2019/03/06

VMEC-BOOZXFORM-READFLD memo

(VMEC ver. 8.50 or later is recommended)

1. Compile-Install

1. Expand STELLOPT.tar.gz
2. Edit "setup.sh" to be customized for your environment
3. run the shell
   - Choose "release"
   - Choose "vmec2000 booz_xform"
   - Choose either with- or without NETCDF support (Note: one should build NETCDF version and non-NETCDF version (text WOUT file and binary BOOZMN file) independently)
   - MPI – no
   - Choose clean or ordinary make
4. After compiling, symbolic links for "xbooz_xfrom" and "xvmec2000" are created in the install directory "/home/HOGE/bin". To keep both the NETCDF and non-NETCDF version, copy the executable files under the install directory by renaming "xvmec2000_cdf", "xvmec2000_txt", and so on.

5. Compile "READFLD_CDF"
   Just "Make" it. It requires libGSPS.a, but if the user does not use any plotting subroutines in the source, the library can be omitted in the compilation (remove "-DGSPS" flag in Makefile).
   This READFLD is compatible both for binary and NETCDF format of boozmn file.
   The code is MPI parallelized to speed up the calculation of volume elements and so on required specifically for FORTEC-3D code.

Note : netcdf and hdf5 libraries are required to compile these programs to handle netcdf files.

2. Run VMEC-Boozxform

1. Edit "run-vmec-boozxform.sh"
   Note: As above, one should choose either NETCDF version or non-NETCDF version

   The shell script automatically make the "in_booz.***" input file.
   According to the explanation in VMEC wiki
   (https://bitbucket.org/lazerson_princeton/stellopt/wiki/Home) , set the number of poloidal and toroidal harmonics, and the flux surfaces to be chosen.
   Note : In Satake's modified version of BOOZ_XFORM, if '888' is specified for the surface list in in_booz.***, it generates the Boozer-coordinates data for all the surfaces that WOUT file contains. Otherwise, user should modify the script so that all the surface indexes "2 3 4 …. ns" are listed in the third line of in_booz.*** file.

2. Run the script

Messages from VMEC and BOOZ_XFORM are written in “msg-vmec(bzxfm).****” , respectively.

VMEC output : wout_***.nc (NETCDF ver.) or wout_***.txt (non-NETCDF ver.)
BOOZ_XFORM output: boozmn_***. nc (NETCDF ver.) or boozmn.*** (non-NETCDF ver.)

In the case of NETCDF, the shell script automatically generate “***.nc.txt” files, which is translation of .nc file to ascii readable format.

3. Run READFLD_CDF

1. prepare “input-read.***” and “input-prof.***” files
   - In “input-read” file, the file name “boozmn_****(.nc)” is specified by “fileext”
   - In case of non-CDF VMEC and BOOZ_XFORM, “wout_txt” should be given.
     - This “wout_txt” is the string appearing in middle of the wout_***.txt file, usually same as the “***” part of the WOUT file name itself.
     - When reading the TASK3D output of WOUT file, user needs to check the string by oneself.
     - Switch to change NETCDF or not by “lcdfbin=.true. (or .false.)”
   - Details of the other input parameters are explained later.
2. Run the script “sub-readfld.sh”
3. The subroutine which reads the boozmn file is “iodisk_cdf” (for NETCDF file) or “io_bin_boozmn” (for binary file).

   Contents of the data file are (suffix “_b” stands for “in Boozer coordinates”) :
   bmnc_b : B_mn Cos Fourier components
   rmnc_b : R_mn Cos 〃
   zmns_b : Z_mn Sin 〃
   pmns_b : ϕ _mn Sin 〃 (relation b/w Boozer $\zeta \Leftrightarrow$ cylinder ϕ toroidal angles)
   gmnc_b : Fourier components of the Jacobian in Boozer coordinates

   If lasym_inp==.true., then up-down asymmetric components for these variables above are also contained. (exchange Sin $\Leftrightarrow$ Cos)

   The followings are flux-surface functions:
   iota_b : rotational transform
   phi_b : toroidal flux
   phip_b : = d(phi)/ds
   bvco_b : poloidal current
   buco_b : toroidal current

4. READFLD also reads the following quantities from WOUT file.
   Rmajor_p : Major radius
   Aminor_p : Minor radius
   VolavgB : volume-average B
   volume_p : plasma volume

4. Input parameters for READFLD

- **input-read.******
  namelist/NEWBZ

  - mmx : how many Fourier modes of B etc. are chosen from Boozmn output (mmx_as for up-down asymmetry components wheh lasym=.true.). Note that total number of Fourier mode is mmx+1, since (m,n)=(0,0) mode is added.
  - kmsh : radial mesh numbers for Spline fitting of B, n, T, iota, etc. kmsh ~ 50 is recommended.
  - nlim, mlim : |m|>mlim, |n|>nlim modes are omitted when choosing Fourier modes (=0 : no limitation)
  - lmask : =.true. if user wants to remove specific (m,n) modes from the B-field spectrum. If .true., then the list of masked modes are given by file #20, "input-mask.***" in the following form:

```
#cos mode mask
2                          ← number of modes to be masked
1    0    1                ← index, Cos-(m, n) mode to be neglected
2    0    36
#sin mode mask             ← in case lasym=.true.
3
1    0    16
2    0    17
3    0    1
```

  - dcheck : =.true. if user wants to check all the Bmn spectrum contained in boozmn output. Data is written in debug93.*** file.
  - lrchk, ltsmap : Convert the boozmn output so that the equilibrium data sent to FORTEC-3D becomes right-handed coordinate system. **lrchk=.true.、ltsmap=.false. is recommended.**
    - ✧ Note : Because of the transformation, sometimes the direction of J and B vectors are opposite to that in VMEC calculation. FORTEC-3D always sees that toroidal magnetic flux is positive.
    - ✧ Iota (=1/q) may be negative in Boozer coordinates.
  - bmag : B-field strength can be magnified by this factor.
  - ifile : How to give (R,a,B0) for normalization in READFLD_CDF
    - ✧ **=0 : from WOUT file (recommended)**
    - ✧ =1 : from input-prof file
  - iswrho : how to choose effective minor radius (anorm) in FORTEC-3D
    =0 : from toroidal flux and B0 chosen by ifile switch (old fashion)
    =1 : anorm=Aminor_p in VMEC (recommended)
    =2 : anorm=a99 in the input parameter
    Note: In any case, Bnorm is defined so that psi_edge=0.5*Bnorm*anorm^2 is satisfied.

  - itype : How to give the n_i ,T_i and T_e profiles
    - ✧ =0 : Old-fashioned FORTEC-3D , in exp-form
    - ✧ **=1 : 10th-order polynomials in rho=(r/a). Same as in GSRAKE (recommended)**
    - ✧ =2 : exp*tanh function, same as in GT5D
    - ✧ =3 : TJ-II, Velasco' way
    - ✧ **=4 : Read table data from #19 file and make spline-fitted profile (recommended)**

    Example of the profile data file "prof-fortec_sample.dat" is contained in

READFLD_EXAMPLE (please contact Satake where to download the files) . It should have the following form:

```
-------------
51            ← the first line shows the number of radial data points
#          rho       ni[m^-3]        Te[eV]        Ti[eV]        Er[V/m]   ← header lines are skipped
  0.000E-02    2.527E+19    2.006E+03    2.045E+03     0.000E+02
  1.000E-02    2.526E+19    2.005E+03    2.043E+03    -3.215E+02
  3.000E-02    2.523E+19    2.002E+03    2.035E+03    -9.980E+02
  5.000E-02    2.517E+19    1.996E+03    2.020E+03    -1.459E+03
  7.000E-02    2.507E+19    1.988E+03    1.997E+03    -1.862E+03
          ...
          ...
  9.700E-01    3.791E+18    1.493E+02    2.633E+02    -9.129E+03
  9.900E-01    3.076E+18    1.414E+02    1.784E+02    -1.200E+04
--------------
```

Arbitral interval of radial mesh points are allowed.

Note :

- In case of itype=0,1,2,3, the coefficients to specify the n and T functions are given in "input-prof.***" file.
- It is recommended that the profile data has rho=0.00 line for smooth fitting to the magnetic axis.
- n,T, Er profile data should have [1/m^3] ,[keV], and [V/m] units, respectively. One can magnify the (n,T,Er) values by the input parameters dfac, tfac, efac in "input-prof" file to adjust the unit of the profile data.
  For example, if the n, T ,Er profiles table is given as above, tfac=1.0d-3, dfac=efac=1.0 so that unit of T becomes [keV].
- In case of itype=4, Er profile input is required only if efac≠0. If efac>0., then the 5th column of prof-fortec file is read and interpolated. Fitted Er profile data appears in "debug92.****" file. which can be used as an input file of FORTEC-3D to specify the Er profile. See § 3.2 of FORTEC-3D manual, the explanation of input-er***.dat file.

- lasym: true for up-down asymmetry (single-null tokamak), false for stellarators.
- lcdfbin : true if boozmn and wout data files are NetCDF format, otherwise false.
- fileext : the name "boozmn_***(.nc)"
- wout_txt : the string appear in the middle of wout file (required only if lcdfbin=.false.).
- lcnorm : always =.false. (only for debug purpose)

namelist/GSRAKE_IN

- ifgsrake : = .true. if GSRAKE input file is required
- ifbr : = .true. if the effect of tangential magnetic drift ($\propto$dB/dr) is included in GSRAKE calculation. For numerical stability, .false. is recommended.
- ifprof: =.true : for Satake's modified GSARKE (give n,T and dn/dr dT/dr table data directry to GSARAKE) ,
  =.false. : polynomial coefficients are sent to GSRAKE (original).
- nrho: radial mesh points on which GSRAKE solves neoclassical fluxes
- nercell : radial mesh points for flux and Er evaluation in FORTEC-3D.

Note : nrho and nercell can be different. nercell can also be different from nrcell explained below, but in near future nercell will be abolished and unified to nrcell.

It is recommended to set nrho=nercell=nrcell.

namelist/ V_ELEMENT

- nacell,nrcell,nzcell： (theta,rho,zeta)-cells for collision and weight-averaging calculation.
- ndivz: Number of toroidal period of the system. full torus=1, 1/18 torus=18。LHD=10、W7-X=5, etc. Usually equals to nfp in VMEC.
- erra, idvin,idivzin：control parameters for the evaluation of volumes of the cells. Do not need to change.
- lnewwflx：=.false. is default
- ifvolem: =1 (on) is default

namelist/ZAHYOIN

- npsi, ntheta, nzeta：meshes to plot flux surface shape
- ztrange：range of toroidal angle to plot the cross-section shapes (× π)
- nguess：test points to find phi=const. poloidal cross-section, 200~500 is enough.

- **input_prof.******
  - dn0, ti0, te0：polynomial or function fitting coefficients for density and temperature
    Meaning of the coefficients differ according to the switch itype. See the subroutines of ntfuncX in setfld.f90 to understand the functions.
    In case itype=4, put arbitrary number for each line (ignored)
  - cr0, …：not used any more；just leave it
  - B0, R0, Z0(=0 always), a0： If one needs to specify the normalization factors, set values here (in case ifile=1).
  - zi , nmass：ion charge and mass (relative to H ion)
  - beta0：obsolete
  - a99：When itype=0~3, and if the profile fitting function is regarded as r_eff instead of rho, set the effective minor radius a99 [m]. Set a99=0.0 usually.
  - dfac, tfac, efac：magnification factors for density, temperature, and Er profile.
    These factors are used to adjust the profile input data to [1/m^3], [keV],[V/m].
    efac has effect only if itype=4, and if efac=0, Er profile data is not required.
  - ncurr, ntor, iqfunc, etc.：not used.

5. Output files from READFLD

- res-read: General messages from READFLD
- avs. , avs2.：Data for plotting magnetic field configuration.
  plot-cont.gpl and plot-cont_surf.gpl are sample gnuplot script to draw figures.
- xspctl: Configuration data used in Orbit6 to draw orbits.
- volem,spctl：unimportant：check cell volume and magnetic field spectrum
- cell_rphiz：unimportant：Relationship of the cell position (nrcell,nacell,nzcell) in Boozer coodinates and (R,phi,Z) in lab. frame. plot_cell-pos.gpl is a sample script.
- **field-data：Configuration data for FORTEC-3D.**
- debug91：To check the n and T profile

- debug92 ; If itype=4 and efac>0.0, E_r radial fitting profile data is created here.
  Note : to use this as input for FORTEC-3D, set “inief=-1500” in the FORTEC-3D input file.
- debug93 : Bmn spectra data (full data contained in boozmn file).
  plot-bmn.gpl to plot the data by gnuplot