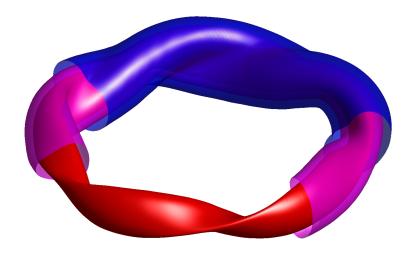
BDISTRIB User Manual



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CHAPTER 1

Overview

This program computes efficiency-ordered distributions of magnetic fields as described in [1]. The main method is described on page 12, and some key definitions are given on page 9.

There are some similarities between this program and the NESCOIL code used to compute stellarator coils [2]. NESCOIL effectively computes the 'inductance' between a plasma surface and a coil surface, meaning the linear relationship by which the current potential on the coil surface gives rise to a normal component of the magnetic field B on the plasma surface. NESCOIL takes the normal component of B on the plasma surface associated with net poloidal coil current plus plasma current, and effectively multiplies the result by the (pseudo)inverse of the inductance matrix, yielding the current potential required to achieve a magnetic surface (zero normal component of B) on the plasma surface. In bdistrib, however, we do not consider net coil current or plasma current, and we compute two inductance matrices instead of one. The two inductance matrices in bdistrib refer to the same outer surface (on which the current potential is defined), but to different surfaces on which the normal B is evaluated. Multiplying one inductance matrix by the (pseudo)inverse of the other gives the so-called 'transfer matrix'. Applying a singular value decomposition (SVD) to this transfer matrix, the singular vectors represent modes of the magnetic field, and the singular values represent the efficiency by which these modes propagate from one toroidal surface to the other.

In bdistrib the three toroidal surfaces are named 'plasma', 'middle', and 'outer', in order from the innermost to outermost. The 'plasma' surface can correspond to the outermost surface of a vmec equilibrium, or it can be a plain circular toroidal surface. The name of the relevant surface appears as a suffix on most variables.

On each surface we use a poloidal angle u and a toroidal angle v, defined as in NESCOIL. The coordinate u lies in the range [0,1]. The surfaces have nfp identical toroidal periods, and an increase in v by 1 corresponds to 1 of these periods. Thus, v increases by nfp in a complete toroidal revolution. In the output file, there is an array v corresponding to one toroidal period, as well as an array v1 corresponding to all nfp toroidal periods. Note that v is proportional to the standard cylindrical angle ϕ : $\phi = 2\pi v/\text{nfp}$. Generally, field lines are not straight in the (u,v) coordinates. On the plasma surface, u is identical to the vmec poloidal angle divided by 2π , while the vmec toroidal angle differs by $2\pi/\text{nfp}$ compared to v.

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In the various variable names in the code and output file, 'r' refers to the position vector, not to a radius. In various arrays with a dimension of length 3, this dimension always corresponds to Cartesian coordinates (x, y, z).

The 'normal' quantities in the code and output file refer to the surface normal vector N = (dr/dv) cross (dr/du) as in the NESCOIL paper. Note that this vector does not have unit magnitude.

1.1 Required libraries

- LIBSTELL (for reading vmec wout files, and for the ezcdf subroutines)
- NetCDF (for writing the output file)
- BLAS/LAPACK (for matrix multiplication and the SVD subroutine)

If OpenMP is available, calculations with the code are parallelized. The plotting and testing functions use python, numpy, and scipy. The plotting routines bdistribPlot and compareSingularValuesPlot use matplotlib.

1.2 Parallelization

The code does not use MPI, and so it runs on a single computing node. However, it is possible to use multiple threads on the node to accelerate computations. The multi-threaded parallelization is done in part using OpenMP and in part using a multi-threaded BLAS routine.

The slowest steps in bdistrib occur when assembling the two inductance matrices. For each of these two matrices, there are two slow steps. The first is computation of the magnetic dipole formula between each pair of points on the two toroidal surfaces. The loop for this computation is parallelized using OpenMP. The other slow step is the integration of this result against each of the basis functions, which is done using matrix multiplication with the BLAS subroutine DGEMM. To parallelize this step you can link bdistrib with a multi-threaded BLAS library, such as the Intel Math Kernel Library (MKL).

1.3 make test

To test that your bdistrib executable is working, you can run make test. Doing so will run bdistrib for some or all of the examples in the examples/ directories. After each example completes, several of the output quantities (typically the singular values of the transfer matrix) will be checked, using the tests.py script in the example's directory. The make test feature is very useful when making changes to the code, since it allows you to check that your code modifications have not broken anything and that previous results can be recovered.

If you run make retest, no new runs of bdistrib will be performed, but the tests.py script will be run on any existing output files in the /examples/ directories.

1.4 Questions, Bugs, and Feedback

We welcome any contributions to the code or documentation. For write permission to the repository, or to report any bugs, provide feedback, or ask questions, contact Matt Landreman at matt.

landreman@gmail.com

CHAPTER 2

Theory

In this section we detail the theoretical background of the bdistrib code. Our discussion closely follows Ref [2] and sections 2.13 - 2.3 of Ref [1].

2.1 Current potential

Consider a surface defined by $\mathbf{r}(u, v)$, i.e. the position vector \mathbf{r} along the surface is parametrized by two coordinates u and v. A vector normal to the surface is

$$\mathbf{N} = \frac{\partial \mathbf{r}}{\partial v} \times \frac{\partial \mathbf{r}}{\partial u}.$$
 (2.1)

(We will follow the same sign convention as [2].) This vector does not generally have unit magnitude; a unit normal vector is

$$\mathbf{n} = \frac{\mathbf{N}}{|\mathbf{n}|}.\tag{2.2}$$

A divergence-free surface current on the surface must have the form

$$\mathbf{K} = \mathbf{n} \times \nabla \Phi \tag{2.3}$$

for a "current potential" Φ . If we now specialize to the case of a toroidal surface, Φ may be not be singly valued if there is net poloidal or toroidal current on the surface. Here we restrict our attention to the single-valued part of Φ .

2.2 Magnetic dipole formula

Let us now examine the magnetic field produced by the surface current (2.3). We begin with the Biot-Savart law for a surface current:

$$\mathbf{B}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int d^2 r' \frac{\mathbf{K}(\mathbf{r}') \times (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3}.$$
 (2.4)

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We specialize to the case in which $u \in [0,1)$ is the poloidal coordinate, and the toroidal coordinate v increases from 0 to 1 in a single toroidal period, where there are n_p identical toroidal periods. (For instance, $n_p = 5$ for W7-X.) In both vmec and bdistrib, n_p is called nfp. Then any area integral on the toroidal surface (such as the integral in (2.4)) can be expressed as

$$\int d^2r \ Q = \sum_{\ell=1}^{n_p} \int_0^1 du \int_0^1 dv \left| \frac{\partial \mathbf{r}}{\partial u} \times \frac{\partial \mathbf{r}}{\partial v} \right| Q = \sum_{\ell=1}^{n_p} \int_0^1 du \int_0^1 dv |\mathbf{N}| Q$$
 (2.5)

for any quantity Q. Thus, (2.4) becomes

$$\mathbf{B}(\mathbf{r}) = \frac{\mu_0}{4\pi} \sum_{\ell'=1}^{n_p} \int_0^1 du' \int_0^1 dv' \frac{1}{|\mathbf{r} - \mathbf{r}'|} \left[\mathbf{N}' \times \nabla' \Phi' \right] \times (\mathbf{r} - \mathbf{r}'). \tag{2.6}$$

We use primes to denote quantities on the surface with the current potential, to distinguish these quantities from the coordinates at which \mathbf{B} is evaluated.

Now observe that $\nabla'\Phi' = (\nabla'u')\partial\Phi'/\partial u' + (\nabla'v')\partial\Phi'/\partial v'$. Also observe (suppressing primes temporarily to reduce clutter)

$$\mathbf{N} \times \nabla u = \left(\frac{\partial \mathbf{r}}{\partial v} \times \frac{\partial \mathbf{r}}{\partial u}\right) \times \nabla u = \left(\frac{\partial \mathbf{r}}{\partial u}\right) \underbrace{\left(\frac{\partial \mathbf{r}}{\partial v} \cdot \nabla u\right)}_{=0} - \left(\frac{\partial \mathbf{r}}{\partial v}\right) \underbrace{\left(\frac{\partial \mathbf{r}}{\partial u} \cdot \nabla u\right)}_{=1} = -\frac{\partial \mathbf{r}}{\partial v}$$
(2.7)

and

$$\mathbf{N} \times \nabla v = \left(\frac{\partial \mathbf{r}}{\partial v} \times \frac{\partial \mathbf{r}}{\partial u}\right) \times \nabla v = \left(\frac{\partial \mathbf{r}}{\partial u}\right) \underbrace{\left(\frac{\partial \mathbf{r}}{\partial v} \cdot \nabla v\right)}_{-1} - \left(\frac{\partial \mathbf{r}}{\partial v}\right) \underbrace{\left(\frac{\partial \mathbf{r}}{\partial u} \cdot \nabla v\right)}_{-2} = \frac{\partial \mathbf{r}}{\partial u}.$$
 (2.8)

Thus, we obtain

$$\mathbf{B}(\mathbf{r}) = \frac{\mu_0}{4\pi} \sum_{\ell'=1}^{n_p} \int_0^1 du' \int_0^1 dv' \frac{1}{|\mathbf{r} - \mathbf{r}'|^3} \left[\frac{\partial \mathbf{r}'}{\partial u'} \frac{\partial \Phi'}{\partial v'} - \frac{\partial \mathbf{r}'}{\partial v'} \frac{\partial \Phi'}{\partial u'} \right] \times (\mathbf{r} - \mathbf{r}'). \tag{2.9}$$

Integrating by parts in u' and v', and using the assumption that Φ is single-valued to drop boundary contributions,

$$\mathbf{B}(\mathbf{r}) = \frac{\mu_0}{4\pi} \sum_{\ell'=1}^{n_p} \int_0^1 du' \int_0^1 dv' \, \Phi' \left[\frac{\partial}{\partial u'} \left(\frac{1}{|\mathbf{r} - \mathbf{r}'|^3} \frac{\partial \mathbf{r}'}{\partial v'} \times (\mathbf{r} - \mathbf{r}') \right) - \frac{\partial}{\partial v'} \left(\frac{1}{|\mathbf{r} - \mathbf{r}'|^3} \frac{\partial \mathbf{r}'}{\partial u'} \times (\mathbf{r} - \mathbf{r}') \right) \right].$$
(2.10)

If the outer derivatives act on the $\partial \mathbf{r}'/\partial v'$ and $\partial \mathbf{r}'/\partial u'$ terms, the resulting contributions cancel, so we can pull these $\partial \mathbf{r}'/\partial \dots$ terms out in front of the outer derivatives:

$$\mathbf{B}(\mathbf{r}) = \frac{\mu_0}{4\pi} \sum_{\ell'=1}^{n_p} \int_0^1 du' \int_0^1 dv' \, \Phi' \left[\frac{\partial \mathbf{r}'}{\partial v'} \times \frac{\partial}{\partial u'} \left(\frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \right) - \frac{\partial \mathbf{r}'}{\partial u'} \times \frac{\partial}{\partial v'} \left(\frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \right) \right]. \tag{2.11}$$

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Next, note that for any scalar w and vector $\mathbf{a}(w)$,

$$\frac{\partial}{\partial w} \left(\frac{\mathbf{a}}{|\mathbf{a}|^3} \right) = \frac{1}{|\mathbf{a}|^3} \frac{\partial \mathbf{a}}{\partial w} - \frac{3}{|\mathbf{a}|^5} \mathbf{a} \mathbf{a} \cdot \frac{\partial \mathbf{a}}{\partial w}.$$
 (2.12)

Using this result, and multiplying (2.11) by an arbitrary vector \mathbf{Y} ,

$$\mathbf{B} \cdot \mathbf{Y} = \frac{\mu_0}{4\pi} \sum_{\ell'=1}^{n_p} \int_0^1 du' \int_0^1 dv' \, \Phi' \left[\dots \right]$$
 (2.13)

- 2.3 Basis functions
- 2.4 Fourier basis
- 2.5 Transfer matrix
- 2.6 Cylindrical approximation

CHAPTER 3

Input Parameters

In this section we describe all the parameters which can be included in the input namelist.

3.1 Resolution parameters

For any new set of surface geometries you consider, you should vary the resolution parameters in this section to make sure they are large enough. These parameters should be large enough that the code results you care about are unchanged under further resolution increases.

nu_plasma

Type: integer *Default*: 64

When it matters: Always

Meaning: Number of grid points in poloidal angle used to evaluate the integral To do: XXX in the outer-to-plasma surface inductance matrix. Often 64 is a good value. It is resonable and common but not mandatory to use the same value for nu_plasma, nu_middle, and nu_outer.

nu_middle

Type: integer *Default*: 64

When it matters: Always

Meaning: Number of grid points in poloidal angle used to evaluate the integral To do: XXX in the outer-to-middle surface inductance matrix. Often 64 is a good value. It is resonable and common but not mandatory to use the same value for nu_plasma, nu_middle, and nu_outer.

$\mathtt{nu_outer}$

Type: integer *Default*: 64

When it matters: Always

Meaning: Number of grid points in poloidal angle used to evaluate the integral To do: XXX in the outer-to-plasma surface and outer-to-middle surface inductance matrices. Often 64 is a good value. It is resonable and common but not mandatory to use the same value for nu_plasma, nu_middle, and nu_outer.

nv_plasma

Type: integer *Default*: 64

When it matters: Always

Meaning: Number of grid points in poloidal angle used to evaluate the integral To do: XXX in the outer-to-plasma surface inductance matrix. A value of 64 is often good when the number of field periods is more than 1. A higher value like 256 may be needed when the number of field periods is 1. It is resonable and common but not mandatory to use the same value for nv_plasma, nv_middle, and nv_outer.

nv_middle

Type: integer *Default*: 64

When it matters: Always

Meaning: Number of grid points in poloidal angle used to evaluate the integral To do: XXX in the outer-to-middle surface inductance matrix. A value of 64 is often good when the number of field periods is more than 1. A higher value like 256 may be needed when the number of field periods is 1. It is resonable and common but not mandatory to use the same value for nv_plasma, nv_middle, and nv_outer.

nv_outer

Type: integer Default: 64

When it matters: Always

Meaning: Number of grid points in poloidal angle used to evaluate the integral To do: XXX in the outer-to-plasma surface and outer-to-middle surface inductance matrices. A value of 64 is often good when the number of field periods is more than 1. A higher value like 256 may be needed when the number of field periods is 1. It is resonable and common but not mandatory to use the same value for nv_plasma, nv_middle, and nv_outer.

mpol_plasma

Type: integer Default: 8

When it matters: Always

Meaning: Maximum poloidal mode number to include for the Fourier basis functions on the plasma surface. The value can be positive or zero. It is resonable and common but not mandatory to use the same value for mpol_plasma, mpol_middle, and mpol_outer.

mpol_middle

Type: integer

Default: 8

When it matters: Always

Meaning: Maximum poloidal mode number to include for the Fourier basis functions on the middle surface. The value can be positive or zero. It is resonable and common but not mandatory to use the same value for mpol_plasma, mpol_middle, and mpol_outer.

mpol_outer

Type: integer Default: 8

When it matters: Always

Meaning: Maximum poloidal mode number to include for the Fourier basis functions on the outer surface. The value can be positive or zero. It is resonable and common but not mandatory to use the same value for mpol_plasma, mpol_middle, and mpol_outer.

ntor_plasma

Type: integer Default: 8

When it matters: Always

Meaning: Maximum toroidal mode number to include for the Fourier basis functions on the plasma surface. The value can be positive or zero. It is resonable and common but not mandatory to use the same value for ntor_plasma, ntor_middle, and ntor_outer. You can set the three ntor parameters to zero to examine only axisymmetric modes.

ntor_middle

Type: integer Default: 8

When it matters: Always

Meaning: Maximum toroidal mode number to include for the Fourier basis functions on the middle surface. The value can be positive or zero. It is resonable and common but not mandatory to use the same value for ntor_plasma, ntor_middle, and ntor_outer. You can set the three ntor parameters to zero to examine only axisymmetric modes.

ntor_outer

Type: integer *Default*: 8

When it matters: Always

Meaning: Maximum toroidal mode number to include for the Fourier basis functions on the outer surface. The value can be positive or zero. It is resonable and common but not mandatory to use the same value for ntor_plasma, ntor_middle, and ntor_outer. You can set the three ntor parameters to zero to examine only axisymmetric modes.

3.2 Geometry parameters for the plasma surface

geometry_option_plasma

Type: integer

Default: 0

When it matters: Always

Meaning: This option controls which type of geometry is used for the plasma surface.

geometry_option_plasma = 0: The plasma surface will be a plain circular torus. The major radius will be RO_plasma. The minor radius will be a_plasma.

geometry_option_plasma = 1: Identical to option 0. (This option exists just for consistency
with geometry_option_middle and geometry_option_outer.)

geometry_option_plasma = 2: The plasma surface will be the last surface in the full radial grid of the vmec file specified by woutFilename. The poloidal angle used will be the normal vmec angle which is not a straight-field-line coordinate.

geometry_option_plasma = 3: The plasma surface will be the last surface in the half radial grid of the vmec file specified by woutFilename. The poloidal angle used will be the normal vmec angle which is not a straight-field-line coordinate.

geometry_option_plasma = 4: The plasma surface will be the last surface in the half radial grid of the vmec file specified by woutFilename. The poloidal angle used will be the straight-field-line coordinate, obtained by shifting the normal vmec poloidal angle by vmec's λ quantity.

geometry_option_plasma = 5: The plasma surface will be the flux surface with normalized poloidal flux efit_psiN taken from the efit file specified by efit_filename.

$R0_plasma$

Type: real Default: 10.0

When it matters: Only when geometry_option_plasma is 0 or 1.

Meaning: Major radius of the plasma surface, when this surface is a plain circular torus.

a_plasma

Type: real Default: 0.5

When it matters: Only when geometry_option_plasma is 0 or 1.

Meaning: Minor radius of the plasma surface, when this surface is a plain circular torus.

nfp_imposed

Type: integer Default: 1

When it matters: Only when geometry_option_plasma is 0 or 1.

Meaning: When the plasma surface is a plain circular torus, only toroidal mode numbers that are a multiple of this parameter will be considered. This parameter thus plays a role like <code>vmec</code>'s <code>nfp</code> (number of field periods), and is used when <code>nfp</code> is not already loaded from a <code>vmec</code> file.

woutFilename

Type: string Default: "

When it matters: Only when geometry_option_plasma is 2, 3, or 4.

Meaning: Name of the vmec wout output file which will be used for the plasma surface. You can

use either a netCDF or ASCII format file.

efit_filename

Type: string Default: "

When it matters: Only when geometry_option_plasma is 5.

Meaning: Name of the efit output file which will be used for the plasma surface.

efit_psiN

Type: real Default: 0.98

When it matters: Only when geometry_option_plasma is 5.

Meaning: Value of normalized poloidal flux at which to select a flux surface from the efit input file. A value of 1 corresponds to the last closed flux surface, and 0 corresponds to the magnetic axis.

efit_num_modes

Type: integer Default: 10

When it matters: Only when geometry_option_plasma is 5.

Meaning: Controls the number of Fourier modes used to represent $R(\theta)$ and $Z(\theta)$ for the shape of the plasma surface. Each of these functions will be expanded in a sum of functions $\sin(m\theta)$ and $\cos(m\theta)$, where m ranges from 0 to efit_num_modes-1.

3.3 Geometry parameters for the middle surface

geometry_option_middle

Type: integer Default: 0

When it matters: Always

Meaning: This option controls which type of geometry is used for the middle surface.

geometry_option_middle = 0: The middle surface will be a plain circular torus. The major radius will be the same as the plasma surface: either RO_plasma if geometry_option_plasma is 0 or 1, or Rmajor_p from the vmec wout file if geometry_option_plasma is 2. The minor radius will be a_middle.

geometry_option_middle = 1: Identical to option 0, except the major radius of the middle surface will be set by R0_middle.

geometry_option_middle = 2: The middle surface will computing by expanding the plasma surface uniformly by a distance separation_middle.

geometry_option_middle = 3: The middle surface will be the 'coil' surface in the NESCOIL 'nescin' input file specified by nescin_filename_middle.

R0_middle

Type: real Default: 10.0

When it matters: Only when geometry_option_middle is 1.

Meaning: Major radius of the middle surface, when this surface is a plain circular torus.

a_middle

Type: real Default: 1.0

When it matters: Only when geometry_option_middle is 0 or 1.

Meaning: Minor radius of the middle surface, when this surface is a plain circular torus.

separation_middle

Type: real Default: 0.2

When it matters: Only when geometry_option_middle is 2.

Meaning: Amount by which the middle surface is offset from the plasma surface.

nescin_filename_middle

Type: string Default: "

When it matters: Only when geometry_option_middle is 3.

Meaning: Name of a NESCOIL nescin input file. The coil surface from this file will be used as

the middle surface for bdistrib.

3.4 Geometry parameters for the outer surface

geometry_option_outer

Type: integer *Default*: 0

When it matters: Always

Meaning: This option controls which type of geometry is used for the outer surface.

geometry_option_outer = 0: The outer surface will be a plain circular torus. The major radius will be RO_outer. The minor radius will be a_outer.

geometry_option_outer = 1: Identical to option 0.

geometry_option_outer = 2: The outer surface will computing by expanding the plasma surface uniformly by a distance separation_outer.

geometry_option_outer = 3: The outer surface will be the 'coil' surface from the NESCOIL 'nescin' input file specified by nescin_filename_outer.

R0_outer

Type: real Default: 10.0

When it matters: Only when geometry_option_outer is 1.

Meaning: Major radius of the outer surface, when this surface is a plain circular torus.

a outer

Type: real Default: 1.5

When it matters: Only when geometry_option_outer is 0 or 1.

Meaning: Minor radius of the outer surface, when this surface is a plain circular torus.

separation_outer

Type: real Default: 0.4

When it matters: Only when geometry_option_outer is 2.

Meaning: Amount by which the outer surface is offset from the plasma surface. (Not the offset

between the outer and *middle* surfaces!).

nescin_filename_outer

Type: string Default: "

When it matters: Only when geometry_option_outer is 3.

Meaning: Name of a NESCOIL nescin input file. The coil surface from this file will be used as

the outer surface for bdistrib.

3.5 Other parameters

basis_set_option

Type: integer Default: 1

When it matters: Always

Meaning: Determines which set of basis functions is used.

basis_set_option = 1: Use $\sin(2\pi[mu + nv])$ basis functions.

basis_set_option = 2: Use $\cos(2\pi[mu + nv])$ basis functions.

basis_set_option = 3: Use both $\sin(2\pi[mu+nv])$ and $\cos(2\pi[mu+nv])$ basis functions.

pseudoinverse_thresholds

Type: real array *Default*: 1e-12

When it matters: Always

Meaning: To form the pseudoinverse of the outer-to-middle inductance matrix, singular values larger than this threshold will be replaced by their inverse, whereas singular values smaller than this threshold will be replaced by zero. You can supply more than one threshold value in order to compare results for different choices. Good threshold values are in the range 1e-6 to 1e-13, i.e. small compared to 1 but larger than machine precision.

n_singular_vectors_to_save

Type: integer *Default*: 12

When it matters: Always

Meaning: Number of columns of U and V to save in the output file, where U and V are the matrices of left and right singular vectors of the transfer matrix, $T = U\Sigma V^T$. Regardless of this parameter, all singular *values* will be saved in the output file.

save_level

Type: integer Default: 2

When it matters: Always

Meaning: Option related determining how many variables are saved in the netCDF output file. The larger the value, the smaller the output file.

save_level = 0: Save everything.

save_level = 1: Save everything except the inductance matrices.

save_level = 2: Save everything except the inductance matrices and the drdu, drdv, and normal arrays.

References

- [1] A. Boozer. Nucl. Fusion, 55, 025001 (2015).
- [2] P. Merkel. Nucl. Fusion, 27, 867 (1987).