobal::broadcast_inputs(), allglobal::check_inputs(), dforce(), dfp200(), evaluate_dbb(), evaluate_dmupfdx(), fcn1(), fcn2(), final_diagnostics(), sphdf5::hdfint(), hesian(), lforce(), ma02aa(), sphdf5::mirror_input_to_outfile(), newton(), preset(), rzaxis(), spec(), and allglobal::wrtend().

7.47 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::wmanual** = .false.
- logical **inputlist::wrzaxis** = .false.
- logical **inputlist::wpackxi** = .false.
- logical **inputlist::wvolume** = .false.
- logical **inputlist::wcoords** = .false.
- logical **inputlist::wbasefn** = .false.
- logical **inputlist::wmemory** = .false.
- logical **inputlist::wmetrix** = .false.
- logical **inputlist::wma00aa** = .false.

- logical **inputlist::wmatrix** = .false.
- logical **inputlist::wspsmat** = .false.
- logical **inputlist::wspsint** = .false.
- logical **inputlist::wmp00ac** = .false.
- logical **inputlist::wma02aa** = .false.
- logical **inputlist::wpackab** = .false.
- logical **inputlist::wtr00ab** = .false.
- logical **inputlist::wcurent** = .false.
- logical **inputlist::wdf00ab** = .false.
- logical **inputlist::wlforce** = .false.
- logical **inputlist::wintghs** = .false.
- logical **inputlist::wmtrxhs** = .false.
- logical **inputlist::wlbpol** = .false.
- logical **inputlist::wbrcast** = .false.
- logical **inputlist::wdfp100** = .false.
- logical **inputlist::wdfp200** = .false.
- logical **inputlist::wdforce** = .false.
- logical **inputlist::wnewton** = .false.
- logical **inputlist::wcasing** = .false.
- logical **inputlist::wbnorml** = .false.
- logical **inputlist::wjo00aa** = .false.
- logical **inputlist::wpp00aa** = .false.
- logical **inputlist::wpp00ab** = .false.
- logical **inputlist::wbfield** = .false.
- logical **inputlist::wstzxyz** = .false.
- logical **inputlist::whesian** = .false.
- logical **inputlist::wra00aa** = .false.
- logical **inputlist::wnumrec** = .false.
- logical **inputlist::wdcuhre** = .false.
- logical **inputlist::wminpack** = .false.
- logical **inputlist::wiqpack** = .false.
- logical **inputlist::wrksuite** = .false.
- logical **inputlist::wi1mach** = .false.
- logical **inputlist::wd1mach** = .false.
- logical **inputlist::wilut** = .false.
- logical **inputlist::witers** = .false.
- logical **inputlist::wsphdf5** = .false.
- logical **inputlist::wpreset** = .false.
- logical **inputlist::wglobal** = .false.
- logical **inputlist::wxspech** = .false.
- logical inputlist::wbuild_vector_potential = .false.
- logical **inputlist::wreadin** = .false.

  write screen output of readin()
- logical **inputlist::wwrtend** = .false.

  write screen output of wrtend()
- logical **inputlist::wmacros** = .false.

  write screen output from expanded macros

7.47.1 Detailed Description

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

7.47.2 Variable Documentation

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

Todo : what is this?

8 Module Documentation

8.1 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 **write_spec_namelist** ()
- 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 $|curlB\text{-}mu*B|$ *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**

  number of independent degrees of freedom in angle transformation;

- real, dimension(:,:,:), allocatable **dlambdaout**
- 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 **hdffdrz**

  derivatives of B^2 at the interfaces wrt geometry 2D Hessian;
- real, dimension(:,:,:,:,:), allocatable **denergydrr**

  derivatives of energy at the interfaces wrt geometry 3D Hessian;
- real, dimension(:,:,:,:,:), allocatable **denergydrz**

  derivatives of energy at the interfaces wrt geometry 3D Hessian;

- real, dimension(:,:,:,:,:), allocatable **denergydzr**
  derivatives of energy at the interfaces wrt geometry 3D Hessian;
- real, dimension(:,:,:,:,:), allocatable **denergydzz**
  derivatives of energy at the interfaces wrt geometry 3D Hessian;
- 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 (?)
- logical **lhessian2dallocated**
  flag to indicate that 2D Hessian matrix is allocated (?)
- real, dimension(:,:), allocatable **hessian2d**
  Hessian 2D.
- real, dimension(:,:), allocatable **dessian2d**
  derivative Hessian 2D
- logical **lhessian3dallocated**
  flag to indicate that 2D Hessian matrix is allocated (?)
- real, dimension(:,:), allocatable **hessian3d**
  Hessian 3D.
- real, dimension(:,:), allocatable **dessian3d**
  derivative Hessian 3D
- 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

8.1.1 Detailed Description

global variable storage used as "workspace" throughout the code

8.1.2 Function/Subroutine Documentation

8.1.2.1 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,

$$Isurf_i \rightarrow Isurf_i \cdot \frac{curtor}{\sum_{i=1}^{Mvol-1} Isurf_i + Ivol_i} Ivol_i \rightarrow Ivol_i \cdot \frac{curtor}{\sum_{i=1}^{Mvol-1} Isurf_i + Ivol_i} \tag{258}$$

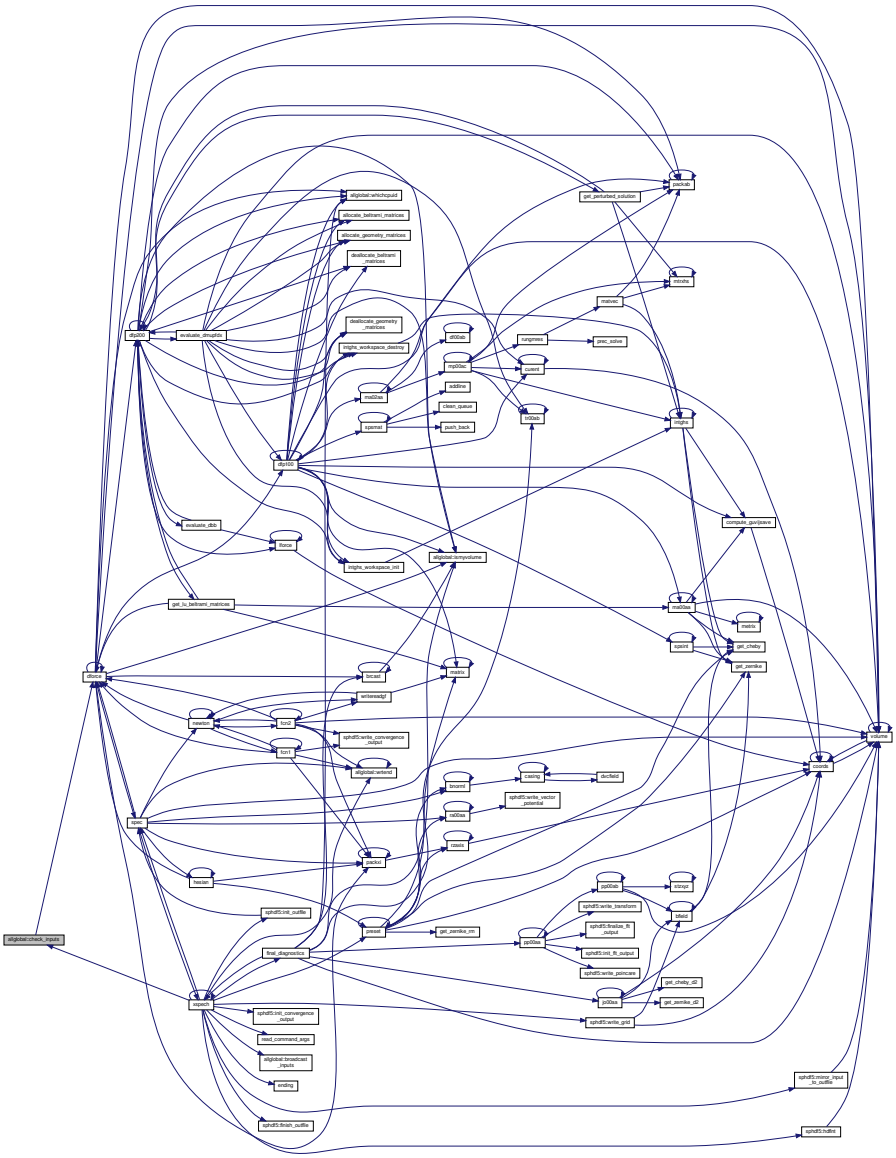
Finally, the volume current in the vacuum region is set to 0.

reading of numericlist
reading of locallist
reading of globallist
reading of diagnosticslist
reading of screenlist

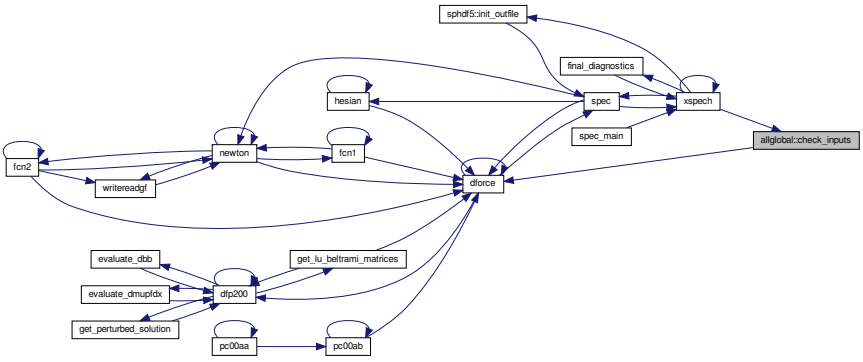
References inputlist::bnc, inputlist::c05factor, inputlist::c05xmax, inputlist::c05xtol, cpus, inputlist::curpol, inputlist::curtor, dforce(), inputlist::dpp, inputlist::dqq, inputlist::drz, inputlist::epsgmres, inputlist::epsilon, inputlist::epsilu, inputlist::escale, inputlist::forcetol, inputlist::gamma, 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, 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:



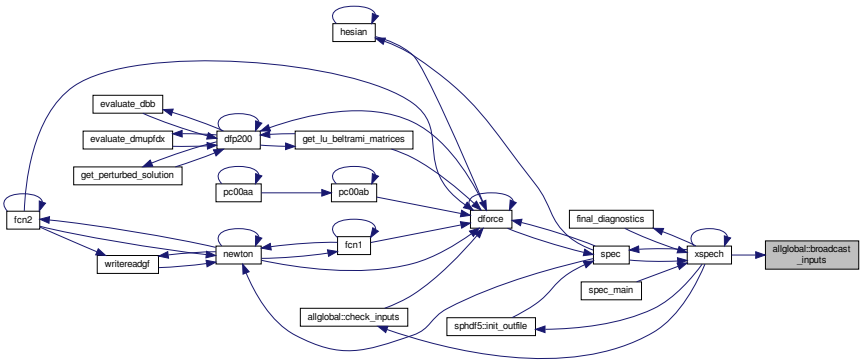
Here is the caller graph for this function:



8.1.2.2 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::ltransform, 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:



8.1.2.3 ismyvolume() `subroutine allglobal::ismyvolume (`

`integer, intent(in) vvol )`

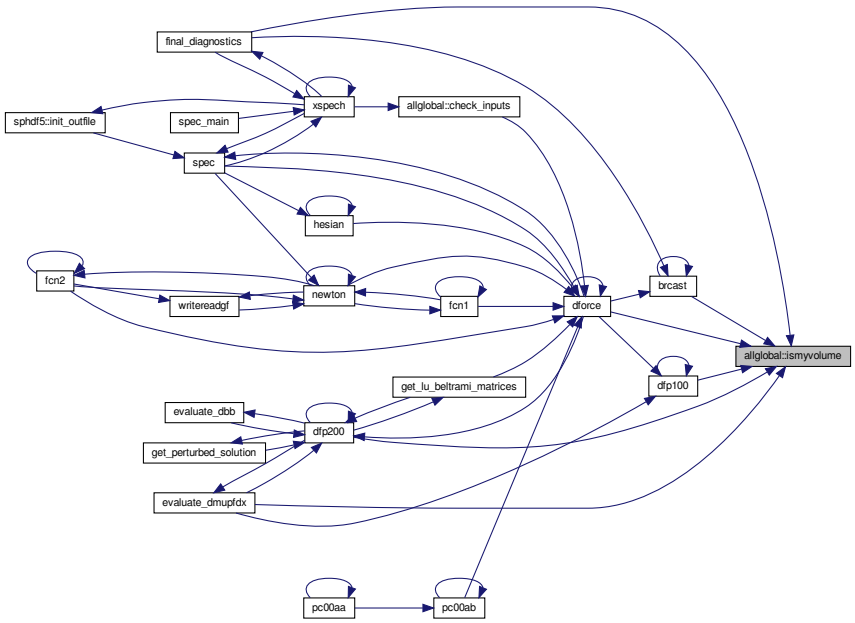
Check if volume vvol is associated to the corresponding MPI node.
The global variable `IsMyVolumeValue` is updated to 0 or 1, depending on `vvol` . A value of -1 is set if an error occured.

Parameters

vvol	volume to check

References ismyvolumevalue, myid, and ncpu.
Referenced by brcast(), dforce(), dfp100(), dfp200(), evaluate_dmupfdx(), and final_diagnostics().

Here is the caller graph for this function:



8.2 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** = 3.21

  version of SPEC

8.2.1 Detailed Description

some constants used throughout the code

8.3 cputiming Module Reference

timing variables

Variables

- real **tmanual** = 0.0
- real **manualt** = 0.0
- real **trzaxis** = 0.0
- real **rzaxist** = 0.0
- real **tpackxi** = 0.0
- real **packxit** = 0.0
- real **tvolume** = 0.0
- real **volumet** = 0.0
- real **tcoords** = 0.0
- real **coordst** = 0.0
- real **tbasefn** = 0.0
- real **basefnt** = 0.0
- real **tmemory** = 0.0
- real **memoryt** = 0.0
- real **tmetrix** = 0.0
- real **metrixt** = 0.0

- real **tma00aa** = 0.0
- real **ma00aat** = 0.0
- real **tmatrix** = 0.0
- real **matrixt** = 0.0
- real **tspsmat** = 0.0
- real **spsmatt** = 0.0
- real **tspsint** = 0.0
- real **spsintt** = 0.0
- real **tmp00ac** = 0.0
- real **mp00act** = 0.0
- real **tma02aa** = 0.0
- real **ma02aat** = 0.0
- real **tpackab** = 0.0
- real **packabt** = 0.0
- real **ttr00ab** = 0.0
- real **tr00abt** = 0.0
- real **tcurent** = 0.0
- real **curentt** = 0.0
- real **tdf00ab** = 0.0
- real **df00abt** = 0.0
- real **tlforce** = 0.0
- real **lforcet** = 0.0
- real **tintghs** = 0.0
- real **intghst** = 0.0
- real **tmtrxhs** = 0.0
- real **mtrxhst** = 0.0
- real **tlbpol** = 0.0
- real **lbpolt** = 0.0
- real **tbrcast** = 0.0
- real **brcastt** = 0.0
- real **tdfp100** = 0.0
- real **dfp100t** = 0.0
- real **tdfp200** = 0.0
- real **dfp200t** = 0.0
- real **tdforce** = 0.0
- real **dforcet** = 0.0
- real **tnewton** = 0.0
- real **newtont** = 0.0
- real **tcasing** = 0.0
- real **casingt** = 0.0
- real **tbnorml** = 0.0
- real **bnormlt** = 0.0
- real **tjo00aa** = 0.0
- real **jo00aat** = 0.0
- real **tpp00aa** = 0.0
- real **pp00aat** = 0.0
- real **tpp00ab** = 0.0
- real **pp00abt** = 0.0
- real **tbfield** = 0.0
- real **bfieldt** = 0.0
- real **tstzxyz** = 0.0
- real **stzxyzt** = 0.0
- real **thesian** = 0.0
- real **hesiant** = 0.0
- real **tra00aa** = 0.0

- real **ra00aat** = 0.0
- real **tnumrec** = 0.0
- real **numrect** = 0.0
- real **tdcuhre** = 0.0
- real **dcuhret** = 0.0
- real **tminpack** = 0.0
- real **minpackt** = 0.0
- real **tiqpack** = 0.0
- real **iqpackt** = 0.0
- real **trksuite** = 0.0
- real **rksuitet** = 0.0
- real **ti1mach** = 0.0
- real **i1macht** = 0.0
- real **td1mach** = 0.0
- real **d1macht** = 0.0
- real **tilut** = 0.0
- real **ilutt** = 0.0
- real **titers** = 0.0
- real **iterst** = 0.0
- real **tsphdf5** = 0.0
- real **sphdf5t** = 0.0
- real **tpreset** = 0.0
- real **presett** = 0.0
- real **tglobal** = 0.0
- real **globalt** = 0.0
- real **txspech** = 0.0
- real **xspecht** = 0.0
- real **tinputlist** = 0.0
- real **inputlistt** = 0.0
- real **treadin** = 0.0
- real **twrtend** = 0.0

8.3.1 Detailed Description

timing variables

8.4 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 (?)

8.4.1 Detailed Description

Interface to FFTW library.

8.5 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;

8.5.1 Detailed Description

central definition of file units to avoid conflicts

8.6 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;

8.6.1 Detailed Description

...todo...

8.7 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 (?)

8.7.1 Detailed Description

timing of Newton iterations

8.8 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;

8.8.1 Detailed Description

platform-dependant numerical resolution

8.9 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 "/iterations")
- integer(hid_t) **dt_energy_id**

  Memory datatype identifier (for "Energy" dataset in "/iterations")
- integer(hid_t) **dt_forceerr_id**

  Memory datatype identifier (for "ForceErr" dataset in "/iterations")
- integer(hid_t) **dt_irbc_id**

  Memory datatype identifier (for "iRbc" dataset in "/iterations")
- integer(hid_t) **dt_izbs_id**

  Memory datatype identifier (for "iZbs" dataset in "/iterations")
- integer(hid_t) **dt_irbs_id**

Memory datatype identifier (for "iRbs" dataset in "/iterations")

- integer(hid_t) **dt_izbc_id**

  Memory datatype identifier (for "iZbc" dataset in "/iterations")

- 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.

8.9.1 Detailed Description

writing the HDF5 output file

8.10 typedefns Module Reference

type definitions for custom datatypes

Data Types

- type derivative

  $\mathrm{d}\mathbf{B}/\mathrm{d}\mathbf{X}$ *(?) More...*
- type matrixlu
- type subgrid

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

8.10.1 Detailed Description

type definitions for custom datatypes

8.10.2 Data Type Documentation

8.10.2.1 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?

Class Members

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

8.10.2.2 type typedefns::matrixlu

8.10.2.3 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

9 Data Type Documentation

9.1 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**

9.1.1 Detailed Description

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

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

9.1.2 Member Data Documentation

9.1.2.1 efmn `real, dimension(:,:), allocatable intghs_module::intghs_workspace::efmn`
This is efmn.

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

This is ofmn.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- src/intghs.f90

10 File Documentation

10.1 src/basefn.f90 File Reference

Polynomials evaluation.

Functions/Subroutines

- subroutine get_cheby (lss, lrad, cheby)

  Get the Chebyshev polynomials with zeroth, first derivatives.
- subroutine get_cheby_d2 (lss, lrad, cheby)

  Get the Chebyshev polynomials with zeroth, first and second derivatives The Chebyshev polynomial has been recombined and rescaled. See get_cheby for more detail.
- subroutine get_zernike (r, lrad, mpol, zernike)

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

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

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

10.1.1 Detailed Description

Polynomials evaluation.

10.1.2 Function/Subroutine Documentation

10.1.2.1 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.

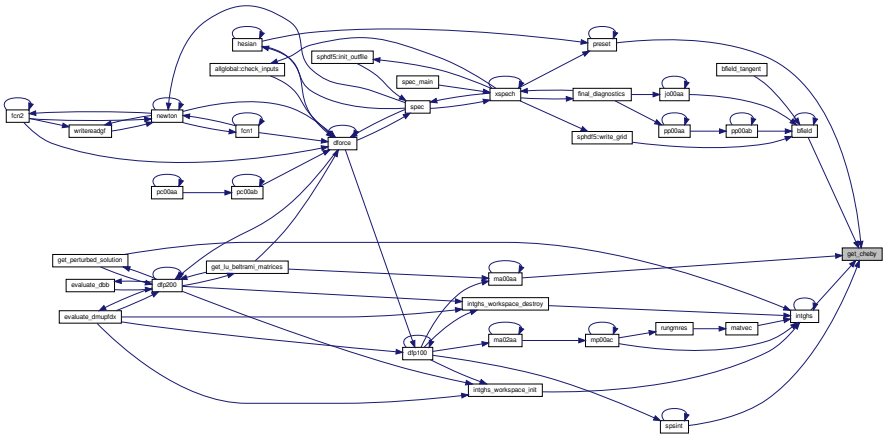
$$T_0(s) = 1,$$
$$T_1(s) = s,$$
$$T_{l+1}(s) = 2sT_l(s) - T_{l-1}(s).$$

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:



10.1.2.2 get_cheby_d2() `subroutine get_cheby_d2 (`

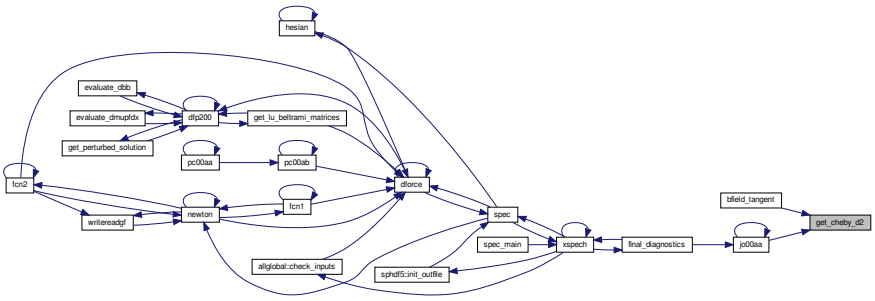
```
real, intent(in) lss,
integer, intent(in) lrad,
real, dimension(0:lrad,0:2), intent(inout) cheby )
```

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:



10.1.2.3 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

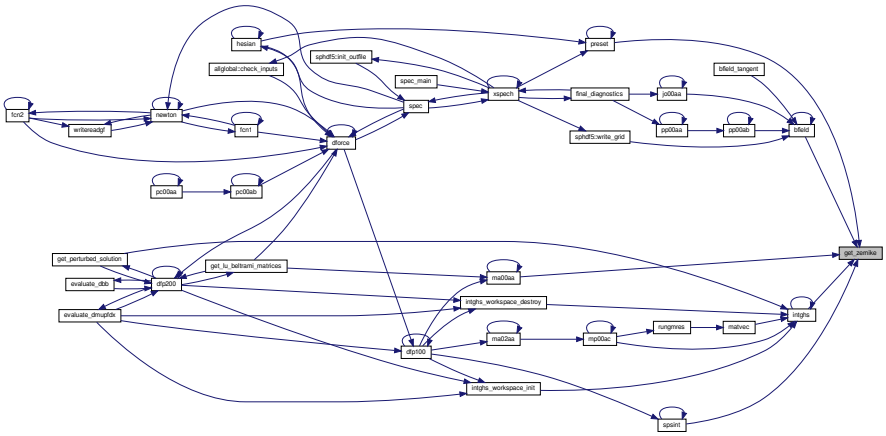
$$\hat{R}_l^m = \frac{1}{l+1}R_l^m.$$

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:



10.1.2.4 get_zernike_d2()

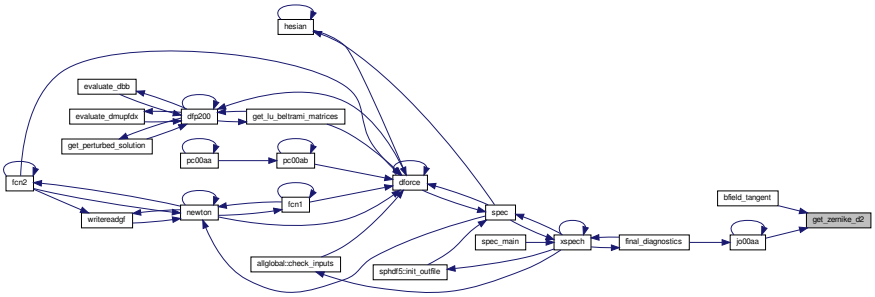
```
subroutine get_zernike_d2 (
    real, intent(in) r,
    integer, intent(in) lrad,
    integer, intent(in) mpol,
    real, dimension(0:lrad,0:mpol,0:2), intent(inout) zernike )
```

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:



10.1.2.5 get_zernike_rm()

```
subroutine get_zernike_rm (
    real, intent(in) r,
```

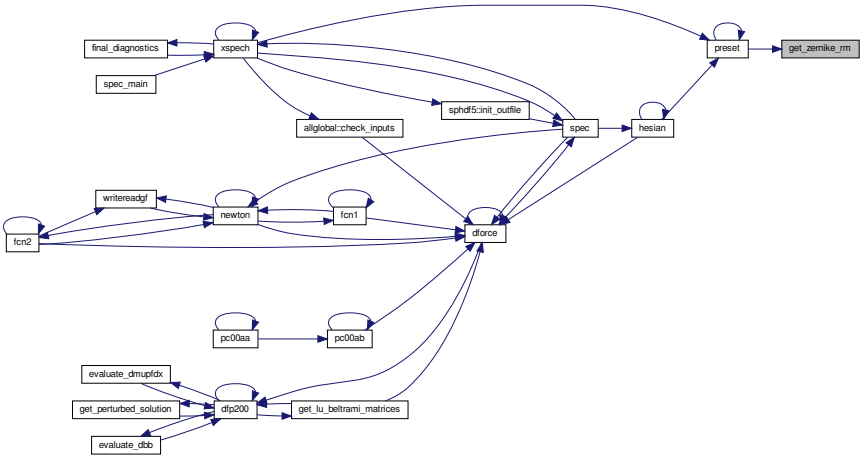
```
integer, intent(in) lrad,
integer, intent(in) mpol,
real, dimension(0:lrad,0:mpol), intent(inout) zernike )
```

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:



10.2 src/bfield.f90 File Reference

Returns $\dot{s} \equiv B^s / B^\zeta$ and $\dot{\theta} \equiv B^\theta / B^\zeta$.

Functions/Subroutines

- subroutine bfield (zeta, st, Bst)

  Compute the magnetic field.
- subroutine bfield_tangent (zeta, st, Bst)

  compute the tangential magnetic field

10.2.1 Detailed Description

Returns $\dot{s} \equiv B^s / B^\zeta$ and $\dot{\theta} \equiv B^\theta / B^\zeta$.

10.2.2 Function/Subroutine Documentation

10.2.2.1 bfield_tangent()

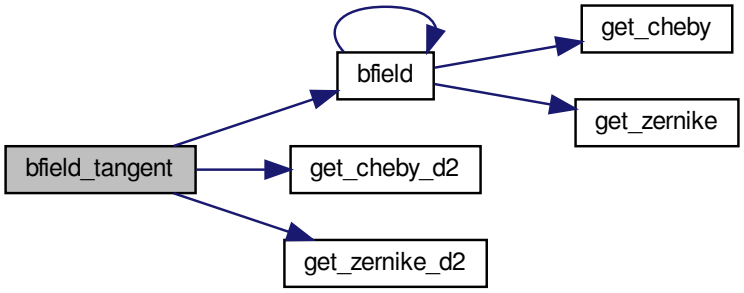
```
subroutine bfield_tangent (
    real, intent(in) zeta,
    real, dimension(1:6), intent(in) st,
    real, dimension(1:6), intent(out) Bst )
```

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:



10.3 src/bnorml.f90 File Reference

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

Functions/Subroutines

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

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

10.3.1 Detailed Description

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

10.4 src/brcast.f90 File Reference

Broadcasts Beltrami fields, profiles, . . .

Functions/Subroutines

- subroutine brcast (lvol)

  Broadcasts Beltrami fields, profiles, . . .

10.4.1 Detailed Description

Broadcasts Beltrami fields, profiles, . . .

10.5 src/casing.f90 File Reference

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

Functions/Subroutines

- subroutine casing (teta, zeta, gBn, icasing)

  Constructs the field created by the plasma currents, at an arbitrary, external location using virtual casing.
- subroutine dvcfield (Ndim, tz, Nfun, vcintegrand)

  Differential virtual casing integrand.

10.5.1 Detailed Description

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

10.6 src/coords.f90 File Reference

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

Functions/Subroutines

- subroutine coords (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.

10.6.1 Detailed Description

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

10.7 src/curent.f90 File Reference

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

Functions/Subroutines

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

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

10.7.1 Detailed Description

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

10.8 src/df00ab.f90 File Reference

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

Functions/Subroutines

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

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

10.8.1 Detailed Description

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

10.9 src/dforce.f90 File Reference

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

Functions/Subroutines

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

  Calculates $\mathbf{F}(\mathbf{x})$, 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)

10.9.1 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 $\nabla\mathbf{F}$.

10.10 src/dfp100.f90 File Reference

Split the work between MPI nodes and evaluate the global constraint.

Functions/Subroutines

- subroutine dfp100 (Ndofgl, x, Fvec, LComputeDerivatives)

  Split the work between MPI nodes and evaluate the global constraint.

10.10.1 Detailed Description

Split the work between MPI nodes and evaluate the global constraint.

10.10.2 Function/Subroutine Documentation

10.10.2.1 dfp100()

```
subroutine dfp100 (
    integer Ndofgl,
    real, dimension(1:mvol-1) x,
    real, dimension(1:ndofgl) Fvec,
    logical LComputeDerivatives )
```

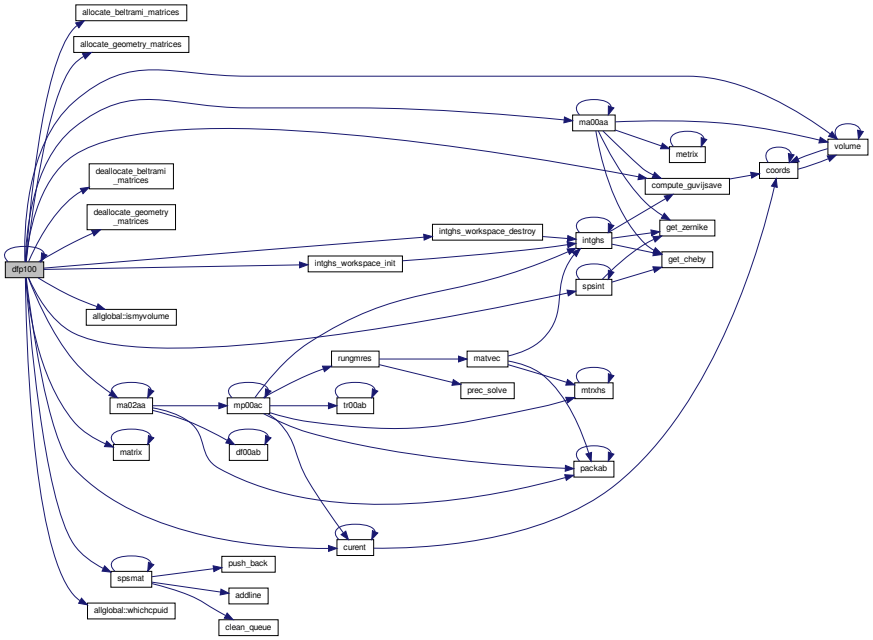
Split the work between MPI nodes and evaluate the global constraint.

Parameters

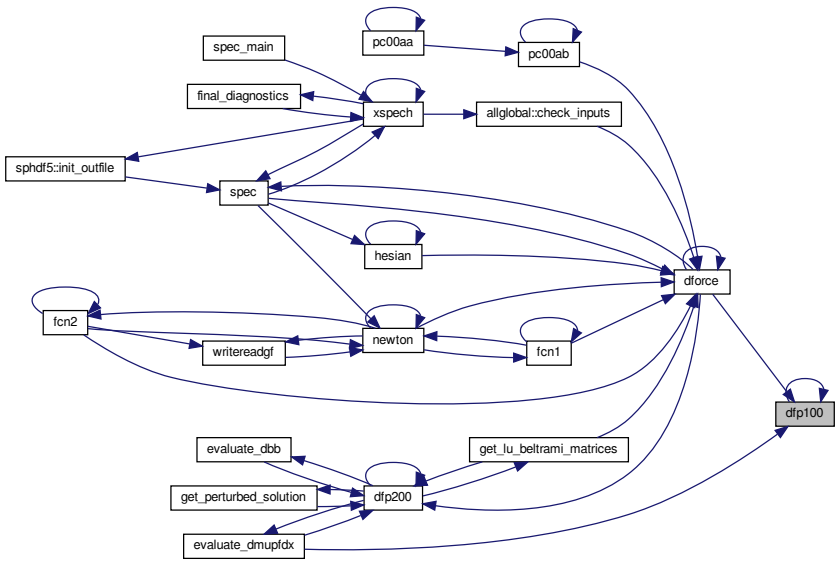
Ndofgl	
x	
Fvec	
LComputeDerivatives	

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(), dfp100(), 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, allglobal::in, intghs_workspace_destroy(), intghs_workspace_init(), allglobal::ipdtdpf, allglobal::iquad, allglobal::ismyvolume(), allglobal::ismyvolumevalue, inputlist::isurf, allglobal::izbs, inputlist::lconstraint, allglobal::lcoordinatesingularity, inputlist::lfreebound, allglobal::liluprecond, allglobal::localconstraint, allglobal::lplasmaregion, inputlist::lrad, allglobal::lsavedguvij, allglobal::lvacuumregion, ma00aa(), ma02aa(), matrix(), allglobal::mbpsi, allglobal::mn, allglobal::mpi_comm_spec, constants::mu0, allglobal::myid, allglobal::nadof, allglobal::ncpu, allglobal::notmatrixfree, allglobal::nt, inputlist::nvol, allglobal::nz, constants::one, fileunits::ounit, constants::pi, constants::pi2, allglobal::solution, spsint(), spsmat(), allglobal::tdstcc, allglobal::tdstcs, allglobal::tdstsc,

allglobal::tdstss, allglobal::tdszcc, allglobal::tdszcs, 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(), dfp100(), and evaluate_dmupfdx().
Here is the call graph for this function:



Here is the caller graph for this function:



10.11 src/dfp200.f90 File Reference

Given the field consistent with the constraints and the geometry, computes local quantites related to the force evaluation.

Functions/Subroutines

- subroutine dfp200 (LcomputeDerivatives, vvol)

  Given the field consistent with the constraints and the geometry, computes local quantites related to the force evaluation.
- subroutine get_lu_beltrami_matrices (vvol, oBI, NN)

  get LU Beltrami matrices
- subroutine get_perturbed_solution (vvol, oBI, NN)

  This routine evaluates the value of the magnetic field once the interface is perturbed using matrix perturbation theory.
- subroutine evaluate_dmupfdx (innout, idof, ii, issym, irz)

  Evaluate mu and psip derivatives and store them in dmupfdx.
- subroutine evaluate_dbb (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.
- subroutine **hessian_dffdrz** (lvol, idof, innout, issym, irz, ii, dBB, XX, YY, length, dRR, dZZ, dII, dLL, dPP, Ntz)
- subroutine **hessian3d_dffdrz** (lvol, idof, innout, issym, irz, ii, dBB, XX, YY, length, dRR, dZZ, dII, dLL, dPP, Ntz)

10.11.1 Detailed Description

Given the field consistent with the constraints and the geometry, computes local quantites related to the force evaluation.

10.11.2 Function/Subroutine Documentation

10.11.2.1 dfp200() `subroutine dfp200 (`

```
logical, intent(in) LcomputeDerivatives,
integer vvol )
```

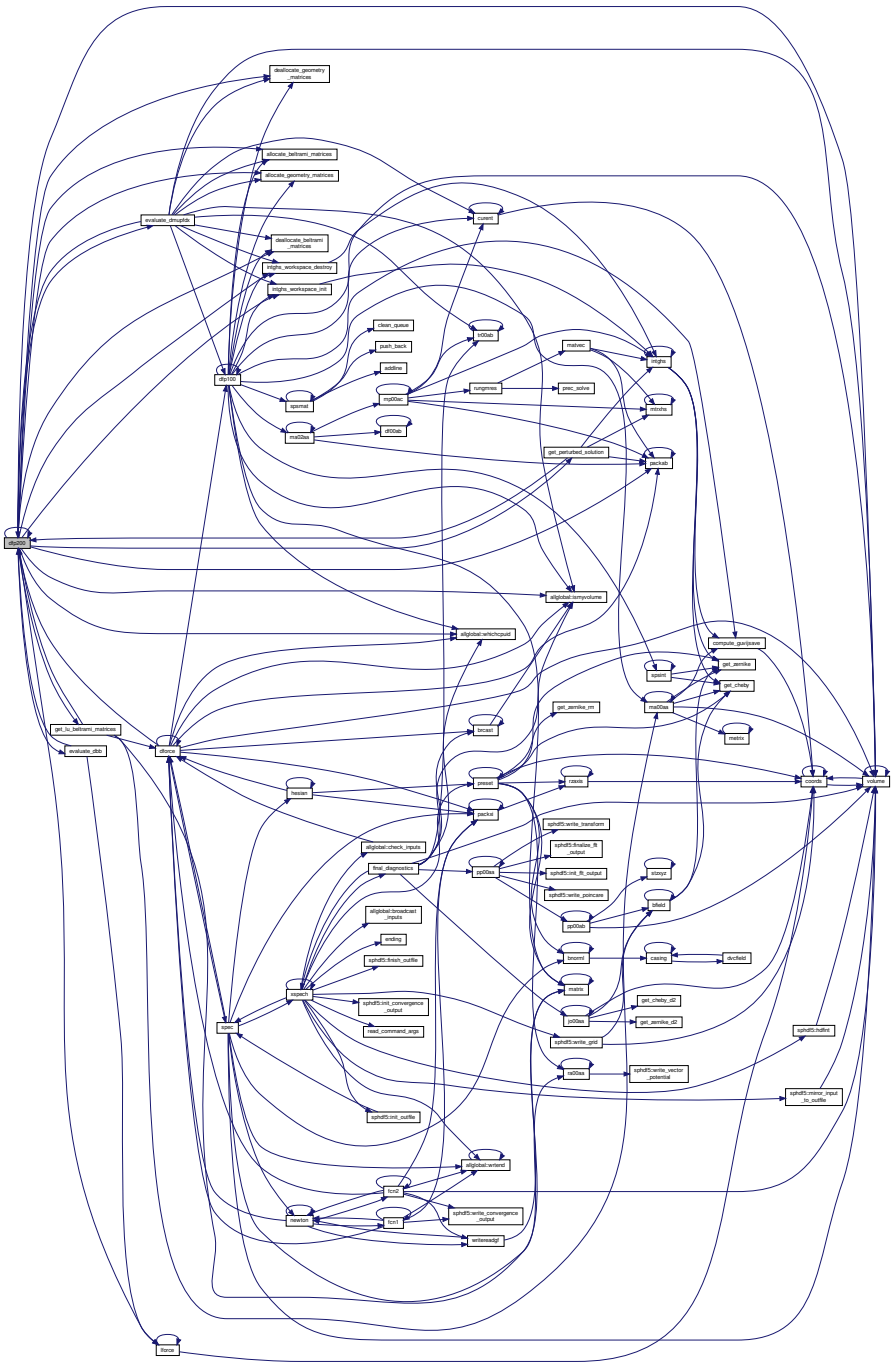
Given the field consistent with the constraints and the geometry, computes local quantites related to the force evaluation.

Parameters

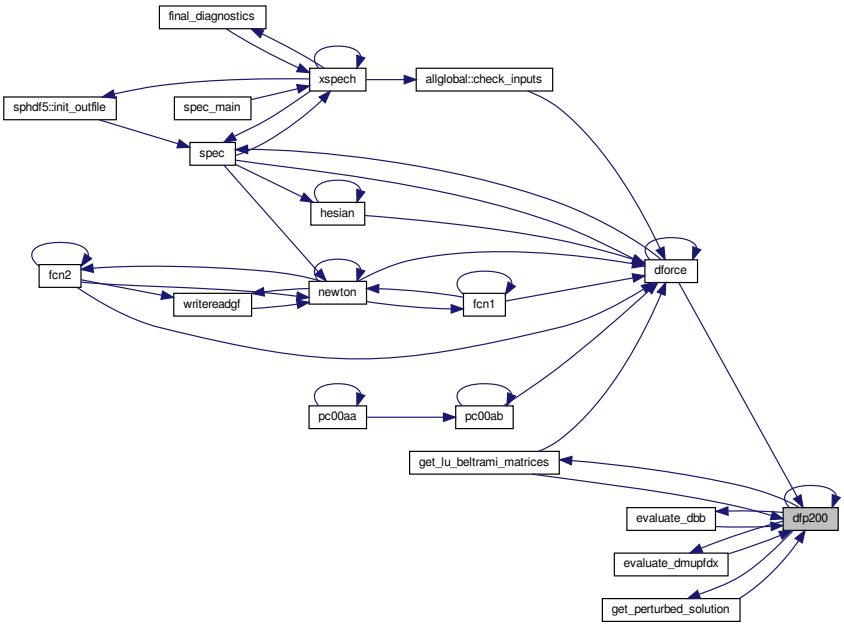
LcomputeDerivatives	
vvol	

References inputlist::adiabatic, allocate_beltrami_matrices(), allocate_geometry_matrices(), allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::bbweight, allglobal::bemn, allglobal::bomn, allglobal::btemn, allglobal::cfmn, allglobal::comn, allglobal::cosi, allglobal::cpus, allglobal::dbbdmp, allglobal::dbdx, deallocate_beltrami_matrices(), deallocate_geometry_matrices(), allglobal::denergydrr, allglobal::denergydzr, allglobal::dessian, allglobal::dffdrz, dfp200(), allglobal::diotadxup, allglobal::ditgpdxtp, allglobal::dma, allglobal::dmb, allglobal::dmd, allglobal::dmg, allglobal::dmupfdx, allglobal::dpflux, allglobal::drij, allglobal::drodr, allglobal::drodz, allglobal::dtflux, allglobal::dvolume, allglobal::dzij, allglobal::dzodr, allglobal::dzodz, allglobal::efmn, inputlist::epsilon, evaluate_dbb(), evaluate_dmupfdx(), allglobal::evmn, inputlist::gamma, get_lu_beltrami_matrices(), get_perturbed_solution(), allglobal::guvij, constants::half, allglobal::hessian, allglobal::iemn, inputlist::igeometry, allglobal::ijreal, allglobal::im, allglobal::in, intghs_workspace_destroy(), intghs_workspace_init(), allglobal::iomn, allglobal::iquad, allglobal::irbc, allglobal::irbs, allglobal::irij, allglobal::ismyvolume(), allglobal::ismyvolumevalue, allglobal::izbc, allglobal::izbs, allglobal::izij, inputlist::lcheck, inputlist::lconstraint, allglobal::lcoordinatesingularity, inputlist::lextrap, inputlist::lfindzero, lforce(), inputlist::lfreebound, allglobal::lgdof, allglobal::lhessian2dallocated, allglobal::lhessian3dallocated, allglobal::lhessianallocated, inputlist::lhmatrix, allglobal::lmns, allglobal::localconstraint, allglobal::lplasmaregion, inputlist::lrad, allglobal::lvacuumregion, allglobal::mmpp, allglobal::mn, allglobal::mne, allglobal::mns, allglobal::mpi_comm_spec, inputlist::mpol, inputlist::mu, allglobal::myid, allglobal::nadof, allglobal::ncpu, allglobal::notstellsym, allglobal::nt, inputlist::ntor, allglobal::ntz, inputlist::nvol, allglobal::nz, allglobal::odmn, allglobal::ofmn, constants::one, fileunits::ounit, packab(), inputlist::pscale, allglobal::psifactor, allglobal::rij, allglobal::semn, allglobal::sfmn, allglobal::sg, allglobal::simn, allglobal::sini, numerical::small, allglobal::solution, allglobal::somn, allglobal::sweight, inputlist::tflux,

allglobal::trij, constants::two, allglobal::tzij, volume(), allglobal::vvolume, allglobal::whichcpuid(), inputlist::wmacros, allglobal::yesstellsym, constants::zero, and allglobal::zij.
Referenced by dforce(), dfp200(), 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:



10.11.2.2 get_lu_beltrami_matrices()

```
subroutine get_lu_beltrami_matrices (
    integer, intent(in) vvol,
    type(matrixlu), intent(inout) oBI,
    integer, intent(in) NN )
```

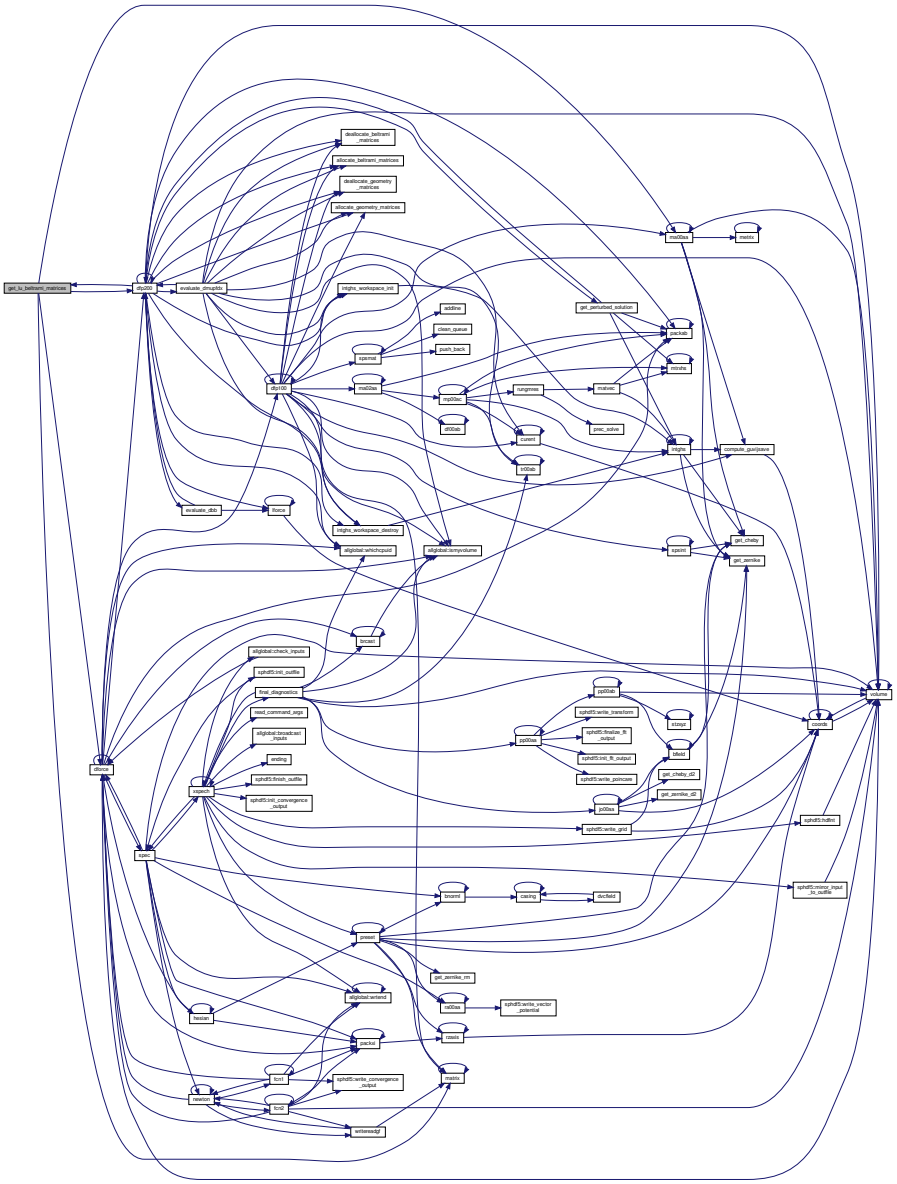
get LU Beltrami matrices

Parameters

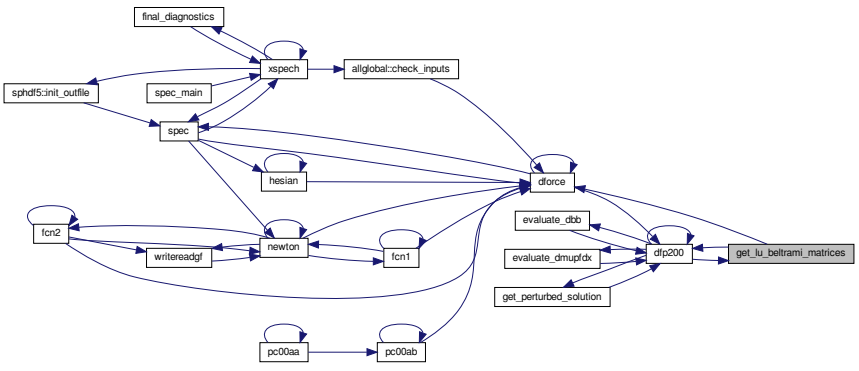
vvol	
oBI	
NN	

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:



10.11.2.3 get_perturbed_solution()

```
subroutine get_perturbed_solution (
    integer, intent(in) vvol,
    type(matrixlu), intent(inout) oBI,
    integer, intent(in) NN )
```

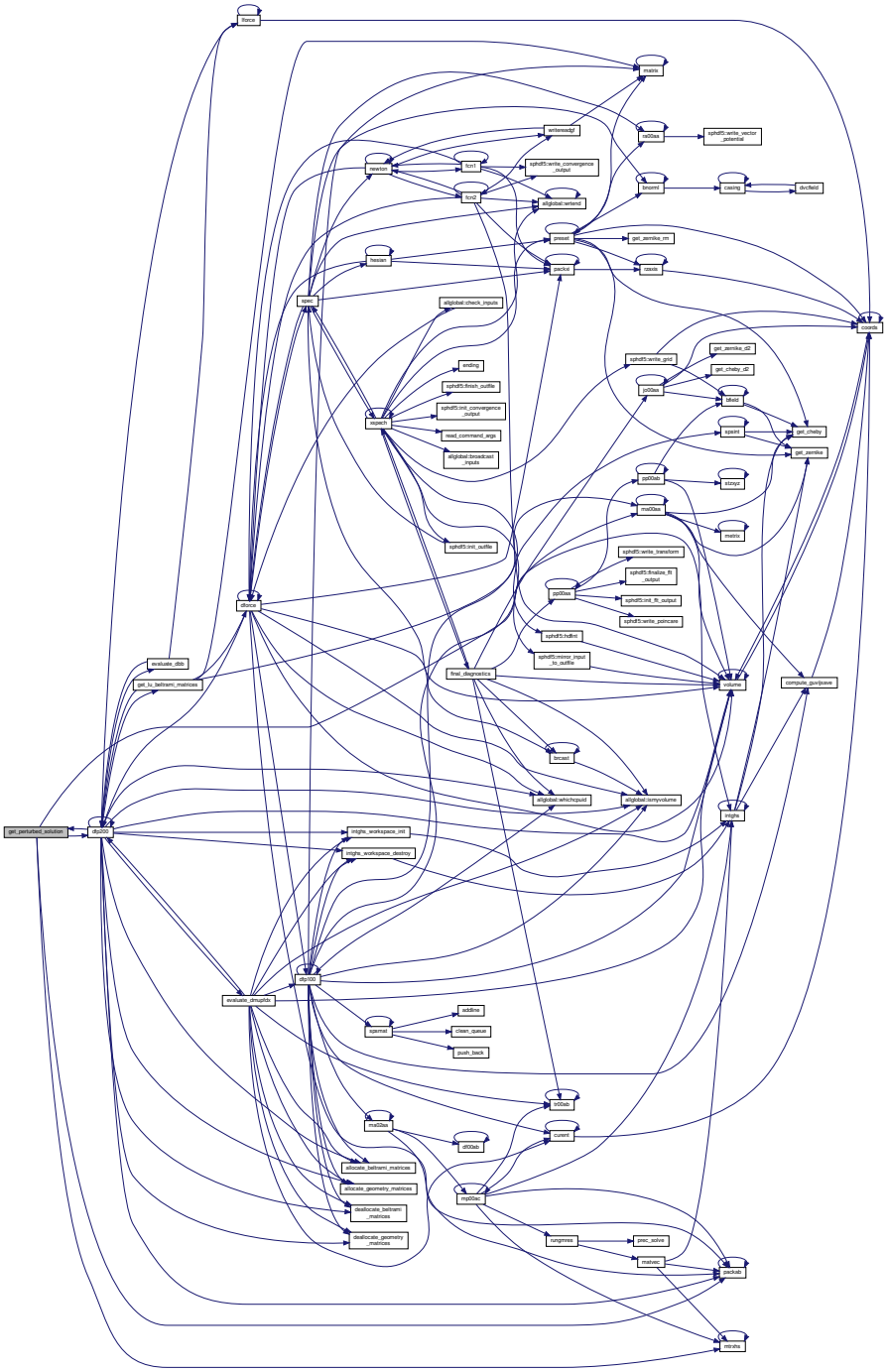
This routine evaluates the value of the magnetic field once the interface is perturbed using matrix perturbation theory.

Parameters

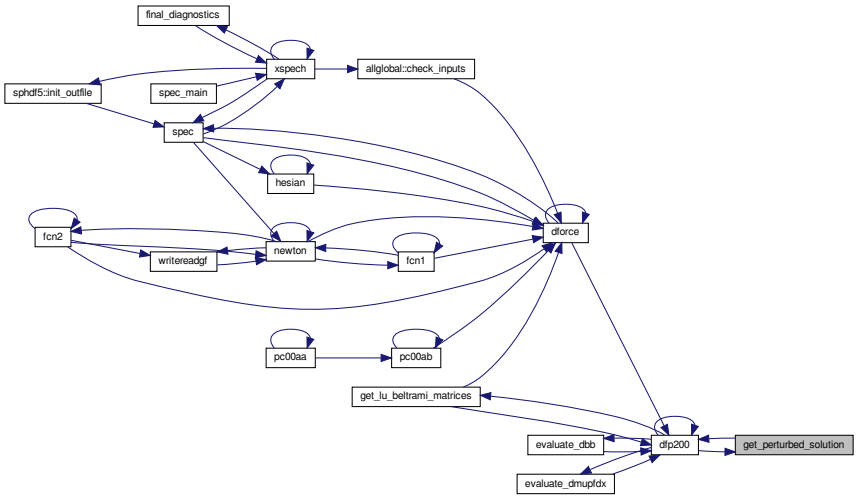
vvol	
oBI	
NN	

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:



10.11.2.4 evaluate_dmupfdx()

```
subroutine evaluate_dmupfdx (
    integer innout,
    integer idof,
    integer ii,
    integer issym,
    integer irz )
```

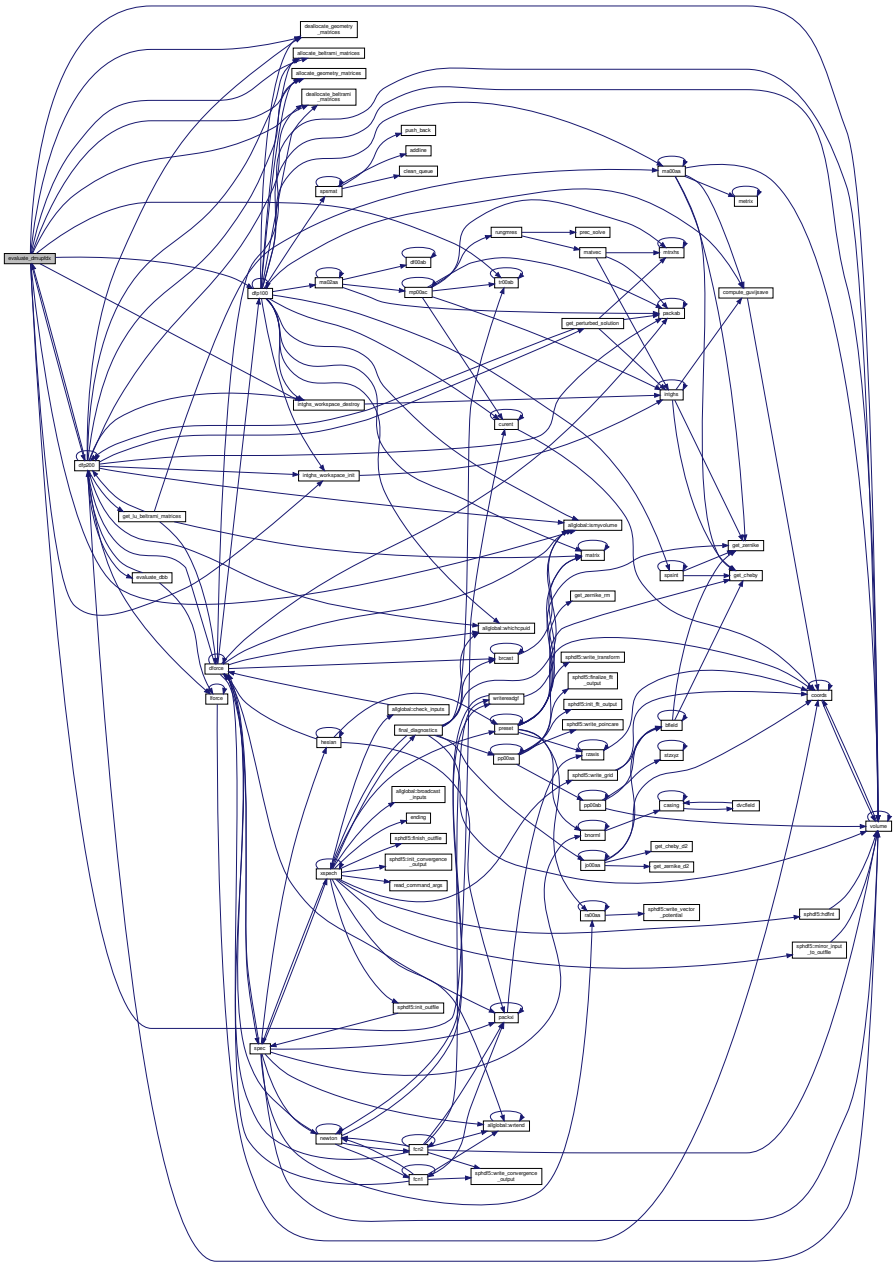
Evaluate mu and psip derivatives and store them in dmupfdx.

Parameters

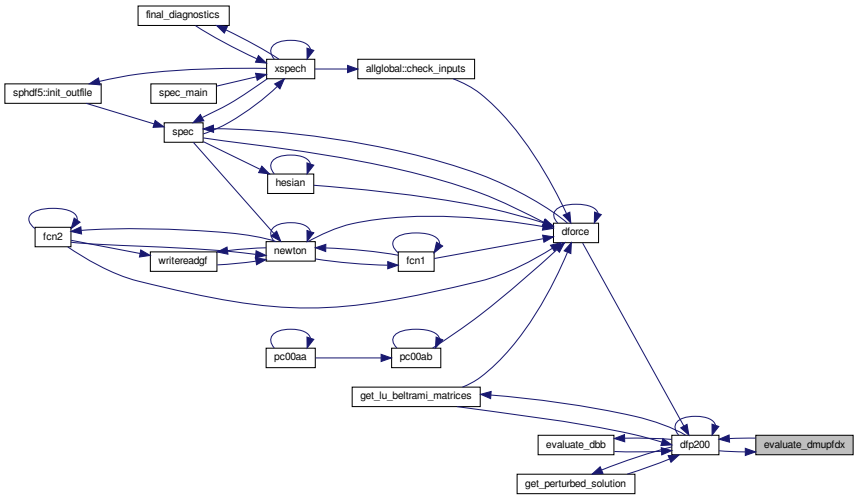
innout	
idof	
ii	
issym	
irz	

References allocate_beltrami_matrices(), allocate_geometry_matrices(), allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::btemn, allglobal::cpus, curent(), allglobal::dbdx, deallocate_beltrami_matrices(), deallocate_geometry_matrices(), dfp100(), dfp200(), allglobal::diotadxup, allglobal::ditgpdxtp, allglobal::dma, allglobal::dmb, allglobal::dmd, allglobal::dmg, allglobal::dmupfdx, allglobal::dpflux, inputlist::drz, allglobal::dtflux, allglobal::dvolume, constants::half, inputlist::igeometry, allglobal::im, allglobal::in, intghs_workspace_destroy(), intghs_workspace_init(), allglobal::ipdtdpf, allglobal::iquad, allglobal::irbc, allglobal::irbs, allglobal::ismyvolume(), allglobal::ismyvolumevalue, allglobal::izbc, allglobal::izbs, inputlist::lcheck, inputlist::lconstraint, allglobal::lcoordinatesingularity, inputlist::lfreebound, allglobal::lmns, allglobal::localconstraint, allglobal::lplasmaregion, inputlist::lrad, allglobal::lvacuumregion, allglobal::mn, allglobal::mne, allglobal::mns, allglobal::mpi_comm_spec, inputlist::mu, inputlist::mupftol, allglobal::myid, allglobal::nadof, allglobal::ncpu, allglobal::ngdof, allglobal::nt, inputlist::nvol, allglobal::nz, constants::one, fileunits::ounit, allglobal::psifactor, allglobal::rij, numerical::small, allglobal::sweight, tr00ab(), constants::two, volume(), allglobal::vvolume, inputlist::wmacros, allglobal::xoffset, constants::zero, and allglobal::zij.
Referenced by dfp200().

Here is the call graph for this function:



Here is the caller graph for this function:



10.11.2.5 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

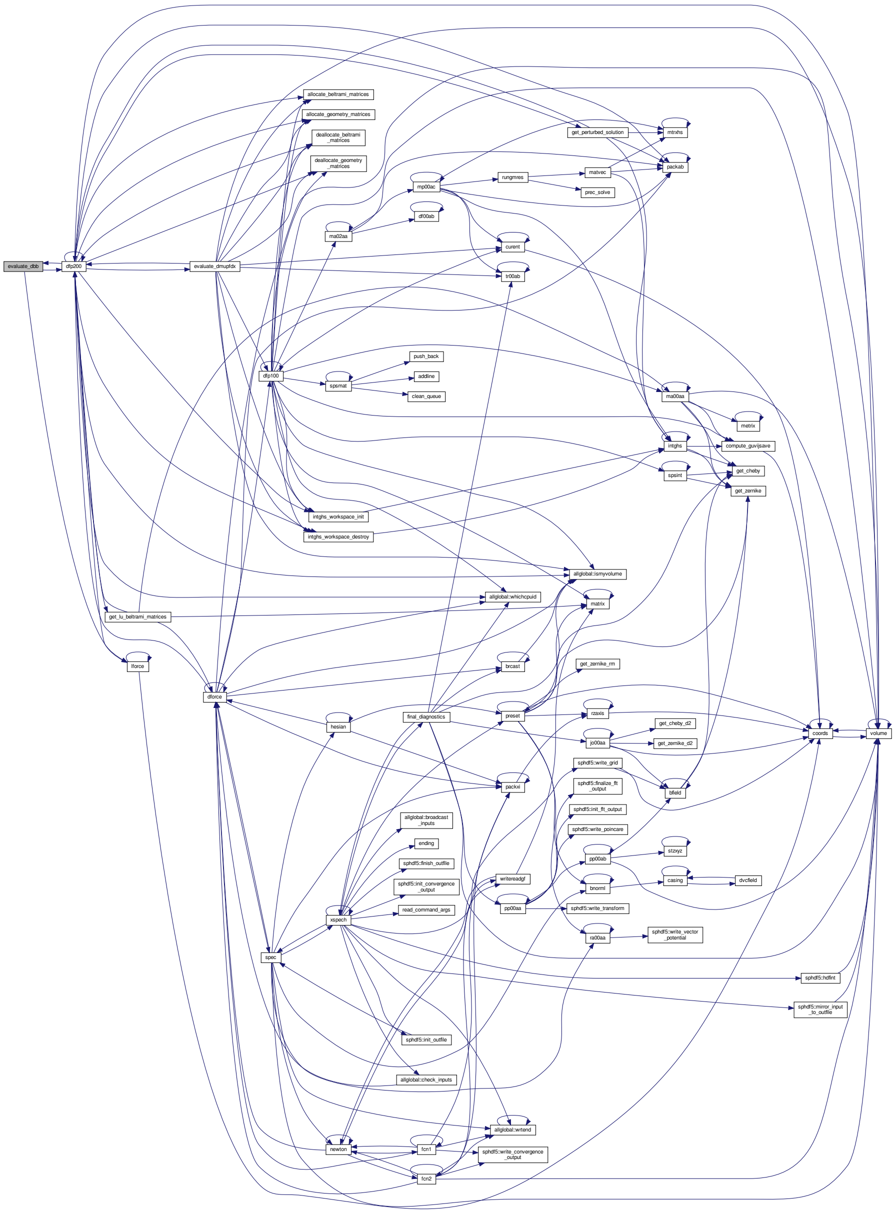
lvol	
idof	
innout	
issym	
irz	
ii	
dBB	
XX	
YY	
length	
dRR	

Parameters

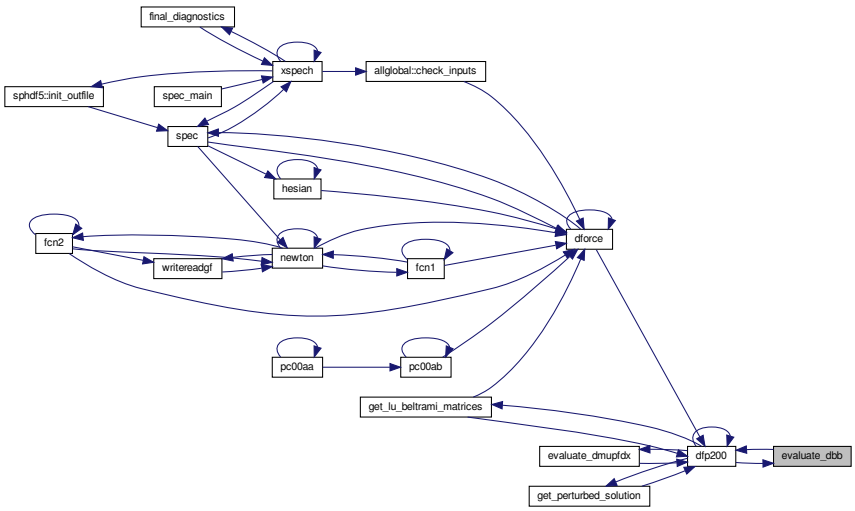
dZZ	
dII	
dLL	
dPP	
Ntz	
LcomputeDerivatives	

References inputlist::adiabatic, allglobal::bbweight, allglobal::cfmn, allglobal::comn, allglobal::cosi, allglobal::cpus, allglobal::dbbdmp, allglobal::dbdx, allglobal::denergydrr, allglobal::denergydrz, allglobal::denergydzr, allglobal::denergydzz, allglobal::dffdrz, dfp200(), allglobal::dpflux, allglobal::drij, allglobal::drodr, allglobal::drodz, inputlist::drz, allglobal::dvolume, allglobal::dzij, allglobal::dzodr, allglobal::dzodz, allglobal::efmn, inputlist::epsilon, allglobal::evmn, inputlist::gamma, allglobal::guvij, constants::half, allglobal::hdffdrz, inputlist::igeometry, allglobal::ijreal, allglobal::im, allglobal::in, allglobal::iquad, allglobal::irbc, allglobal::irbs, allglobal::irij, allglobal::izbc, allglobal::izbs, allglobal::izij, inputlist::lcheck, inputlist::lconstraint, allglobal::lcoordinatesingularity, lforce(), allglobal::lgdof, allglobal::lhessian3dallocated, allglobal::localconstraint, allglobal::lplasmaregion, inputlist::lrad, allglobal::lvacuumregion, allglobal::mmpp, allglobal::mn, allglobal::mns, allglobal::mpi_comm_spec, allglobal::myid, allglobal::nadof, allglobal::ncpu, allglobal::ngdof, allglobal::notstellsym, allglobal::nt, inputlist::ntor, inputlist::nvol, allglobal::nz, allglobal::odmn, allglobal::ofmn, constants::one, fileunits::ounit, inputlist::pscale, allglobal::psifactor, allglobal::rij, allglobal::sfmn, allglobal::sg, allglobal::simn, allglobal::sini, numerical::small, allglobal::sweight, allglobal::trij, constants::two, allglobal::tzij, allglobal::vvolume, inputlist::wmacros, allglobal::xoffset, allglobal::yesstellsym, constants::zero, and allglobal::zij.
Referenced by dfp200().

Here is the call graph for this function:



Here is the caller graph for this function:



10.12 src/global.f90 File Reference

Defines input namelists and global variables, and opens some output files.

Data Types

- type typedefns::subgrid

  used for quantities which have different resolutions in different volumes, e.g. the vector potential More...
- type typedefns::matrixlu
- type typedefns::derivative

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

Modules

- module constants

  some constants used throughout the code
- module numerical

  platform-dependant numerical resolution
- module fileunits

  central definition of file units to avoid conflicts
- module cputiming

  timing variables
- module typedefns

  type definitions for custom datatypes
- module allglobal

  global variable storage used as "workspace" throughout the code
- module fftw_interface

  Interface to FFTW library.

Functions/Subroutines

- subroutine **fileunits::mute** (action)
- subroutine **allglobal::build_vector_potential** (lvol, iocons, aderiv, tderiv)
- subroutine **allglobal::set_mpi_comm** (comm)
- subroutine **allglobal::read_inputlists_from_file** ()
- subroutine **allglobal::write_spec_namelist** ()
- 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** = 3.21

  version of SPEC
- real, parameter **numerical::machprec** = 1.11e-16

  machine precision: 0.5$*$*epsilon(one) for 64 bit double precision*
- real, parameter **numerical::vsmall** = 100$*$machprec

  very small number
- real, parameter **numerical::small** = 10000$*$machprec

  small number
- real, parameter **numerical::sqrtmachprec** = sqrt(machprec)

  square root of machine precision
- real, parameter **numerical::logtolerance** = 1.0e-32

  this is used to avoid taking alog10(zero); see e.g. dforce;
- integer **fileunits::iunit** = 10

  input; used in global/readin:ext.sp, global/wrtend:ext.sp.end
- integer **fileunits::ounit** = 6

  screen output;
- integer **fileunits::gunit** = 13

  wall geometry; used in wa00aa
- integer **fileunits::aunit** = 11

  vector potential; used in ra00aa:.ext.AtAzmn;
- integer **fileunits::dunit** = 12

  derivative matrix; used in newton:.ext.GF;
- integer **fileunits::hunit** = 14

  eigenvalues of Hessian; under re-construction;
- integer **fileunits::munit** = 14

  matrix elements of Hessian;
- integer **fileunits::lunit** = 20

  local unit; used in lunit+myid: pp00aa:.ext.poincare,.ext.transform;
- integer **fileunits::vunit** = 15

  for examination of adaptive quadrature; used in casing:.ext.vcint;
- real **cputiming::tmanual** = 0.0
- real **cputiming::manualt** = 0.0
- real **cputiming::trzaxis** = 0.0
- real **cputiming::rzaxist** = 0.0
- real **cputiming::tpackxi** = 0.0
- real **cputiming::packxit** = 0.0
- real **cputiming::tvolume** = 0.0

- real **cputiming::volumet** = 0.0
- real **cputiming::tcoords** = 0.0
- real **cputiming::coordst** = 0.0
- real **cputiming::tbasefn** = 0.0
- real **cputiming::basefnt** = 0.0
- real **cputiming::tmemory** = 0.0
- real **cputiming::memoryt** = 0.0
- real **cputiming::tmetrix** = 0.0
- real **cputiming::metrixt** = 0.0
- real **cputiming::tma00aa** = 0.0
- real **cputiming::ma00aat** = 0.0
- real **cputiming::tmatrix** = 0.0
- real **cputiming::matrixt** = 0.0
- real **cputiming::tspsmat** = 0.0
- real **cputiming::spsmatt** = 0.0
- real **cputiming::tspsint** = 0.0
- real **cputiming::spsintt** = 0.0
- real **cputiming::tmp00ac** = 0.0
- real **cputiming::mp00act** = 0.0
- real **cputiming::tma02aa** = 0.0
- real **cputiming::ma02aat** = 0.0
- real **cputiming::tpackab** = 0.0
- real **cputiming::packabt** = 0.0
- real **cputiming::ttr00ab** = 0.0
- real **cputiming::tr00abt** = 0.0
- real **cputiming::tcurent** = 0.0
- real **cputiming::curentt** = 0.0
- real **cputiming::tdf00ab** = 0.0
- real **cputiming::df00abt** = 0.0
- real **cputiming::tlforce** = 0.0
- real **cputiming::lforcet** = 0.0
- real **cputiming::tintghs** = 0.0
- real **cputiming::intghst** = 0.0
- real **cputiming::tmtrxhs** = 0.0
- real **cputiming::mtrxhst** = 0.0
- real **cputiming::tlbpol** = 0.0
- real **cputiming::lbpolt** = 0.0
- real **cputiming::tbrcast** = 0.0
- real **cputiming::brcastt** = 0.0
- real **cputiming::tdfp100** = 0.0
- real **cputiming::dfp100t** = 0.0
- real **cputiming::tdfp200** = 0.0
- real **cputiming::dfp200t** = 0.0
- real **cputiming::tdforce** = 0.0
- real **cputiming::dforcet** = 0.0
- real **cputiming::tnewton** = 0.0
- real **cputiming::newtont** = 0.0
- real **cputiming::tcasing** = 0.0
- real **cputiming::casingt** = 0.0
- real **cputiming::tbnorml** = 0.0
- real **cputiming::bnormlt** = 0.0
- real **cputiming::tjo00aa** = 0.0
- real **cputiming::jo00aat** = 0.0
- real **cputiming::tpp00aa** = 0.0
- real **cputiming::pp00aat** = 0.0

- real **cputiming::tpp00ab** = 0.0
- real **cputiming::pp00abt** = 0.0
- real **cputiming::tbfield** = 0.0
- real **cputiming::bfieldt** = 0.0
- real **cputiming::tstzxyz** = 0.0
- real **cputiming::stzxyzt** = 0.0
- real **cputiming::thesian** = 0.0
- real **cputiming::hesiant** = 0.0
- real **cputiming::tra00aa** = 0.0
- real **cputiming::ra00aat** = 0.0
- real **cputiming::tnumrec** = 0.0
- real **cputiming::numrect** = 0.0
- real **cputiming::tdcuhre** = 0.0
- real **cputiming::dcuhret** = 0.0
- real **cputiming::tminpack** = 0.0
- real **cputiming::minpackt** = 0.0
- real **cputiming::tiqpack** = 0.0
- real **cputiming::iqpackt** = 0.0
- real **cputiming::trksuite** = 0.0
- real **cputiming::rksuitet** = 0.0
- real **cputiming::ti1mach** = 0.0
- real **cputiming::i1macht** = 0.0
- real **cputiming::td1mach** = 0.0
- real **cputiming::d1macht** = 0.0
- real **cputiming::tilut** = 0.0
- real **cputiming::ilutt** = 0.0
- real **cputiming::titers** = 0.0
- real **cputiming::iterst** = 0.0
- real **cputiming::tsphdf5** = 0.0
- real **cputiming::sphdf5t** = 0.0
- real **cputiming::tpreset** = 0.0
- real **cputiming::presett** = 0.0
- real **cputiming::tglobal** = 0.0
- real **cputiming::globalt** = 0.0
- real **cputiming::txspech** = 0.0
- real **cputiming::xspecht** = 0.0
- real **cputiming::tinputlist** = 0.0
- real **cputiming::inputlistt** = 0.0
- real **cputiming::treadin** = 0.0
- real **cputiming::twrtend** = 0.0
- integer **allglobal::myid**

  MPI rank of current CPU.
- integer **allglobal::ncpu**

  number of MPI tasks
- integer **allglobal::ismyvolumevalue**

  flag to indicate if a CPU is operating on its assigned volume
- real **allglobal::cpus**

  initial time
- integer **allglobal::mpi_comm_spec**

  SPEC MPI communicator.
- logical **allglobal::skip_write** = .false.
- real **allglobal::pi2nfp**
- real **allglobal::pi2pi2nfp**
- real **allglobal::pi2pi2nfphalf**

- real **allglobal::pi2pi2nfpquart**
- character(len=1000) **allglobal::ext**
- real **allglobal::forceerr**

  total force-imbalance
- real **allglobal::energy**

  MHD energy.
- real, dimension(:), allocatable **allglobal::ipdt**
- real, dimension(:,:), allocatable **allglobal::ipdtdpf**

  Toroidal pressure-driven current.
- integer **allglobal::mvol**
- logical **allglobal::yesstellsym**

  internal shorthand copies of Istellsym, which is an integer input;
- logical **allglobal::notstellsym**

  internal shorthand copies of Istellsym, which is an integer input;
- logical **allglobal::yesmatrixfree**
- logical **allglobal::notmatrixfree**

  to use matrix-free method or not
- real, dimension(:,:), allocatable **allglobal::cheby**

  local workspace for evaluation of Chebychev polynomials
- real, dimension(:,:,:), allocatable **allglobal::zernike**

  local workspace for evaluation of Zernike polynomials
- real, dimension(:,:,:), allocatable **allglobal::tt**

  derivatives of Chebyshev polynomials at the inner and outer interfaces;
- real, dimension(:,:,:,:), allocatable **allglobal::rtt**

  derivatives of Zernike polynomials at the inner and outer interfaces;
- real, dimension(:,:), allocatable **allglobal::rtm**

  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-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**

  number of independent degrees of freedom in angle transformation;
- real, dimension(:,:,:), allocatable **allglobal::dlambdaout**
- 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::hdffdrz**

  derivatives of B^2 at the interfaces wrt geometry 2D Hessian;
- real, dimension(:,:,:,:,:), allocatable **allglobal::denergydrr**

  derivatives of energy at the interfaces wrt geometry 3D Hessian;
- real, dimension(:,:,:,:,:), allocatable **allglobal::denergydrz**

  derivatives of energy at the interfaces wrt geometry 3D Hessian;
- real, dimension(:,:,:,:,:), allocatable **allglobal::denergydzr**

  derivatives of energy at the interfaces wrt geometry 3D Hessian;
- real, dimension(:,:,:,:,:), allocatable **allglobal::denergydzz**

  derivatives of energy at the interfaces wrt geometry 3D Hessian;
- 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 (?)
- logical **allglobal::lhessian2dallocated**

  flag to indicate that 2D Hessian matrix is allocated (?)
- real, dimension(:,:), allocatable **allglobal::hessian2d**

  Hessian 2D.
- real, dimension(:,:), allocatable **allglobal::dessian2d**

  derivative Hessian 2D
- logical **allglobal::lhessian3dallocated**

  flag to indicate that 2D Hessian matrix is allocated (?)
- real, dimension(:,:), allocatable **allglobal::hessian3d**

  Hessian 3D.
- real, dimension(:,:), allocatable **allglobal::dessian3d**

  derivative Hessian 3D
- 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 (?)

10.12.1 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,

$$R_l(\theta,\zeta) = \sum_j R_{j,l}\cos(m_j\theta - n_j\zeta), \tag{259}$$

$$Z_l(\theta,\zeta) = \sum_j Z_{j,l}\sin(m_j\theta - n_j\zeta). \tag{260}$$

- These harmonics are read from the `ext.sp` file and come directly after the namelists described above. The required format is as follows:

$$\begin{array}{cccccccccc} m_1 & n_1 & R_{1,0} & Z_{1,0} & R_{1,1} & Z_{1,1} & ... & R_{1,N} & Z_{1,N} \\ m_2 & n_2 & R_{2,0} & Z_{2,0} & R_{2,1} & Z_{2,1} & ... & R_{2,N} & Z_{2,N} \\ ... & & & & & & & & \\ m_j & n_j & R_{j,0} & Z_{j,0} & R_{j,1} & Z_{j,1} & ... & R_{j,N} & Z_{j,N} \\ ... & & & & & & & & \end{array} \tag{261}$$

- 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.

10.12.2 Data Type Documentation

10.12.2.1 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	

10.12.2.2 type typedefns::matrixlu

10.12.2.3 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?

10.13 src/hesian.f90 File Reference

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

Functions/Subroutines

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

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

10.13.1 Detailed Description

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

10.14 src/inputlist.f90 File Reference

Input namelists.

Functions/Subroutines

- subroutine **inputlist::initialize_inputs**

Variables

- integer, parameter **inputlist::mnvol** = 256

  The maximum value of `Nvol` is `MNvol=256`.
- integer, parameter **inputlist::mmpol** = 128

  The maximum value of `Mpol` is `MNpol=64`.
- integer, parameter **inputlist::mntor** = 128

  The maximum value of `Ntor` is `MNtor=64`.
- integer inputlist::igeometry = 3

  selects Cartesian, cylindrical or toroidal geometry;
- integer **inputlist::istellsym** = 1

  stellarator symmetry is enforced if `Istellsym==1`
- integer **inputlist::lfreebound** = 0

  compute vacuum field surrounding plasma

- real **inputlist::phiedge** = 1.0

  total enclosed toroidal magnetic flux;
- real **inputlist::curtor** = 0.0

  total enclosed (toroidal) plasma current;
- real **inputlist::curpol** = 0.0

  total enclosed (poloidal) linking current;
- real **inputlist::gamma** = 0.0

  adiabatic index; cannot set $|\gamma| = 1$
- integer inputlist::nfp = 1

  field periodicity
- integer inputlist::nvol = 1

  number of volumes
- integer inputlist::mpol = 0

  number of poloidal Fourier harmonics
- integer inputlist::ntor = 0

  number of toroidal Fourier harmonics
- integer, dimension(1:mnvol+1) inputlist::lrad = 4

  Chebyshev resolution in each volume.
- integer inputlist::lconstraint = -1

  selects constraints; primarily used in ma02aa() and mp00ac().
- real, dimension(1:mnvol+1) inputlist::tflux = 0.0

  toroidal flux, 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
- logical **inputlist::ltransform** = .false.

  to evaluate iota and straight field line coordinates
- real **inputlist::fudge** = 1.0e-00

  redundant
- real **inputlist::scaling** = 1.0e-00

  redundant
- logical **inputlist::wmanual** = .false.
- logical **inputlist::wrzaxis** = .false.
- logical **inputlist::wpackxi** = .false.
- logical **inputlist::wvolume** = .false.
- logical **inputlist::wcoords** = .false.
- logical **inputlist::wbasefn** = .false.
- logical **inputlist::wmemory** = .false.
- logical **inputlist::wmetrix** = .false.

- logical **inputlist::wma00aa** = .false.
- logical **inputlist::wmatrix** = .false.
- logical **inputlist::wspsmat** = .false.
- logical **inputlist::wspsint** = .false.
- logical **inputlist::wmp00ac** = .false.
- logical **inputlist::wma02aa** = .false.
- logical **inputlist::wpackab** = .false.
- logical **inputlist::wtr00ab** = .false.
- logical **inputlist::wcurent** = .false.
- logical **inputlist::wdf00ab** = .false.
- logical **inputlist::wlforce** = .false.
- logical **inputlist::wintghs** = .false.
- logical **inputlist::wmtrxhs** = .false.
- logical **inputlist::wlbpol** = .false.
- logical **inputlist::wbrcast** = .false.
- logical **inputlist::wdfp100** = .false.
- logical **inputlist::wdfp200** = .false.
- logical **inputlist::wdforce** = .false.
- logical **inputlist::wnewton** = .false.
- logical **inputlist::wcasing** = .false.
- logical **inputlist::wbnorml** = .false.
- logical **inputlist::wjo00aa** = .false.
- logical **inputlist::wpp00aa** = .false.
- logical **inputlist::wpp00ab** = .false.
- logical **inputlist::wbfield** = .false.
- logical **inputlist::wstzxyz** = .false.
- logical **inputlist::whesian** = .false.
- logical **inputlist::wra00aa** = .false.
- logical **inputlist::wnumrec** = .false.
- logical **inputlist::wdcuhre** = .false.
- logical **inputlist::wminpack** = .false.
- logical **inputlist::wiqpack** = .false.
- logical **inputlist::wrksuite** = .false.
- logical **inputlist::wi1mach** = .false.
- logical **inputlist::wd1mach** = .false.
- logical **inputlist::wilut** = .false.
- logical **inputlist::witers** = .false.
- logical **inputlist::wsphdf5** = .false.
- logical **inputlist::wpreset** = .false.
- logical **inputlist::wglobal** = .false.
- logical **inputlist::wxspech** = .false.
- logical inputlist::wbuild_vector_potential = .false.
- logical **inputlist::wreadin** = .false.

  write screen output of readin()
- logical **inputlist::wwrtend** = .false.

  write screen output of wrtend()
- logical **inputlist::wmacros** = .false.

  write screen output from expanded macros

10.14.1 Detailed Description

Input namelists.

10.15 src/intghs.f90 File Reference

Calculates volume integrals of Chebyshev-polynomials and covariant field for Hessian computation.

Data Types

- type intghs_module::intghs_workspace

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

Functions/Subroutines

- subroutine intghs (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.

10.15.1 Detailed Description

Calculates volume integrals of Chebyshev-polynomials and covariant field for Hessian computation.

10.15.2 Function/Subroutine Documentation

10.15.2.1 intghs()

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

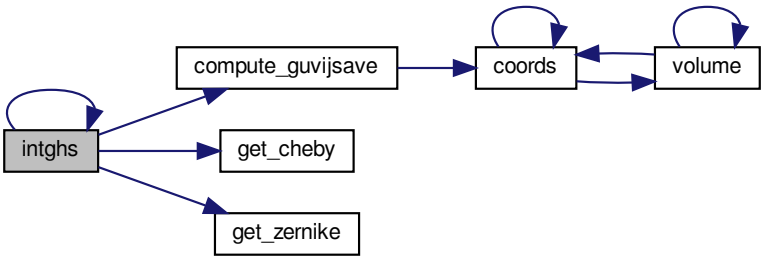
Calculates volume integrals of Chebyshev polynomials and covariant field products.

Parameters

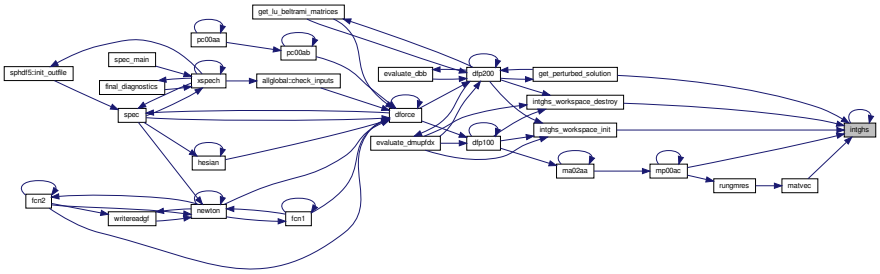
lquad	
mn	
lvol	
lrad	
idx	

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, intghs(), 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, 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(), 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:



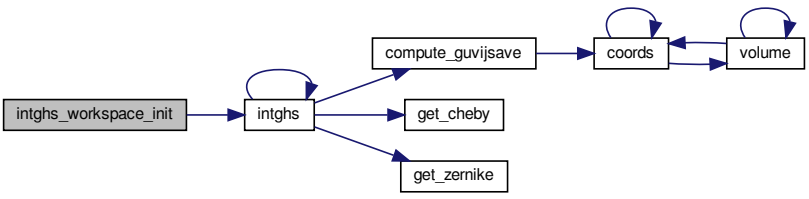
10.15.2.2 intghs_workspace_init() `subroutine intghs_workspace_init ( integer, intent(in) lvol )`

init workspace

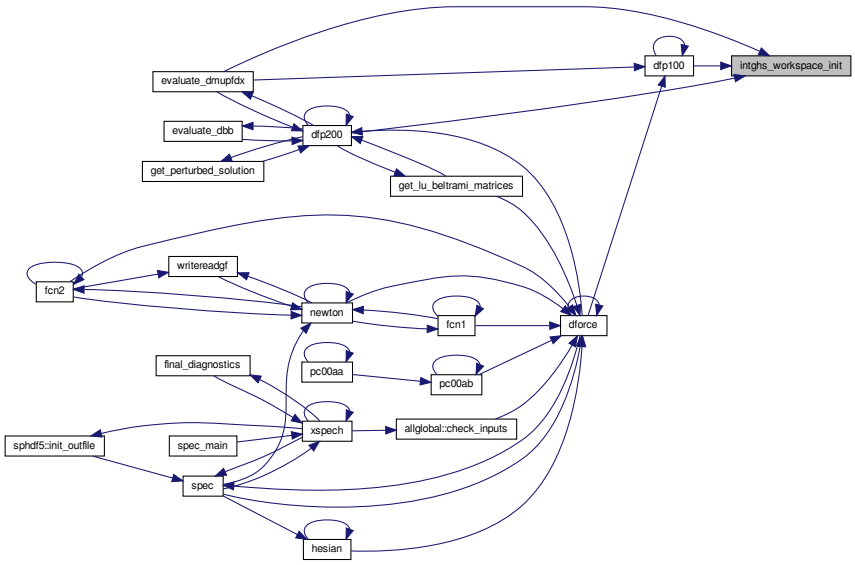
Parameters

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:



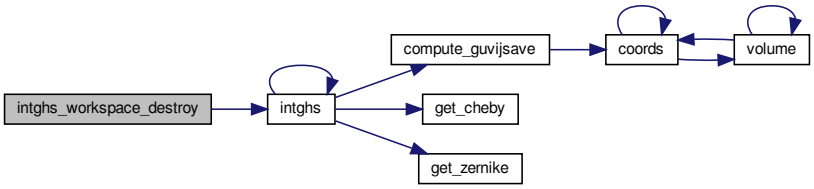
10.15.2.3 intghs_workspace_destroy() `subroutine intghs_workspace_destroy`

free workspace

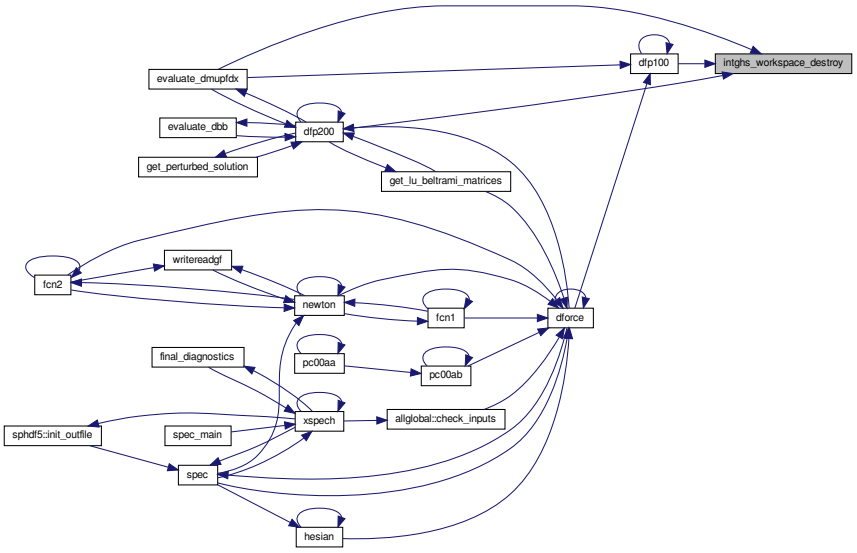
Parameters

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:



10.16 src/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, $\nabla \times \mathbf{B} - \mu \mathbf{B}$.

10.16.1 Detailed Description

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

10.17 src/lforce.f90 File Reference

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

Functions/Subroutines

- subroutine 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, $\mathcal{I}_i$.

10.17.1 Detailed Description

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

10.18 src/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.

10.18.1 Detailed Description

Calculates volume integrals of Chebyshev polynomials and metric element products.

10.19 src/ma02aa.f90 File Reference

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

Functions/Subroutines

- subroutine ma02aa (lvol, NN)

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

10.19.1 Detailed Description

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

10.20 src/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)

10.20.1 Detailed Description

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

10.21 src/memory.f90 File Reference

memory management module

Functions/Subroutines

- subroutine allocate_beltrami_matrices (vvol, LcomputeDerivatives)

  allocate Beltrami matrices
- subroutine deallocate_beltrami_matrices (LcomputeDerivatives)

  deallocate Beltrami matrices
- subroutine allocate_geometry_matrices (vvol, LcomputeDerivatives)

  allocate geometry matrices
- subroutine deallocate_geometry_matrices (LcomputeDerivatives)

  deallocate geometry matrices

10.21.1 Detailed Description

memory management module

10.21.2 Function/Subroutine Documentation

10.21.2.1 allocate_beltrami_matrices()

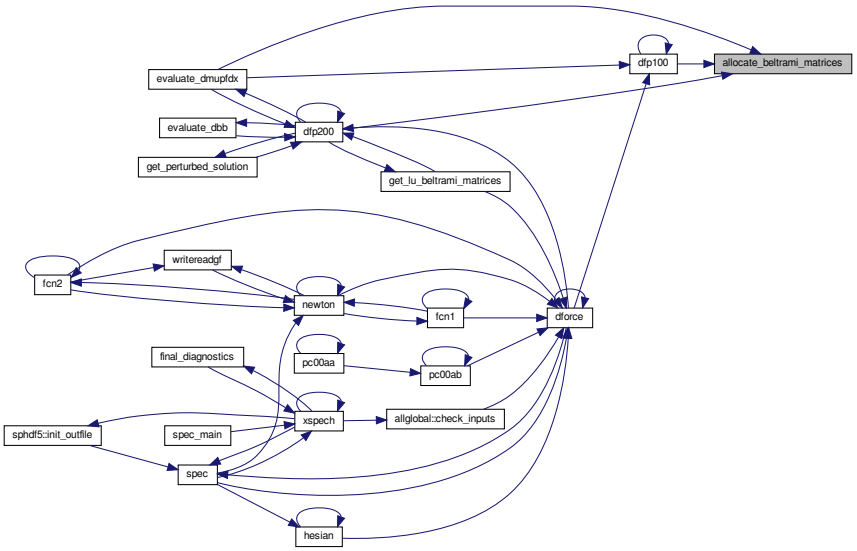
```
subroutine allocate_beltrami_matrices (
    integer, intent(in) vvol,
    logical, intent(in) LcomputeDerivatives )
```

allocate Beltrami matrices

Parameters

vvol	
LcomputeDerivatives	

References allglobal::adotx, allglobal::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:



10.21.2.2 deallocate_beltrami_matrices()

```
subroutine deallocate_beltrami_matrices (
    logical, intent(in) LcomputeDerivatives )
```

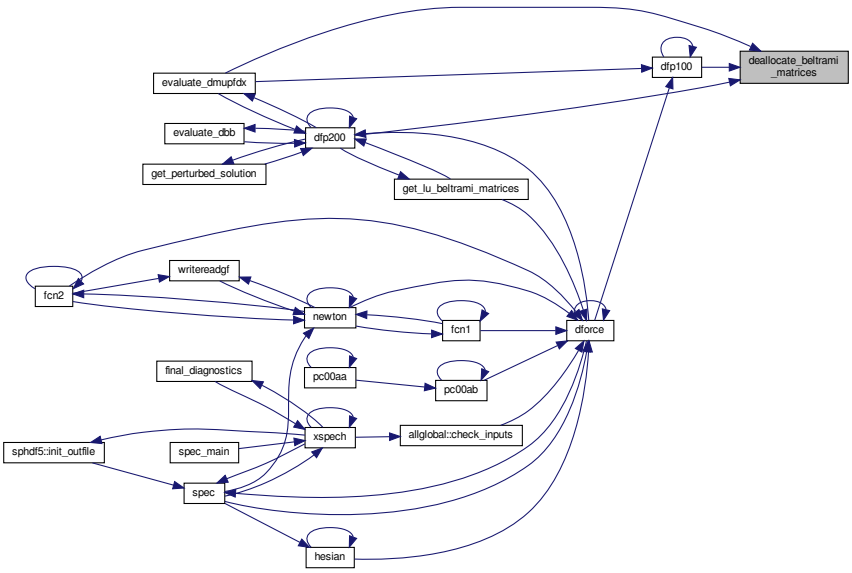
deallocate Beltrami matrices

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:



10.21.2.3 allocate_geometry_matrices() `subroutine allocate_geometry_matrices ( integer vvol, logical, intent(in) LcomputeDerivatives )`

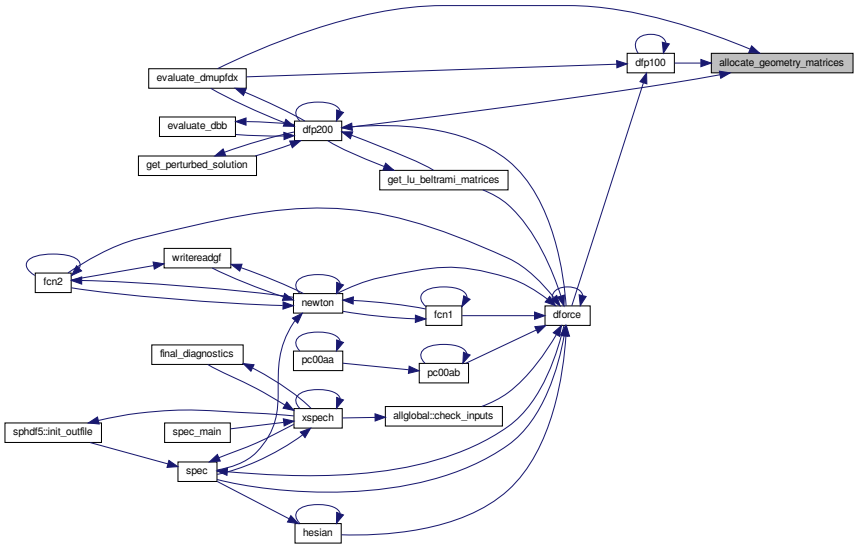
allocate geometry matrices

Parameters

vvol	
LcomputeDerivatives	

References allglobal::ddttcc, allglobal::ddttcs, allglobal::ddttsc, allglobal::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:



10.21.2.4 deallocate_geometry_matrices() `subroutine deallocate_geometry_matrices ( logical, intent(in) LcomputeDerivatives )`

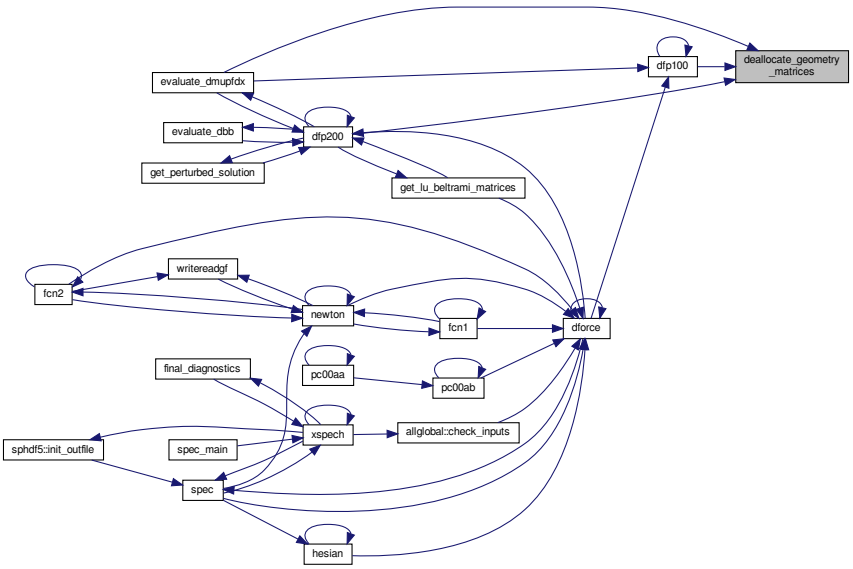
deallocate geometry matrices

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:



10.22 src/metrix.f90 File Reference

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

Functions/Subroutines

- subroutine metrix (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

10.22.1 Detailed Description

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

10.22.2 Function/Subroutine Documentation

10.22.2.1 compute_guvijsave()

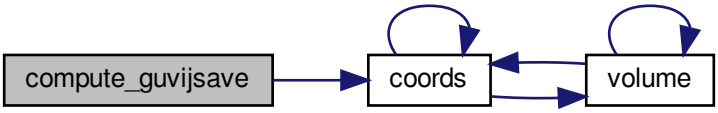
```
subroutine compute_guvijsave (
    integer, intent(in) lquad,
    integer, intent(in) vvol,
    integer, intent(in) ideriv,
    integer, intent(in) Lcurvature )
```

compute guvijsave

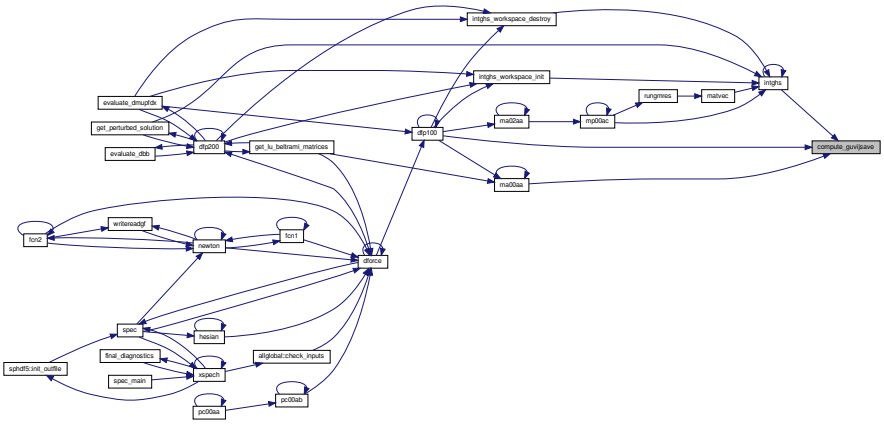
Parameters

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:



10.23 src/mp00ac.f90 File Reference

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

Functions/Subroutines

- subroutine mp00ac (Ndof, Xdof, Fdof, Ddof, Ldfjac, iflag)

  Solves Beltrami/vacuum (linear) system, given matrices.
  unpacking fluxes, helicity multiplier
- subroutine rungmres (n, nrestart, mu, vvol, rhs, sol, ipar, fpar, wk, nw, guess, a, au, jau, ju, iperm, ierr)

  run GMRES
- subroutine matvec (n, x, ax, a, mu, vvol)

  compute a.x by either by coumputing it directly, or using a matrix free method
- subroutine prec_solve (n, vecin, vecout, au, jau, ju, iperm)

  apply the preconditioner

10.23.1 Detailed Description

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

10.23.2 Function/Subroutine Documentation

10.23.2.1 rungmres()

```
subroutine rungmres (
    integer n,
    integer nrestart,
    real mu,
    integer vvol,
    real, dimension(1:n) rhs,
    real, dimension(1:n) sol,
    integer, dimension(16) ipar,
    real, dimension(16) fpar,
    real, dimension(1:nw) wk,
    integer nw,
    real, dimension(n) guess,
    real, dimension(*) a,
    real, dimension(*) au,
    integer, dimension(*) jau,
    integer, dimension(*) ju,
    integer, dimension(*) iperm,
    integer ierr )
```

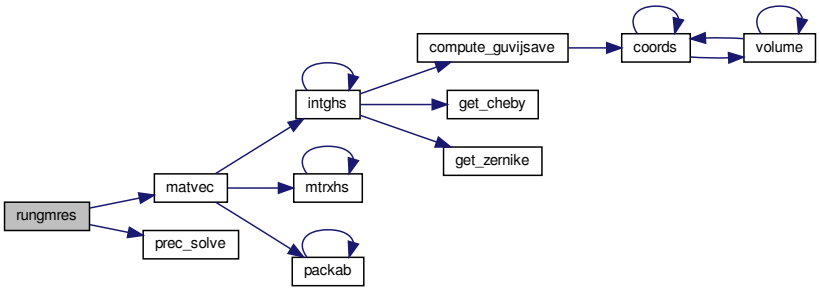
run GMRES

Parameters

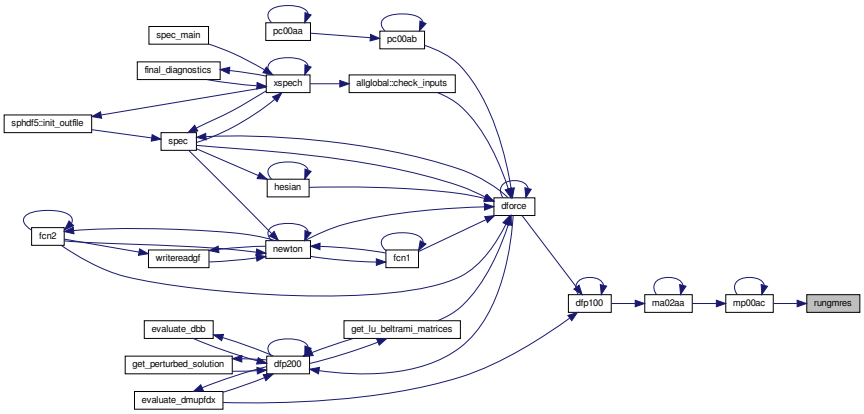
n	
nrestart	
mu	
vvol	
rhs	
sol	
ipar	
fpar	
wk	
nw	
guess	
a	
au	
jau	
ju	
iperm	
ierr	

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:



10.23.2.2 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 )
```

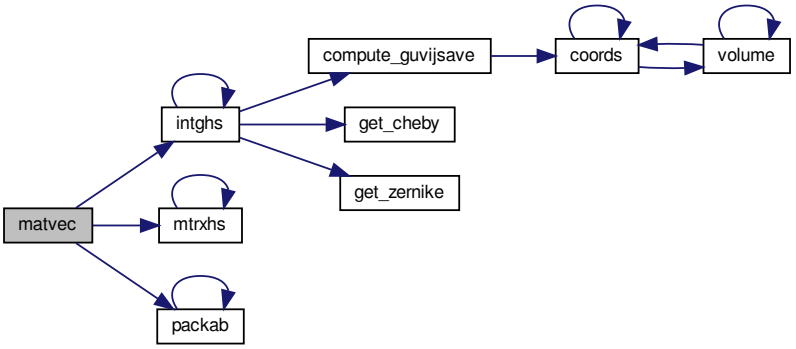
compute a.x by either by coumputing it directly, or using a matrix free method

Parameters

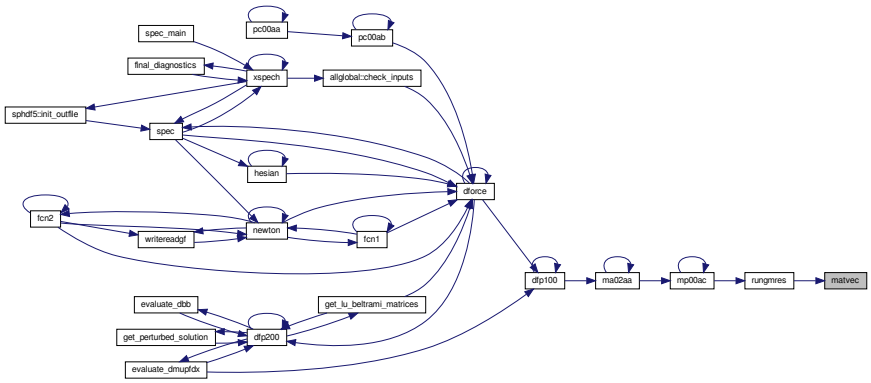
n	
x	
ax	
a	
mu	
vvol	

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:



10.23.2.3 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

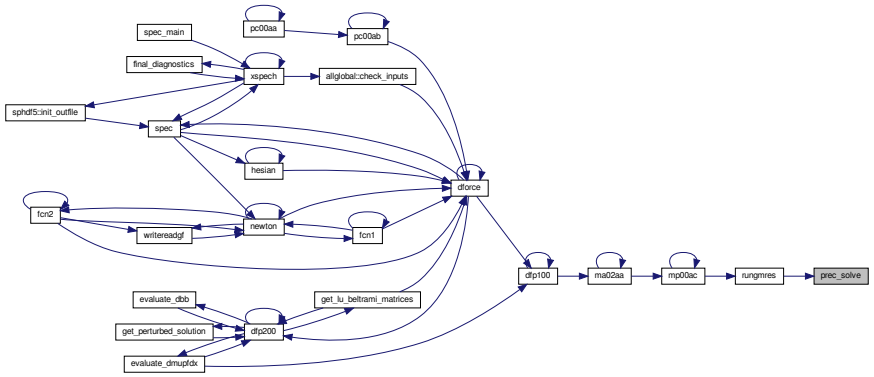
Parameters

n	
vecin	
vecout	
au	
jau	
ju	

Parameters

iperm	

Referenced by rungmres().
Here is the caller graph for this function:



10.24 src/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.

10.24.1 Detailed Description

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

10.25 src/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)

  Objective to be given to the Newton solver, using only function values.
- subroutine fcn2 (NGdof, xx, fvec, fjac, Ldfjac, irevcm)

  Objective to be given to the Newton solver, using function values and derivatives.

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 (?)

10.25.1 Detailed Description

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

10.26 src/packab.f90 File Reference

Packs, and unpacks, Beltrami field solution vector; $\mathbf{a} \equiv \{A_{\theta,e,i,l}, A_{\zeta,e,i,l}, \text{etc.}\}$.

Functions/Subroutines

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

  Packs and unpacks Beltrami field solution vector.

10.26.1 Detailed Description

Packs, and unpacks, Beltrami field solution vector; $\mathbf{a} \equiv \{A_{\theta,e,i,l}, A_{\zeta,e,i,l}, \text{etc.}\}$.

10.27 src/packxi.f90 File Reference

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

Functions/Subroutines

- subroutine packxi (NGdof, position, Mvol, mn, iRbc, iZbs, iRbs, iZbc, packorunpack, LComputeDerivatives, LComputeAxis)

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

10.27.1 Detailed Description

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

10.28 src/pc00aa.f90 File Reference

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

Functions/Subroutines

- subroutine pc00aa (NGdof, position, Nvol, mn, ie04dgf)

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

10.28.1 Detailed Description

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

10.29 src/pc00ab.f90 File Reference

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

Functions/Subroutines

- subroutine pc00ab (mode, NGdof, Position, Energy, Gradient, nstate, iuser, ruser)

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

10.29.1 Detailed Description

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

10.30 src/pp00aa.f90 File Reference

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

Functions/Subroutines

- subroutine pp00aa

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

10.30.1 Detailed Description

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

10.31 src/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).

10.31.1 Detailed Description

Follows magnetic fieldline using ode-integration routine from rksuite.f .

10.32 src/preset.f90 File Reference

Allocates and initializes internal arrays.

Functions/Subroutines

- subroutine preset

  Allocates and initializes internal arrays.

10.32.1 Detailed Description

Allocates and initializes internal arrays.

10.33 src/ra00aa.f90 File Reference

Writes vector potential to .ext.sp.A .

Functions/Subroutines

- subroutine ra00aa (writeorread)

  Writes vector potential to .ext.sp.A .

10.33.1 Detailed Description

Writes vector potential to .ext.sp.A .

10.34 src/rzaxis.f90 File Reference

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

Functions/Subroutines

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

  The coordinate axis is assigned via a poloidal average over an arbitrary surface.
- subroutine **fndiff_rzaxis** (Mvol, mn, ivol, jRbc, jRbs, jZbc, JZbs, imn, irz, issym)

10.34.1 Detailed Description

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

10.35 src/sphdf5.f90 File Reference

Writes all the output information to `ext.sp.h5`.

Modules

- module sphdf5

  writing the HDF5 output file

Functions/Subroutines

- subroutine **sphdf5::init_outfile**

  Initialize the interface to the HDF5 library and open the output file.
- subroutine sphdf5::mirror_input_to_outfile

  Mirror input variables into output file.
- subroutine sphdf5::init_convergence_output

  Prepare convergence evolution output.
- subroutine **sphdf5::write_convergence_output** (nDcalls, ForceErr)

  Write convergence output (evolution of interface geometry, force, etc).
- subroutine sphdf5::write_grid

  Write the magnetic field on a grid.
- subroutine sphdf5::init_flt_output (numTrajTotal)

  Initialize field line tracing output group and create array datasets.
- subroutine sphdf5::write_poincare (offset, data, success)

  Write a hyperslab of Poincare data corresponding to the output of one parallel worker.
- subroutine sphdf5::write_transform (offset, length, lvol, diotadxup, fiota)

  Write the rotational transform output from field line following.
- subroutine sphdf5::finalize_flt_output

  Finalize Poincare output.
- subroutine sphdf5::write_vector_potential (sumLrad, allAte, allAze, allAto, allAzo)

  Write the magnetic vector potential Fourier harmonics to the output file group `/vector_potential` .
- subroutine sphdf5::hdfint

  Write the final state of the equilibrium to the output file.
- subroutine **sphdf5::finish_outfile**

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

Variables

- logical, parameter **sphdf5::hdfdebug** = .false.

  global flag to enable verbal diarrhea commenting HDF5 operations
- integer, parameter **sphdf5::internalhdf5msg** = 0

  1: print internal HDF5 error messages; 0: only error messages from sphdf5
- integer **sphdf5::hdfier**

  error flag for HDF5 library
- integer **sphdf5::rank**

  rank of data to write using macros
- integer(hid_t) **sphdf5::file_id**

  default file ID used in macros
- integer(hid_t) **sphdf5::space_id**

  default dataspace ID used in macros
- integer(hid_t) **sphdf5::dset_id**

  default dataset ID used in macros
- integer(hsize_t), dimension(1:1) **sphdf5::onedims**

  dimension specifier for one-dimensional data used in macros
- integer(hsize_t), dimension(1:2) **sphdf5::twodims**

  dimension specifier for two-dimensional data used in macros
- integer(hsize_t), dimension(1:3) **sphdf5::threedims**

  dimension specifier for three-dimensional data used in macros
- logical **sphdf5::grp_exists**

  flags used to signal if a group already exists
- logical **sphdf5::var_exists**

  flags used to signal if a variable already exists
- integer(hid_t) **sphdf5::iteration_dset_id**

  Dataset identifier for "iteration".
- integer(hid_t) **sphdf5::dataspace**

  dataspace for extension by 1 iteration object
- integer(hid_t) **sphdf5::memspace**

  memspace for extension by 1 iteration object
- integer(hsize_t), dimension(1) **sphdf5::old_data_dims**

  current dimensions of "iterations" dataset
- integer(hsize_t), dimension(1) **sphdf5::data_dims**

  new dimensions for "iterations" dataset
- integer(hsize_t), dimension(1) **sphdf5::max_dims**

  maximum dimensions for "iterations" dataset
- integer(hid_t) **sphdf5::plist_id**

  Property list identifier used to activate dataset transfer property.
- integer(hid_t) **sphdf5::dt_ndcalls_id**

  Memory datatype identifier (for "nDcalls" dataset in "/iterations")
- integer(hid_t) **sphdf5::dt_energy_id**

  Memory datatype identifier (for "Energy" dataset in "/iterations")
- integer(hid_t) **sphdf5::dt_forceerr_id**

  Memory datatype identifier (for "ForceErr" dataset in "/iterations")
- integer(hid_t) **sphdf5::dt_irbc_id**

  Memory datatype identifier (for "iRbc" dataset in "/iterations")
- integer(hid_t) **sphdf5::dt_izbs_id**

  Memory datatype identifier (for "iZbs" dataset in "/iterations")
- integer(hid_t) **sphdf5::dt_irbs_id**

Memory datatype identifier (for "iRbs" dataset in "/iterations")

- integer(hid_t) **sphdf5::dt_izbc_id**

  Memory datatype identifier (for "iZbc" dataset in "/iterations")

- 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.

10.35.1 Detailed Description

Writes all the output information to `ext.sp.h5`.
If the output file already exists, it will be deleted and replaced by an empty one, which gets filled in with the updated data. All calls to the HDF5 API are filtered to only happen from MPI rank-0 to be able to use the serial HDF5 library. Parallel HDF5 was considered in the past, but abandoned due to very subtle and irreproducible errors.

10.36 src/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.

10.36.1 Detailed Description

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

10.37 src/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

10.37.1 Detailed Description

Constructs matrices for the precondtioner.

10.37.2 Function/Subroutine Documentation

10.37.2.1 push_back()

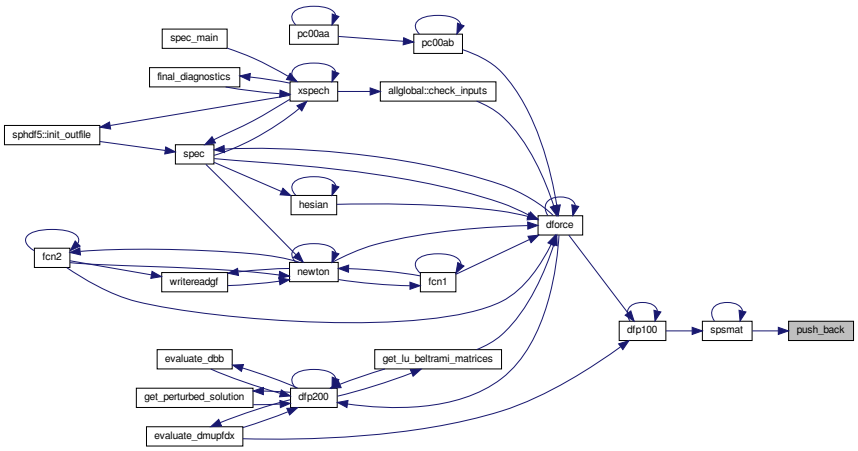
```
subroutine push_back (
    integer, intent(in) iq,
    integer, dimension(4), intent(inout) nq,
    integer, intent(in) NN,
    real, intent(in) vA,
    real, intent(in) vD,
    integer, intent(in) vjA,
    real, dimension(nn,4), intent(inout) qA,
    real, dimension(nn,4), intent(inout) qD,
    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:



10.37.2.2 clean_queue()

```
subroutine clean_queue (
```

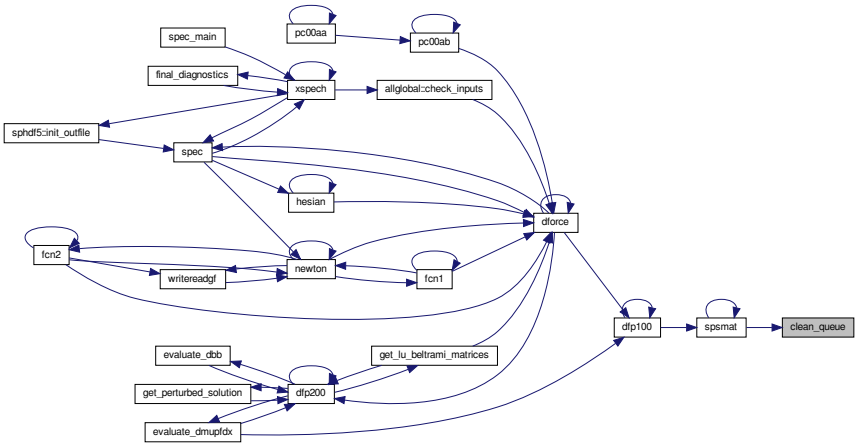
```
integer, dimension(4), intent(inout) nq,
integer, intent(in) NN,
real, dimension(nn,4), intent(inout) qA,
real, dimension(nn,4), intent(inout) qD,
integer, dimension(nn,4), intent(inout) qjA )
```

clean the queue

Parameters

nq	
NN	
qA	
qD	
qjA	

References constants::zero.
Referenced by spsmat().
Here is the caller graph for this function:



10.37.2.3 addline() `subroutine addline (`

```
integer, dimension(4), intent(inout) nq,
integer, intent(inout) NN,
real, dimension(nn,4), intent(inout) qA,
real, dimension(nn,4), intent(inout) qD,
integer, dimension(nn,4), intent(inout) qjA,
integer, intent(inout) ns,
integer, intent(inout) nrow,
real, dimension(*) dMAS,
real, dimension(*) dMDS,
integer, dimension(*) jdMAS,
integer, dimension(*) idMAS )
```

add the content from the queue to the real matrices

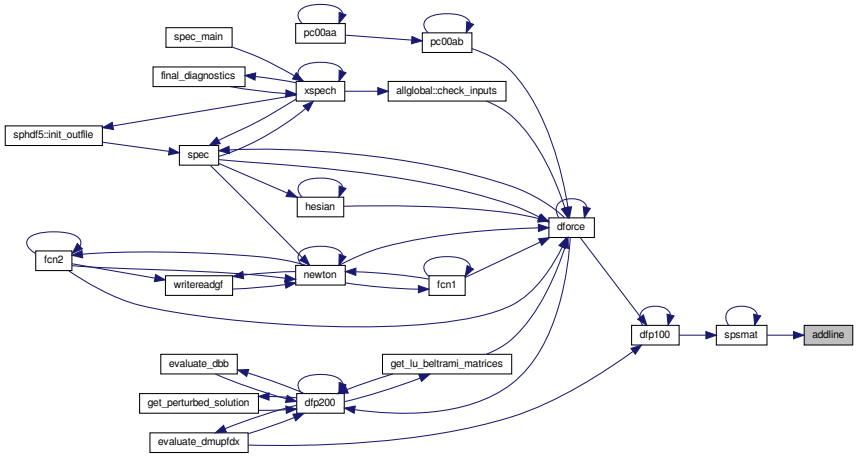
Parameters

nq	
NN	

Parameters

qA	
qD	
qjA	
ns	
nrow	
dMAS	
dMDS	
jdMAS	
idMAS	

Referenced by spsmat().
Here is the caller graph for this function:



10.38 src/stzxyz.f90 File Reference

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

10.38.1 Detailed Description

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

10.39 src/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.

10.39.1 Detailed Description

Calculates rotational transform given an arbitrary tangential field.

10.40 src/volume.f90 File Reference

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

Functions/Subroutines

- subroutine volume (lvol, vflag)

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

10.40.1 Detailed Description

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

10.41 src/wa00aa.f90 File Reference

Constructs smooth approximation to wall.

Modules

- module laplaces

  ...todo...

Functions/Subroutines

- subroutine wa00aa (iwa00aa)

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

  Compute vacuum magnetic scalar potential (?)

Variables

- logical **laplaces::stage1**

  what is this ?
- logical **laplaces::exterior**

  what is this ?
- logical **laplaces::dorm**

  what is this ?
- integer **laplaces::nintervals**

  what is this ?
- integer **laplaces::nsegments**

  what is this ?
- integer **laplaces::ic**

  what is this ?
- integer **laplaces::np4**

  what is this ?
- integer **laplaces::np1**

  what is this ?
- integer, dimension(:), allocatable **laplaces::icint**

  what is this ?
- real **laplaces::originalalpha**

what is this ?

- real, dimension(:), allocatable **laplaces::xpoly**

  what is this ?
- real, dimension(:), allocatable **laplaces::ypoly**

  what is this ?
- real, dimension(:), allocatable **laplaces::phi**

  what is this ?
- real, dimension(:), allocatable **laplaces::phid**

  what is this ?
- real, dimension(:,:), allocatable **laplaces::cc**

  what is this ?
- integer **laplaces::ilength**

  what is this ?
- real **laplaces::totallength**

  what is this ?
- integer **laplaces::niterations**

  counter; eventually redundant; 24 Oct 12;
- integer **laplaces::iangle**

  angle ; eventually redundant; 24 Oct 12;
- real **laplaces::rmid**

  used to define local polar coordinate; eventually redundant; 24 Oct 12;
- real **laplaces::zmid**

  used to define local polar coordinate; eventually redundant; 24 Oct 12;
- real **laplaces::alpha**

  eventually redundant; 24 Oct 12;

10.41.1 Detailed Description

Constructs smooth approximation to wall.

10.42 src/xspech.f90 File Reference

Main program.

Functions/Subroutines

- program spec_main

  Main program of SPEC.
- subroutine xspech

  Main subroutine of SPEC.
- subroutine read_command_args

  Read command-line arguments; in particular, determine input file (name or extension).
- subroutine spec

  This is the main "driver" for the physics part of SPEC.
- subroutine final_diagnostics

  Final diagnostics.
- subroutine **ending**

  Closes output files, writes screen summary.

10.42.1 Detailed Description

Main program.

10.42.2 Function/Subroutine Documentation

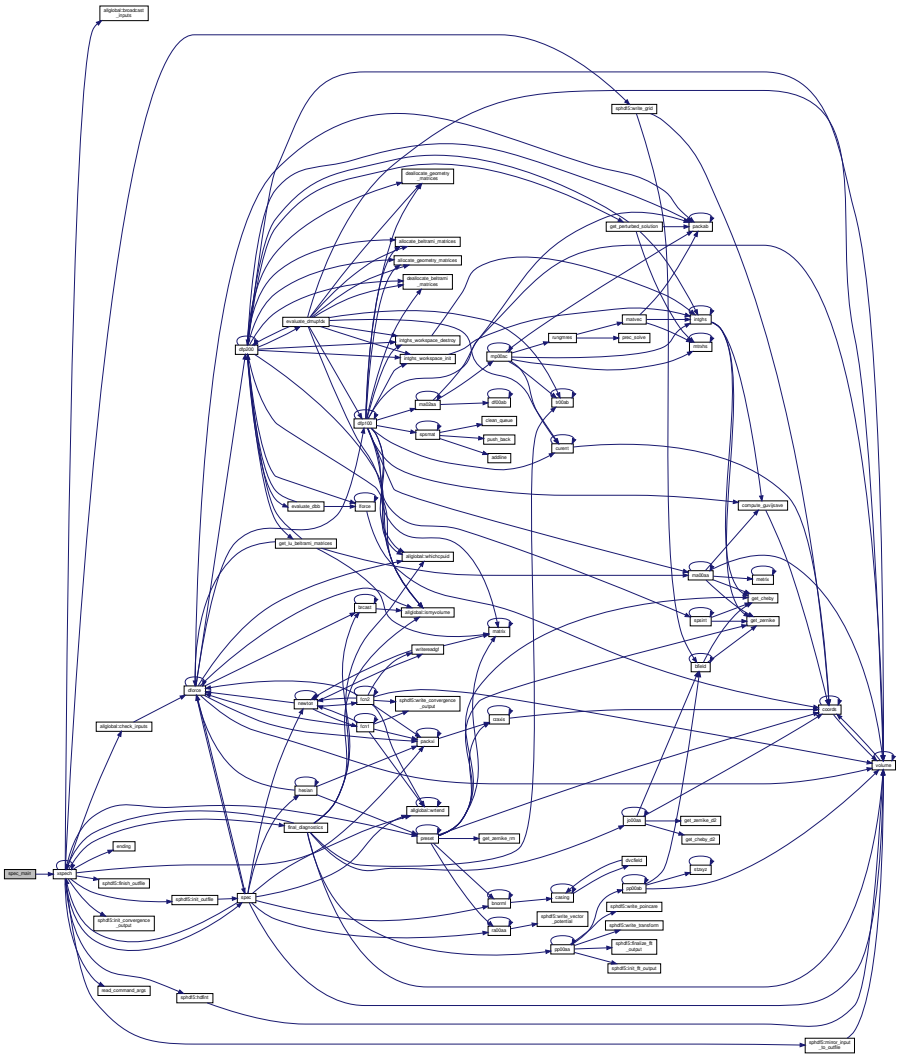
10.42.2.1 spec_main() `program spec_main`

Main program of SPEC.
This only calls the xpech() subroutine to do a stand-alone SPEC run.

Returns

none

References xspech().
Here is the call graph for this function:



10.42.2.2 xspech() `subroutine xspech`

Main subroutine of SPEC.
This orchestrates a stand-alone SPEC run:

- read the input file
- solve the MRxMHD equilibrium (see spec())

- run some diagnostics on the results
- write the output file(s)

reading input, allocating global variables

- The input namelists and geometry are read in via a call to readin() . A full description of the required input is given in global.f90 .
- Most internal variables, global memory etc., are allocated in preset() .
- All quantities in the input file are mirrored into the output file's group `/input` .

preparing output file group iterations

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

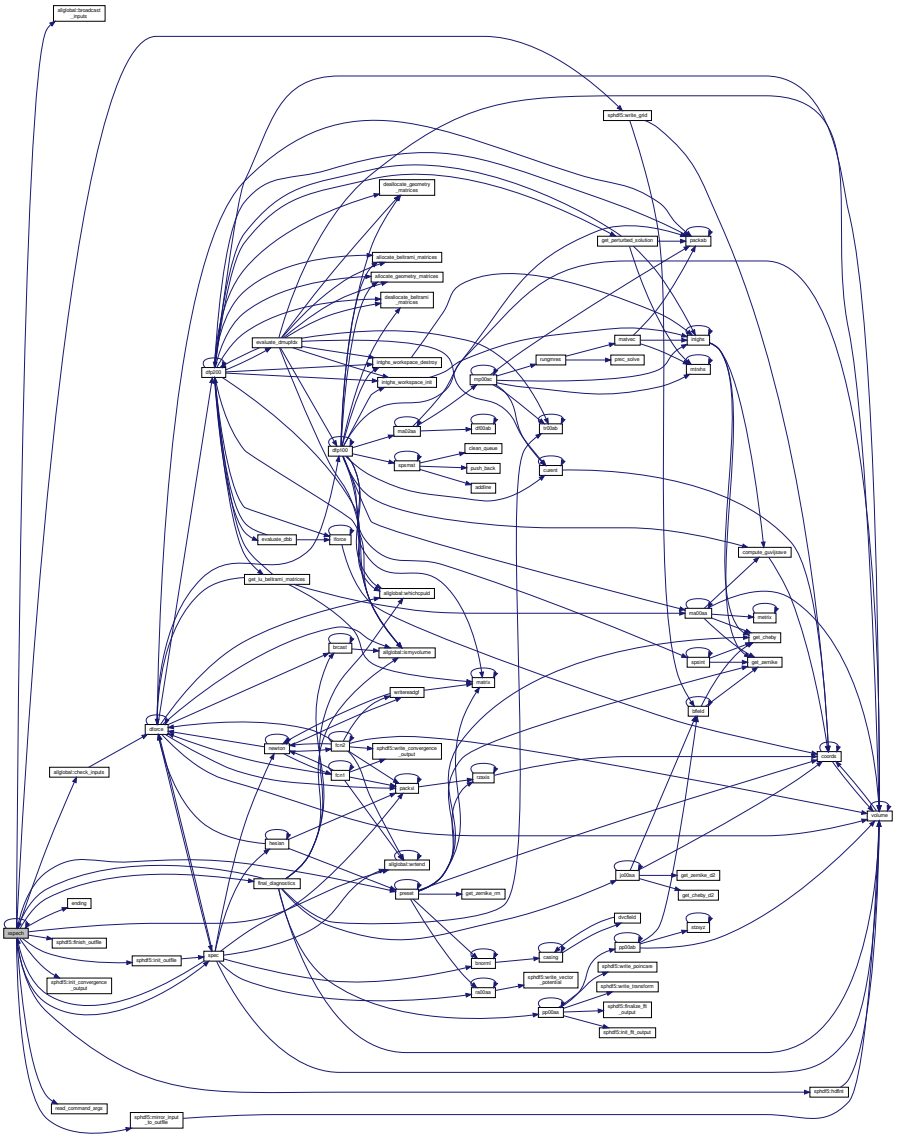
```
DATATYPE  H5T_COMPOUND {
      H5T_NATIVE_INTEGER "nDcalls";
      H5T_NATIVE_DOUBLE "Energy";
      H5T_NATIVE_DOUBLE "ForceErr";
      H5T_ARRAY { [Mvol+1][mn] H5T_NATIVE_DOUBLE } "iRbc";
      H5T_ARRAY { [Mvol+1][mn] H5T_NATIVE_DOUBLE } "iZbs";
      H5T_ARRAY { [Mvol+1][mn] H5T_NATIVE_DOUBLE } "iRbs";
      H5T_ARRAY { [Mvol+1][mn] H5T_NATIVE_DOUBLE } "iZbc";
}
```

restart files

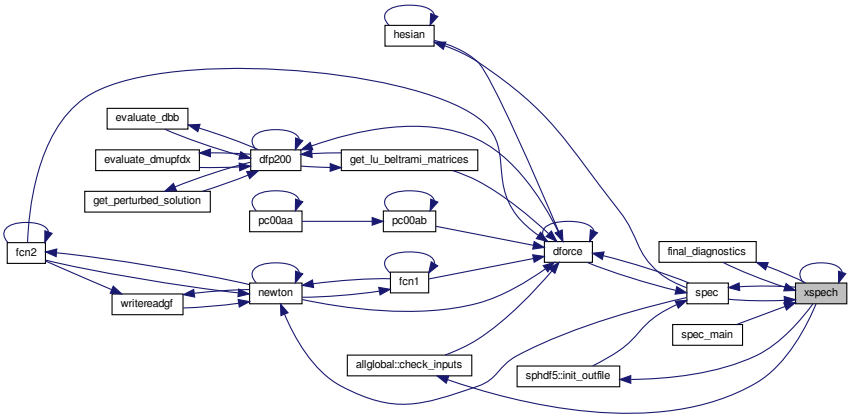
- wrtend() is called to write the restart files.

References allglobal::broadcast_inputs(), allglobal::check_inputs(), allglobal::cpus, ending(), final_diagnostics(), sphdf5::finish_outfile(), sphdf5::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(), allglobal::wrtend(), and xspech().
Referenced by final_diagnostics(), spec(), spec_main(), and xspech().

Here is the call graph for this function:



Here is the caller graph for this function:

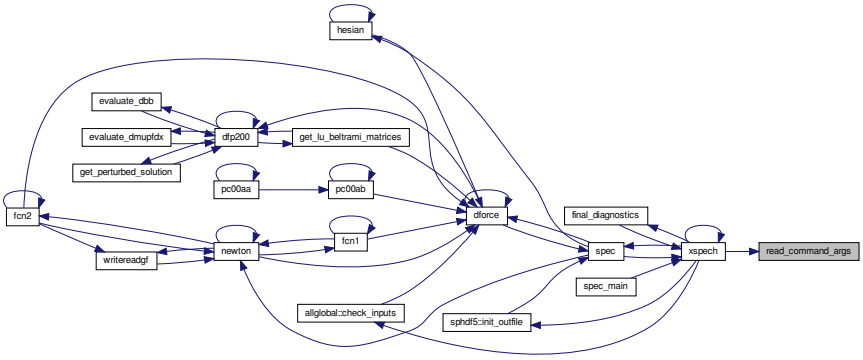


10.42.2.3 read_command_args() `subroutine read_command_args`

Read command-line arguments; in particular, determine input file (name or extension).

- The input file name, `ext` , is given as the first command line input, and the input file itself is then `ext.sp` .
- Alternatively, you can directly specify the input file itself as `ext.sp` .
- You can also generate a template input file using `xspec` -i .
- Or print help information using `xspec` -h .
- Additional command line inputs recognized are:
  - `-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:



10.42.2.4 spec() subroutine spec

This is the main "driver" for the physics part of SPEC.
Picard iterations are performed (if in free-boundary mode) and within each Picard iteration, the fixed-boundary problem is solved (also iteratively). **packing geometrical degrees-of-freedom into vector**

- If `NGdof.gt.0` , where `NGdof` counts the geometrical degrees-of-freedom, i.e. the R_{bc}, Z_{bs}, etc., then packxi() is called to "pack" the geometrical degrees-of-freedom into `position(0:NGdof)` .

initialize adiabatic constants

- If `Ladiabatic.eq.0` , then the "adiabatic constants" in each region, P_v, are calculated as

$$P_v \equiv p_v V_v^\gamma, \tag{262}$$

  where $p_v \equiv$ `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. (262), i.e. $p = P/V^\gamma$.
- The Beltrami/vacuum fields in each region are re-calculated using dforce() .
- If `Lcheck.eq.5` .or. `LHevalues` .or. `LHevectors` .or. `Lperturbed.eq.1` , then the force-gradient matrix is examined using hesian() .

free-boundary: re-computing normal field

- If `Lfreebound.eq.1` and `Lfindzero.gt.0` and `mfreeits.ne.0` , then the magnetic field at the computational boundary produced by the plasma currents is computed using bnorml() .
- The "new" magnetic field at the computational boundary produced by the plasma currents is updated using a Picard scheme:

$$\mathtt{Bns}_i^j = \lambda\, \mathtt{Bns}_i^{j-1} + (1-\lambda)\mathtt{Bns}_i, \tag{263}$$

  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

$$\sum_i |\mathtt{Bns}_i^{j-1} - \mathtt{Bns}_i|/N, \tag{264}$$

  where N is the total number of Fourier harmonics.
- There are several choices that are available:
  - if `mfreeits=-2` : the vacuum magnetic field (really, the normal component of the field produced by the external currents at the computational boundary) required to hold the given equlibrium is written to file. This information is required as input by FOCUS [8] for example. (This option probably needs to revised.)

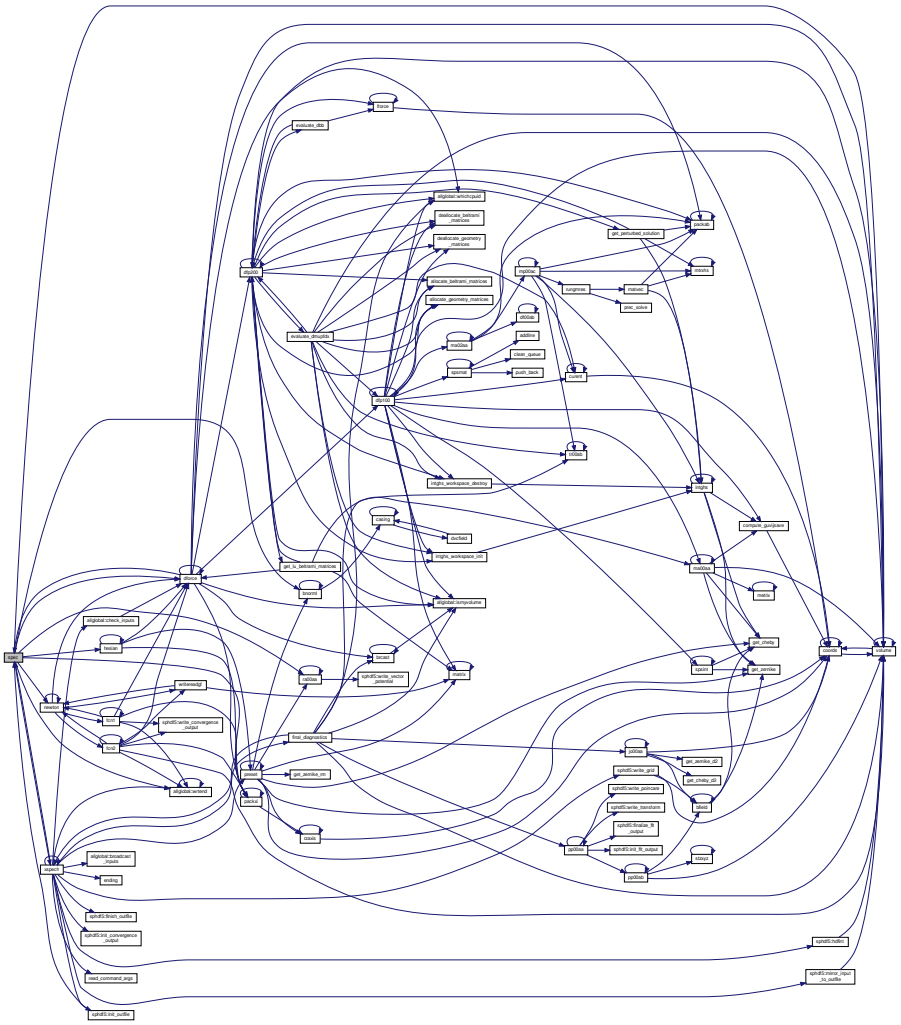
- if mfreeits=-1 : after the plasma field is computed by virtual casing, the vacuum magnetic field is set to exactly balance the plasma field (again, we are really talking about the normal component at the computational boundary.) This will ensure that the computational boundary itself if a flux surface of the total magnetic field.
- if mfreeits=0 : the plasma field at the computational boundary is not updated; no "free-boundary" iterations take place.
- if mfreeits>0 : the plasma field at the computational boundary is updated according to the above blending Eqn. (263), and the free-boundary iterations will continue until either the tolerance condition is met (see gBntol and Eqn. (264)) or the maximum number of free-boundary iterations, namely mfreeits , is reached. For this case, Lzerovac is relevant: if Lzerovac=1 , then the vacuum field is set equal to the normal field at every iteration, which results in the computational boundary being a flux surface. (I am not sure if this is identical to setting mfreeits=-1 ; the logic etc. needs to be revised.)

output files: vector potential

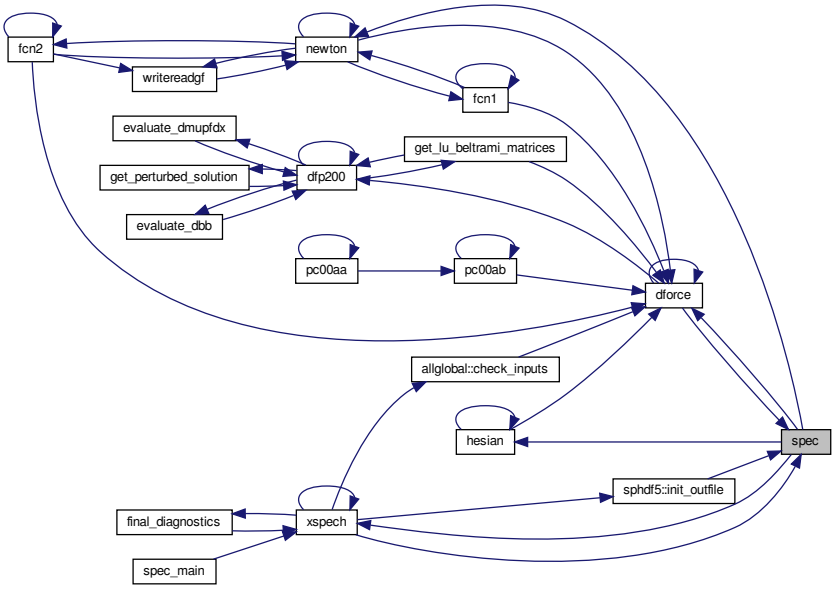
- The vector potential is written to file using ra00aa() .

References inputlist::adiabatic, allglobal::ate, allglobal::ato, allglobal::aze, allglobal::azo, allglobal::bbe, allglobal::bbo, allglobal::beltramierror, bnorml(), allglobal::cfmn, allglobal::cpus, dforce(), allglobal::dma, allglobal::dmb, allglobal::dmd, allglobal::dmg, allglobal::dpflux, allglobal::dtflux, allglobal::efmn, allglobal::first_free_bound, 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, allglobal::mbpsi, inputlist::mfreeits, allglobal::mn, allglobal::mpi_comm_spec, inputlist::mu, constants::mu0, allglobal::myid, allglobal::ncpu, newton(), inputlist::nfp, allglobal::nfreeboundaryiterations, 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, allglobal::solution, inputlist::tflux, inputlist::vcasingtol, constants::version, volume(), numerical::vsmall, allglobal::vvolume, inputlist::wmacros, allglobal::wrtend(), xspech(), allglobal::yesstellsym, inputlist::zbc, inputlist::zbs, and constants::zero.
Referenced by dforce(), sphdf5::init_outfile(), and xspech().

Here is the call graph for this function:



Here is the caller graph for this function:



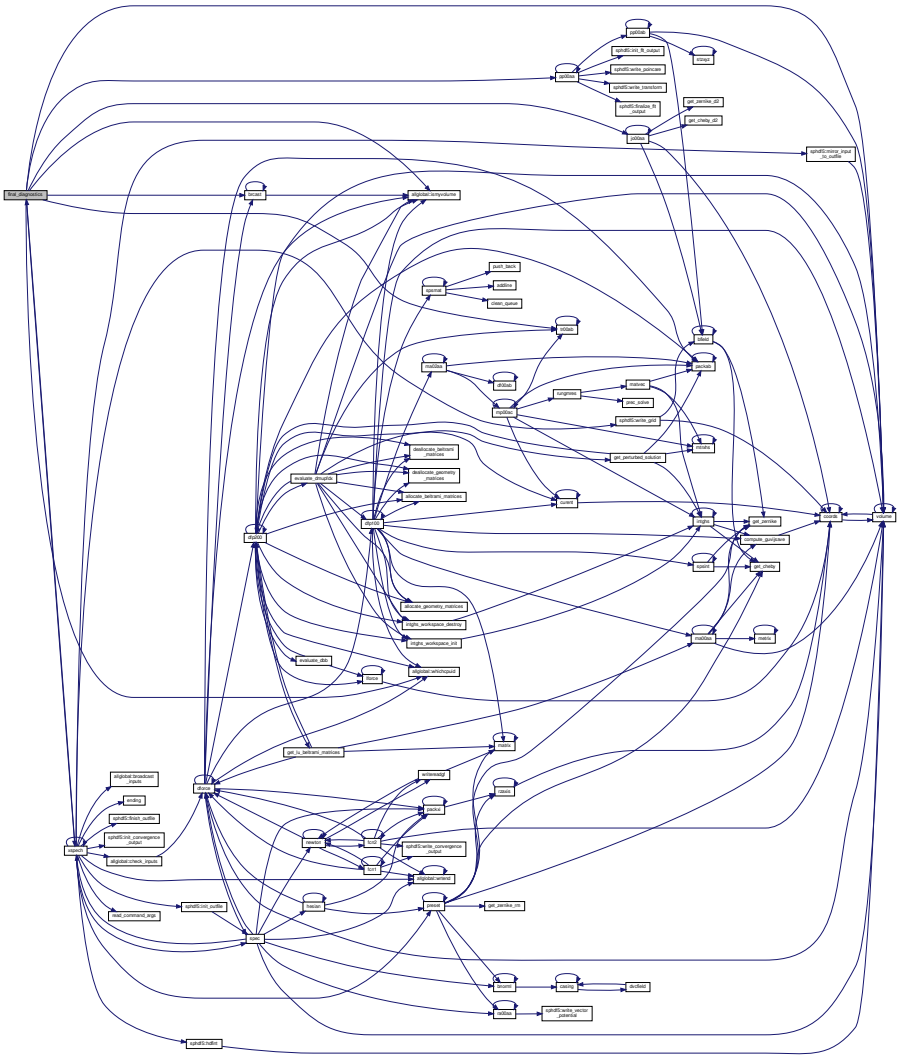
10.42.2.5 final_diagnostics() `subroutine final_diagnostics`

Final diagnostics.

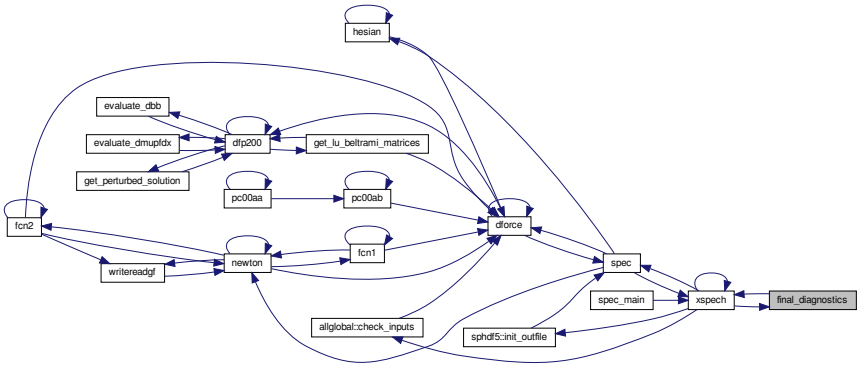
- sc00aa() is called to compute the covariant components of the magnetic field at the interfaces; these are related to the singular currents
- if `Lcheck=1` , jo00aa() is called to compute the error in the Beltrami equation
- pp00aa() is called to construct the Poincare plot by field-line following.

References allglobal::beltramierror, brcast(), allglobal::btemn, allglobal::btomn, allglobal::bzemn, allglobal::bzomn, allglobal::cfmn, allglobal::cpus, allglobal::diotadxup, allglobal::dtflux, allglobal::efmn, inputlist::igeometry, allglobal::imagneticok, allglobal::iquad, allglobal::ismyvolume(), allglobal::ismyvolumevalue, inputlist::isurf, inputlist::ivolume, jo00aa(), inputlist::lcheck, allglobal::lcoordinatesingularity, allglobal::lmns, allglobal::lplasmaregion, inputlist::lsvdiota, inputlist::ltransform, allglobal::lvacuumregion, allglobal::mn, allglobal::mpi_comm_spec, inputlist::mu, allglobal::myid, allglobal::ncpu, inputlist::nppts, inputlist::nptrj, allglobal::nt, allglobal::ntz, inputlist::nvol, allglobal::nz, inputlist::odetol, allglobal::ofmn, constants::one, fileunits::ounit, constants::pi2, pp00aa(), allglobal::sfmn, tr00ab(), volume(), allglobal::whichcpuid(), 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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