

CheasePy

User Guide

Ehab Hassan

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CheasePy is code written in Python to run the CHEASE (*Cubic Hermite Element Axisymmetric Static Equilibrium*) code, which solves the Grad-Shafranov equation for toroidal MHD equilibria using pressure and current profiles and fixed plasma boundaries that is defined by a set of experimental data points (R,Z). The CheesePy code allows an iterative running of the CHEASE code either to check the preservation of MHD equilibria or converging to an experimentally defined total toroidal plasma current by modifying any input quantity.

1 Toroidal MHD Equilibrium

1.1 Grad-Shafranov Equation

The MHD equilibrium equations are given by:

$$\mathbf{J} \times \mathbf{B} = \nabla p \quad (1)$$

$$\nabla \times \mathbf{B} = \mathbf{J} \quad (2)$$

$$\nabla \cdot \mathbf{B} = 0 \quad (3)$$

The magnetic field can be represented as:

$$\mathbf{B} = T\nabla + \nabla\phi \times \nabla\Psi \quad (4)$$

where ϕ is the ignorable toroidal angle and Ψ is the poloidal magnetic flux function.

For static MHD equilibria, the Grad-Shafranov equation is given by:

$$\nabla \cdot \frac{1}{R^2} \nabla \Psi = \frac{j_\phi}{R} = -p'(\Psi) - \frac{1}{R^2} TT'(\Psi) \quad (5)$$

where j_ϕ denotes the toroidal plasma current density, R the major radius of the torus. The nature of the equilibria is determined by the two free functions $p'(\Psi)$ and $TT'(\Psi)$, where the pressure p and the poloidal current flux function T are functions of Ψ only.

The total current everywhere inside the plasma ($\Psi < 0$) is positive and is given by:

$$I = \int j_\phi dS = \int j_\phi (J/R) d\Psi d\chi \quad (6)$$

where J is the Jacobian.

1.2 Current Profiles

To achieve MHD equilibrium CHEASE can treat different current profiles such as:

- The poloidal current flux:

$$TT'(\Psi) \quad (7)$$

- The surface averaged current density:

$$I^*(\Psi) = \frac{\oint j_\phi (J/R) d\chi}{\oint (J/R) d\chi} = -R_0^2 \frac{C_1}{C_0} p'(\Psi) - R_0^2 \frac{C_2}{C_0} \frac{TT'(\Psi)}{\mu_0} \quad (8)$$

- The averaged parallel current:

$$I_\parallel = \frac{\oint \mathbf{J} \cdot \mathbf{B} J d\chi}{\oint \mathbf{B} \cdot \nabla \phi J d\chi} = R_0 \frac{\langle \mathbf{J} \cdot \mathbf{B} \rangle}{\langle T/R^2 \rangle} \quad (9)$$

$$I_\parallel = \frac{\oint \mathbf{J} \cdot \mathbf{B} J d\chi}{\oint \mathbf{B} \cdot \nabla \phi J d\chi} = -R_0 \frac{C_1}{C_2} p'(\Psi) - R_0 \frac{TT'(\Psi)}{\mu_0}(\Psi) \left(1 + \frac{1}{T^2(\Psi)} \frac{C_3}{C_2} \right) \quad (10)$$

- The averaged parallel current density:

$$J_\parallel = \frac{\langle \mathbf{J} \cdot \mathbf{B} \rangle}{B_0} \quad (11)$$

where,

$$\{C_0, C_1, C_2, C_3\} = \oint \left\{ \frac{1}{R}, 1, \frac{1}{R^2}, \frac{|\nabla \Psi|^2}{R^2} \right\} J d\chi \quad (12)$$

$$\langle \mathbf{J} \cdot \mathbf{B} \rangle = -T(\Psi) p'(\Psi) - T'(\Psi) \frac{\langle B^2 \rangle}{\mu_0} \quad (13)$$

$$\langle B^2 \rangle = \frac{\oint B^2 J d\chi}{\oint J d\chi} \quad (14)$$

$$\langle T/R^2 \rangle = \frac{\oint T/R^2 J d\chi}{\oint J d\chi} \quad (15)$$

The toroidal current density can be expressed as:

$$j_\phi = \frac{1}{R} \left(\frac{C_0}{C_2} I^*(\Psi) + \left(\frac{C_1}{C_2} - R^2 \right) p'(\Psi) \right) \quad (16)$$

$$j_\phi = \frac{1}{yR} \left(I_\parallel(\Psi) + \left(\frac{C_1}{C_2} - yR^2 \right) p'(\Psi) \right) \quad (17)$$

where

$$y = 1 + \frac{1}{T^2(\Psi)} \frac{C_3}{C_2} \quad (18)$$

1.3 Normalized Quantities

The normalization used here has the following format:

$$\begin{aligned} \Psi &= B_0 R_0^2 \\ I &= \frac{B_0 R_0}{\mu_0} \quad \text{and} \quad J = \frac{B_0}{\mu_0 R_0} \\ p &= \frac{B_0^2}{\mu_0} \quad \text{and} \quad p' = \frac{B_0}{\mu_0 R_0^2} \\ T &= B_0 R_0 \quad \text{and} \quad T' = \frac{1}{R_0} \quad \text{and} \quad TT' = B_0 \end{aligned}$$

2 CHEASE [Fortran] Code

When CHEASE code runs based on experimental data points it takes as an input three files. The *EXPEQ* file (which is a kind of EFIT file, also known as EQDSK file) which has the experimental equilibrium quantities such as the current profile, in addition to the magnetic configuration. The second file is the *EXPTNZ* file which contains profiles for the ion and electron temperatures (T_i & T_e) and densities (n_i & n_e), in addition to the effective atomic number (Z_{eff}) as a function of the normalized poloidal axis (ψ_N). The CHEASE code also takes the *chease_namelist* file which has the initialization parameters that depend on the plasma fusion machine shot, the type of the input physical quantities, and the run-mode of the CHEASE code. For more information about CHEASE code and the different options for the input parameters in the *chease_namelist* file you may go to their [website](#) which has all the required resources and references.

After a successful run, the CHEASE code produces several output files, but CheasePy code uses only *four* of them. The *EXPEQ.OUT(IN)* output files have specific experimental quantities from the EFIT file depending on the selected values of the input parameters in the *chease_namelist* file, such as pressure (P), poloidal coordinate grid points ($\rho(\psi)$), parallel current density profile ($J_{||}$), etc. *EXPTNZ.OUT(IN)* output file should have exactly the same profiles in the *EXPTNZ* input file but with a higher resolution. CHEASE code also packs several output quantities related to the coordinate systems and physical quantities into an HDF5 file called *ogyropsi.h5*, and it should be noticed here that all the quantities in the HDF5 file have SI units in contrary to the normalized quantities in the *EXPEQ.OUT(IN)* files. CHEASE code also gives a text file as an output that contains all the outcomes similar to the HDF5 file named based on the iteration number to be *ogyropsi.dat*. The CHEASE code produces also several other output files but they aren't needed by CHEASEPY.¹

It should be noticed here that for calculating the MHD equilibrium in the zero iteration the CHEASE code uses an *EXPEQ* file that may have the EFIT or EQDSK format which contains an extensive amount of information about the machine geometry, magnetic configuration, and plasma status. However it can also use a reduced format of the EQDSK file which contains only the required data for the next iteration to run properly. In contrary, the format of the *EXPTNZ* doesn't change from one iteration to another, it has the same profiles but with higher resolution as mentioned above. Some parameters in the *chease_namelist* file need to be changed from one iteration to another, but most of them keep their values. For example, the *NEQDSK* parameter takes 1 when using the EFIT file in EQDSK format, or it takes 0 to create the *EXPEQ* from input/given parameters. We will shed more lights on the description and function of the parameters needed to be modified to properly run the CheasePy code in other sections, but it worth mentioning here that the provided *chease_namelist* file with the CheasePy code has only the parameters that you may need to change based on the case you run such as pressure type (nppfun), current type (nsttp), coordinates resolution (NPSI,NCHI,NS,NT,NISO). Other parameters which are not provided in the basic *chease_namelist* file are set to their default values by CheasePy code in the *namelistcreate()* function, or by the CHEASE code itself. You may also add these parameters to the *chease_namelist* file in case you will change them in a regular basis.

¹CheasePy renames all the required input and output files to include the iteration number at the end of each filename, e.g. CheasePy renames *EXPEQ.OUT* to *EXPEQ_iter000.OUT* after the zeroth iteration and does the same after each iteration for all IN and OUT files. However, in case of the files *ogyropsi.dat* and *ogyropsi.h5*, CheasePy renames them to *chease_iterxxx.dat* and *chease_iterxxx.h5*, respectively, after each iteration.

3 CheasePy [Python] Code

To run the CheasePy code you need to have the CHEASE code compiled first in your local machine as instructed in the CHEASE developer [website](#) and have the executable file named *chease.hdf5* in the same directory² of the *cheasepy.py*³, *runchease.py*⁴, and *efittools.py*⁵ files. Also, you need to have [Anaconda for Python 2.7/3.7 version](#) installed in your local machine, where the *cheasepy.py* script works with both versions of Python (2.7 or 3.7).

3.1 Directory Structure

In the main directory there should be at least two files, *runchease.py* and *chease.hdf5* with the path to *cheasepy.py* and *efittools.py* files being accessible. Also, the path to the files of the desired shot can be set to the ‘*shotpath*’ variable in the *runchease.py* script.

The **shots** folder contains subfolders for each available experimental output measurements. Each shot subfolder is named upon the user choice, but it is preferred to be named after the machine/shot name, e.g. *machine.name_shot.number*, and contains at least a profile file and a equilibrium geometry file with their names formatted to have ‘*the parent folder name*’ then ‘*underscore*’ then the type of data file, e.g. *machine.name_shot.number_FILE.TYPE*:

FLE.TYPE	Description
EQDSK	Geometry Equilibrium and Current and Pressure Profiles (full)
EXPEQ	Geometry Equilibrium and Current and Pressure Profiles (reduced)
EXPTNZ	Electron and Ions Profiles (reduced)
ITERDB	Electron and Ions Profiles (reduced)
PROFILES	A Complete Equilibrium Profiles for Ions, Electrons, Impurities, etc. (full)
CHEASE	A Complete Geometry and Profiles output from a previous Chease run (full)

You may add more shots to the shot folder by following the same method of naming the shot folder and the equilibrium geometry and profile files. Having a wrong name for the shot folder and/or any of its contents might cause *CheasePy* code doesn’t work properly.

CheasePy has the capability to take the electron profiles and ion profiles from different sources, it can also take the pressure profile from the EQDSK (EFIT) file or calculate it from any of the input profile sources.⁶ Because the profiles on each source are projected on its own grid, CheasePy allows users to unify all the provided profiles to a single grid by setting a source for the rhomesh grid.⁷

²It is recommended to set/export the \$PATH to the location of the *cheasepy.py* and *efittools.py* files, and to keep the *runchease.py* file with the *chease.hdf5* executable in the same folder.

³*cheasepy.py* is a Python package that contains all the required functions to perform all operations in the CheasePy code such as profile and geometry files creation, profile and geometry files reading, etc.

⁴*runchease.py* is a Python script that allows the user of CheasePy to setup the sources and types of all input profiles and geometry, and it also allows the user to setup the mode of operation of CheasePy code.

⁵*efittools.py* is a Python package that contains functions to read the efrit, profile, and iterdb files, and calculate the outer most closed magnetic surface that does not have the x-point.

⁶Calculating the pressure from EXPTNZ or ITERDB ignores the contribution of the fast particles (n_b).

⁷Considering both ρ_{ψ_N} and ρ_{ϕ_N} coordinates, CheasePy prefers a rhomesh grid source that has both coordinates to ease the interpolation process in different sources.

3.2 Creating chease_namelist File

The *CheasePy* code starts with copying the required profiles and equilibrium geometry files of the selected shot to the current directory, and then it uses the user-defined namelist parameters in *runchease.py* script file to create the *chease_namelist* file (which is required for CHEASE code to run as we indicated above) using the `create_namelist(setParam={})` function in the *cheasepy.py* package.

There is a long list of CHEASE namelist parameters that are used to set the operation mode of CHEASE code, but working on experimental measurements helps in reducing this list to smaller number of parameters, with all other parameters to set to their default values defined by either CHEASE or CheesePy. A list of the required CHEASE parameters can be found in the *runchease.py* script, and they can be modified based on the provided experimental facts. The namelist parameters are stored in a Python dictionary structure called `namelistVals`⁸ with the namelist parameters are the dictionary keys named as defined in CHEASE code. The value of each namelist parameter can be *single-valued* or *list-of-values* depending on the number of times the input namelist parameters will change from one iteration of running CHEASE to another. For example, if CheesePy runs CHEASE for 11 times but each parameter to the `namelistVals` is *single-valued*, then the same namelist input file created in the zeroth iteration will be used in the other 10 iterations. However, if the parameters in the `namelistVals` are defined as a list of two values, the first value will be used for the zeroth iteration of CHEASE then the second value will be used for the other 10 iterations. Generally, *CheasePy* will create a new *chease_namelist* file based on the number of values in the `namelistVals` and use the latest one for the rest of iterations.

The description of the CHEASE namelist parameters available in the *runchease.py* script can be found in the following table:^{9 10}

Parameter	Default	Description
NS	256	Number of tr-intervals for equilibrium calculation.
NT	256	Number of 0-intervals for equilibrium calculation.
NISO	256	Number of s-intervals to define $I^*(s)$ or $I_{ }(s)$.
NPSI	1024	Number of radial stability-s intervals.
NCHI	1024	Number of poloidal nodes for ballooning.
NRBOX	60	Number of R points used to save equilibrium in EQDSK.
NZBOX	60	Number of Z points used to save equilibrium in EQDSK.
RELAX	0	Under-relaxation parameter used if magnetic axis converges slowly
NSTTP	1	Type of input current profiles: 1= $f f'$, 2= I^* , 3= $I_{ }$, and 4= $J_{ }$.
NPROPT	3	Type of output current profiles: 1= $f f'$, 2= I^* , 3= $I_{ }$, and 4= $J_{ }$.
NPPFUN	8	Type of input pressure profiles: 4= P' and 8= P .
NEQDSK	0	Source of equilibrium geometry: 0=EXPEQ and 1=EQDSK
TENSBND	0	Interpolation weight around the x-point.
COCOS.IN	2	To determine the poloidal coordinate systems from input EXPEQ.
TENSPROF	0	Interpolation weight of the profiles.
COCOS.OUT	12	To determine the poloidal coordinate systems from output EXPEQ.
NRHOMESH	0	Type of input grid: 0= ρ_{ψ_N} and 1= ρ_{ϕ_N} .

The *TENSBND* parameter is set to a negative value, e.g. -1, when running CHEASE with NEQDSK=1, i.e. using the EQDSK file as a source for the equilibrium geometry such as the (R,Z) coordinates for the magnetic boundary surface to eliminate the x-point by interpolation. This is not applicable when with NEQDSK=0 because a EXPEQ file will be constructed in a different way that is explained below.

⁸The `namelistVals` is passed to `setParam` argument in `create_namelist` function.

⁹For a full list of the CHEASE input parameters and their detailed description you may read this reference: [The CHEASE code for toroidal MHD equilibria](#) by H. Lutjens, A. Bondeson, O. Sauster

¹⁰You may read more details about how to choose the values of *cocos_in* and *cocos_out* in the [Tokamak coordinate conventions: COCOS](#) by O.Sauter and S.Yu.Medvedevb.

3.3 Reading Input/Output Files

There are different input/output files that can be used with *CheasePy* such as EQDSK, EXPEQ, EXPTNZ, PROFILES, ITERDB, and CHEASE. Each of these files organizes the data/measurements in a different way, and each input/output file has its own grid type and scale. In the following subsection we will show how a user can use *CheasePy* to read these input/output files, and get *CheasePy* to interpolate these read data/measurements on another grid specified/provided by the user.

3.3.1 Reading 'Profiles' File

The equilibrium profiles of different quantities measured in the fusion reactors, such as electron, ion, impurities, and fast ion densities, toroidal and poloidal speeds, etc. are provided by the sentimentalists, and are usually projected on a ψ_N normalized grid and have the same equilibrium for the physical and geometrical quantities in the *EFIT* file.

CheasePy provides the `read_profiles(profilespath, setParam, **kwargs)` function to read the *profiles* file. This function takes the following arguments:

Argument	Default	Description
exptnzfpath	user-input	The path to the <i>profile</i> file.
setParam	{}	nrhopsi=0 (ρ_{ψ_N}) and nrhopsi=1 (ρ_{ϕ_N}) grid. Zeff=True for Z_{eff} profile or Zeff=False for fixed-value Z_{eff} .
**kwargs	None	Choose a source for the ρ_{ψ_N} and ρ_{ϕ_N} grid to interpolate on.

The first argument, `profilespath`, takes the path to the *profiles* file which **must be** provided by the user. If the second argument, `setParam`, is an empty dictionary, the `read_profiles` function returns all quantities projected on the original grid (ψ_N) provided in the profiles file with the original Z_{eff} profile calculated using this equation:

$$Z_{eff} = \frac{\sum_s n_s Z_s^2}{n_e} \quad (19)$$

However, if **Zeff** key is set in `setParam` to False, all grid points of the Z_{eff} profile is set to the average value of the effective atomic number profile calculated using the equation above.

A source for ψ_N (ρ_{ψ_N}) and ϕ_N (ρ_{ϕ_N}) should be provided in the `**kwargs` input argument, hence setting **nrhopsi** in `setParam` to 0 will return all the profiles interpolated into the new ψ_N (ρ_{ψ_N}) grid provided in the source file, however all the profiles will be interpolated into the new ϕ_N counterpart if **nrhopsi** is set to 1, and `read_profiles` function will return only the new ρ_{ψ_N} , ρ_{ϕ_N} , ψ_N , and ϕ_N grids to the calling function/script.

To provide a source for the grid points, we add the type of that source and a path to the source file to the `**kwargs` input in the `read_profiles` function call. Because the user may request to interpolate the profiles onto ψ_N (ρ_{ψ_N}) and ϕ_N (ρ_{ϕ_N}) grids the source must provide both grids point, otherwise *CheasePy* will **raise** an error in case the interpolation onto the ϕ_N (ρ_{ϕ_N}) grid is requested but the input source doesn't provide both grid points to implement that interpolation.¹¹ Therefore, the type of the sources allowed for interpolating onto a grid of different type, e.g. ϕ_N (ρ_{ϕ_N}), are limited to *CHEASE*, *EQDSK*, and *IMPORTED*.¹² The last source allows you to import ψ_N (ρ_{ψ_N}) and ϕ_N (ρ_{ϕ_N}) directly from any external source, and they will override any other grid provided in *CheasePy*.¹³

¹¹If the user wants to interpolate the profiles onto a new grid of the same type, the source may have only the new grid points, e.g. ψ_N (ρ_{ψ_N}), and provided it to the `**kwargs` argument in `read_profiles` function.

¹²Limiting the sources for the grid to these sources is because they have the q-profile which make it possible to convert from ψ_N (ρ_{ψ_N}) to ϕ_N (ρ_{ϕ_N}) using this formula: $\phi = \int \psi dq$.

¹³The **imported** values is explained more in the description of running *CheasePy* and setting its mode of operation in the *runchease.py* file.

The **read.profiles** function returns all the profiles encapsulated in a dictionary in SI units. The name (=key) and description of the returned profiles are listed in the following table:

Measurement	Description
Te	Electron Temperature
Ti	Ion Temperature
Tb	Fast Ions Temperature
ne	Electron Density
ni	Ion Density
nb	Fast Ions Density
nz	Impurities Density
Pb	Fast Ions Pressure
Zeff	Effective Atomic Number
Vtor	Toroidal Velocity
Vpol	Poloidal Velocity
PSIN	ψ_N
PHIN	ϕ_N (with grid source)
rhopsi	ρ_{ψ_N}
rhotor	ρ_{ϕ_N} (with grid source)
pprime	Total Pressure Gradient
pressure	Total Pressure of All Species

3.3.2 Reading 'EXPTNZ' File

The *EXPTNZ* file is an INPUT/OUTPUT file for *CHEASE* code to provide the density and temperature profiles of the ions and electrons in SI units. The first line of the *EXPTNZ* file shows the number of grid points, grid type, i.e. rhopsi (ρ_{ψ_N}) or rhotor (ρ_{ϕ_N}), and the order of the given profiles, such as electron temperature (T_e), electron density (n_e), effective atomic number (Z_{eff}), ion temperature (T_i), and ion density (n_i), in the file. These profiles are organized in a single column with each of them has a length equals the given number of grid points. The header of a *EXPTNZ* file looks like:

512 rhopsi, Te, ne, Zeff, Ti, ni profiles

CheasePy provides the **read.exptnz(exptnzfpath,setParam,**kwargs)** function to read the *EXPTNZ* file. This function takes the following arguments:

Argument	Default	Description
exptnzfpath	user-input	The path to the <i>EXPTNZ</i> file.
setParam	{}	Select between nrhopsi=0 (ρ_{ψ_N}) and nrhopsi=1 (ρ_{ϕ_N}) grid.
**kwargs	None	Choose a source for the ρ_{ψ_N} and ρ_{ϕ_N} grid to interpolate on.

The first argument, **exptnzfpath**, takes the path to the *EXPTNZ* file which **must be** provided by the user. If the second argument, **setParam**, is an empty dictionary, the **read.exptnz** function returns all quantities projected on the original grid (ρ_{ψ_N}) provided in the *EXPTNZ* file, otherwise, a source for ρ_{ψ_N} and ρ_{ϕ_N} should be provided in the ****kwargs** input argument, hence setting **nrhopsi** in **setParam** to 0 will return all the profiles interpolated into the new ρ_{ψ_N} grid provided in the source file, however all the profiles will be interpolated into the new ρ_{ϕ_N} counterpart if **nrhopsi** is set to 1, and **read.exptnz** function will return only the new ρ_{ψ_N} and ρ_{ϕ_N} grids to the calling function/script and ignore the original grids provided in the *EXPTNZ* file. The source of new grids are passed to the ****kwargs** input argument of the **read.exptnz** function as described in section(3.3.1).

In addition to the input profiles, **read.exptnz** function calculates and returns the density and temperature of the impurities and the total pressure. The total pressure calculated in the **read.exptnz** doesn't include the contribution of the fast ions (if any), which might make the pressure calculated from the *EXPTNZ* file is different from the actual pressure measured in the experiment.¹⁴

¹⁴The actual total pressure measured in the experiment is found in the *profiles* and *EQDSK* files.

The **read.exptnz** function returns all the profiles encapsulated in a dictionary in SI units. The name (=key) and description of the returned profiles are listed in the following table:

Measurement	Description
Te	Electron Temperature
Ti	Ion Temperature
ne	Electron Density
ni	Ion Density
nz	Impurities Density
Zeff	Effective Atomic Number
rhopsi	ρ_{ψ_N}
rhotor	ρ_{ϕ_N} (with grid source)
pprime	Total Pressure Gradient
pressure	Total Pressure of All Species

3.3.3 Reading 'ITERDB' File

The *ITERDB* file provides the density and temperature profiles for electrons, ions, and impurities, in addition to the toroidal velocity defined on a *rhotor* (i.e. ρ_{ϕ_N}) grid and SI units.

CheasePy provides the **read.iterdb(iterdbfpath, setParam, **kwargs)** function to read the *ITERDB* file. This function takes the following arguments:

Argument	Default	Description
iterdbfpath	user-input	The path to the <i>ITERDB</i> file.
setParam	{}	Select between nrhopsi=0 (ρ_{ψ_N}) and nrhopsi=1 (ρ_{ϕ_N}) grid.
**kwargs	None	Choose a source for the ρ_{ψ_N} and ρ_{ϕ_N} grid to interpolate on.

The first argument, **iterdbfpath**, takes the path to the *ITERDB* file which **must be** provided by the user. If the second argument, **setParam**, is an empty dictionary, the **read.iterdb** function returns all quantities projected on the original grid (ρ_{ϕ_N}) provided in the *EXPTNZ* file, otherwise, a source for ρ_{ψ_N} and ρ_{ϕ_N} should be provided in the ****kwargs** input argument, hence setting **nrhopsi** in **setParam** to 0 will return all the profiles interpolated into the new ρ_{ψ_N} grid provided in the source file, however all the profiles will be interpolated into the new ρ_{ϕ_N} counterpart if **nrhopsi** is set to 1, and **read.iterdb** function will return only the new ρ_{ψ_N} and ρ_{ϕ_N} grids to the calling function/script and ignore the original grids provided in the *ITERDB* file. The source of new grids are passed to the ****kwargs** input argument of the **read.iterdb** function as described in section(3.3.1).

In addition to the input profiles, **read.iterdb** function calculates and returns the total pressure. The total pressure calculated in the **read.iterdb** doesn't include the contribution of the fast ions (if any).

The **read.iterdb** function returns all the profiles encapsulated in a dictionary in SI units. The name (=key) and description of the returned profiles are listed in the following table:

Measurement	Description
Te	Electron Temperature
Ti	Ion Temperature
ne	Electron Density
ni	Ion Density
nz	Impurities Density
Zeff	Effective Atomic Number
Vtor	Toroidal Velocity
rhopsi	ρ_{ψ_N} (with grid source)
rhotor	ρ_{ϕ_N}
pprime	Total Pressure Gradient
pressure	Total Pressure of All Species

3.3.4 Reading ‘EXPEQ’ File

The *EXPEQ* file is an INPUT/OUTPUT file for *CHEASE* that provides the equilibrium pressure and current profiles on a specific grid. The *EXPEQ* file also provides the equilibrium geometry, such as the (r,z) components of the last closed magnetic surface.¹⁵ All profiles and geometries provided in *EXPEQ* file are ‘normalized’ using the equations in section(1.3).

Because of the variety of profiles and grid types that can be used in the *EXPEQ* file, each profile and grid type is assigned a numeric value to refer to it. These numbers are written in the two lines after the list of (r,z) coordinates in the *EXPEQ* file. The first number in the first line specifies the number of grid points of the ρ_{ψ_N} or ρ_{ϕ_N} coordinates. The second number in the first line is ‘NPPFUN’ and it takes 8 for *pressure* or 4 for *pressure gradient* depending on which one is included in the *EXPEQ* file. The first number in the second line is ‘NSTTP’ and it takes 1 for the *current flux density* (ff'), 2 for *surface current* (I^*), 3 for *parallel current* ($I_{||}$), or 4 for *parallel current density* ($J_{||}$). The second number in the second line is ‘NRHOMESH’ and it takes 0 for *rhopsi* (ρ_{ψ_N}) or 1 for *rhotor* (ρ_{ϕ_N}).

CheasePy provides the `read_expeq(expeqfpath, setParam, **kwargs)` function to read the *EXPEQ* file. This function takes the following arguments:

Argument	Default	Description
expeqfpath	user-input	The path to the <i>EXPEQ</i> file.
setParam	{}	Select between nrhopsi=0 (ρ_{ψ_N}) and nrhopsi=1 (ρ_{ϕ_N}) grid.
**kwargs	None	Choose a source for the ρ_{ψ_N} and ρ_{ϕ_N} grid to interpolate on.

The first argument, `expeqfpath`, takes the path to the *EXPEQ* file which **must be** provided by the user. If the second argument, `setParam`, is an empty dictionary, the `read_expeq` function returns all quantities projected on the original grid (ρ_{ψ_N} or ρ_{ϕ_N}) provided in the *EXPEQ* file, otherwise, a source for ρ_{ψ_N} and ρ_{ϕ_N} should be provided in the `**kwargs` input argument, hence setting **nrhopsi** in `setParam` to 0 will return all the profiles interpolated into the new ρ_{ψ_N} grid provided in the source file, however all the profiles will be interpolated into the new ρ_{ϕ_N} counterpart if **nrhopsi** is set to 1, and `read_expeq` function will return only the new ρ_{ψ_N} and ρ_{ϕ_N} grids to the calling function/script and ignore the original grids provided in the *EXPEQ* file. The source of new grids are passed to the `**kwargs` input argument of the `read_expeq` function as described in section(3.3.1).

The `read_expeq` function returns all the ‘normalized’ pressure profiles and equilibrium geometry encapsulated in a dictionary. The name (=key) and description of the returned profiles are listed in the following table:

Measurement	Description
epsilon	Inverse aspect ratio
zgeom	Geometric mean of z-mesh
pedge	Pressure at the Edge
nRZmesh	Size of (r,z) mesh
nrhomesh	Size of ρ_{ψ_N} or ρ_{ϕ_N} grid
nrhotype	0 = ρ_{ψ_N} or 1 = ρ_{ϕ_N}
nsttp	1 = ff' , 2 = I^* , 3 = $I_{ }$, and 4 = $J_{ }$
nppfun	8 = P or 4 = P'
rhopsi	ρ_{ψ_N} (if nrhotype = 0)
rhotor	ρ_{ϕ_N} (if nrhotype = 1)
pprime	Total Pressure Gradient (if nppfun = 4)
pressure	Total Pressure of All Species (if nppfun = 8)
ffprime	current flux density (if nsttp = 1)
Istr	surface current (if nsttp = 2)
Iprl	parallel current (if nsttp = 3)
Jprl	parallel current density (if nsttp = 4)

¹⁵This magnetic surface should not include any singular point, i.e. x-point, not to cause a problem in finding a state of MHD equilibrium in *CHEASE* code, or an incomplete simulation with an exit error.

It worth mention that if the value of ‘*NPROPT*’ parameter in the *chease_namelist* file is set to a different value of the ‘*NSTTP*’, *CHEASE* uses the current profile that corresponds to the ‘*NPROPT*’ number in the output *EXPEQ* file instead of the one corresponds to the ‘*NSTTP*’. In addition, the sign of the ‘*NPROPT*’ number is flipped to negative if ‘*NPPFUN*’ is set to 8 and kept positive otherwise. A different value for ‘*NPROPT*’ from its ‘*NSTTP*’ counterpart is needed to run *CHEASE* in an iterative mode with a different input current profile. Hence, we make *CHEASE* to output the desired current profile in the output *EXPEQ* file by setting ‘*NPROPT*’ to the number corresponding that current profile.

3.3.5 Reading ‘EQDSK’ File

The *EQDSK* file is an INPUT/OUTPUT file for *CHEASE* that provides the equilibrium pressure, such as the pressure ($P(\psi)$) and pressure gradient ($dP/d\psi$), and equilibrium current, such as the current flux ($ff' = fdf/d\psi$). It also provides the equilibrium geometry, such as the (r,z) components of the last closed magnetic surface, the safety factor (q) profile, the poloidal mesh ($\psi(R, Z)$), and enough information to construct the ψ_N , ϕ_N , ρ_{ψ_N} and ρ_{ϕ_N} grids. All equilibrium profiles and geometries provided in the *EQDSK* file are given in the SI units.

CheasePy provides the `read_eqdsk(eqdskfpath, setParam, Normalized, **kwargs)` function to read the *EQDSK* file. This function takes the following arguments:

Argument	Default	Description
eqdskfpath	user-input	The path to the <i>EQDSK</i> file.
setParam	{}	Select between nrhopsi=0 (ρ_{ψ_N}) and nrhopsi=1 (ρ_{ϕ_N}) grid.
Normalized	False	Return quantities in SI units (False) or Normalized (True).
**kwargs	None	Choose a source for the ρ_{ψ_N} and ρ_{ϕ_N} grid to interpolate on.

The first argument, `eqdskfpath`, takes the path to the *EQDSK* file which **must be** provided by the user. If the second argument, `setParam`, is an empty dictionary, the `read_eqdsk` function returns all quantities projected on the original ϕ_N grid provided in the *EQDSK* file, otherwise, a source for ψ_N and ϕ_N should be provided in the `**kwargs` input argument, hence setting `nrhopsi` in `setParam` to 0 will return all the profiles interpolated into the new ψ_N grid provided in the source file, however all the profiles will be interpolated into the new ϕ_N counterpart if `nrhopsi` is set to 1, and `read_eqdsk` function will return only the new ψ_N , ϕ_N , ρ_{ψ_N} , and ρ_{ϕ_N} grids to the calling function/script and ignore the original grids provided in the *EQDSK* file. The source of new grids are passed to the `**kwargs` input argument of the `read_eqdsk` function as described in section(3.3.1).

The `read_eqdsk` function returns all the profiles and equilibrium geometry encapsulated in a dictionary. The name (=key) and description of the returned profiles are listed in the following table:¹⁶

Measurement	Description
q	Safety Factor Profile
BCTR	Toroidal B at Magnetic Axis
RCTR	R-Coordinate at Magnetic Axis
CURNT	Total Experimental Toroidal Current
PSIN	ψ_N
PHIN	ϕ_N (with grid source)
rhopsi	ρ_{ψ_N}
rhotor	ρ_{ϕ_N} (with grid source)
rbound	r-coordinate of magnetic boundary surface
zbound	z-coordinate of magnetic boundary surface
pprime	Total Pressure Gradient ($P'(\psi)$)
pressure	Total Pressure of All Species ($P(\psi)$)
ffprime	current flux function ($ff'(\psi)$)

¹⁶Due to the long list of parameters returned from the `read_eqdsk` function after reading the *EQDSK* file, we ONLY listed here those are used frequently by *CheasePy* code. The `read_efit_file` function has a full list of all parameters that are read from the *EQDSK* file. This [link](#) has a full description of the *EQDSK* parameters.

3.3.6 Reading 'CHEASE' File

The *CHEASE* file is an OUTPUT file for *CHEASE* that provides the density and temperature for electrons, ions, and impurities, equilibrium pressure and currents, equilibrium geometry, safety factor (q) profile, and poloidal and toroidal grids. All equilibrium profiles and geometries provided in the *CHEASE* file are given in the SI units.

CheasePy provides the `read_chease(cheasepath, setParam, Normalized, **kwargs)` function to read the *CHEASE* file. This function takes the following arguments:

Argument	Default	Description
cheasepath	user-input	The path to the <i>CHEASE</i> file.
setParam	{}	Select between nrhopsi=0 (ρ_{ψ_N}) and nrhopsi=1 (ρ_{ϕ_N}) grid.
Normalized	False	Return quantities in SI units (False) or Normalized (True).
**kwargs	None	Choose a source for the ρ_{ψ_N} and ρ_{ϕ_N} grid to interpolate on.

The first argument, `cheasepath`, takes the path to the *CHEASE* file which **must be** provided by the user. If the second argument, `setParam`, is an empty dictionary, the `read_chease` function returns all quantities projected on the original ϕ_N grid provided in the *CHEASE* file, otherwise, a source for ψ_N and ϕ_N should be provided in the `**kwargs` input argument, hence setting **nrhopsi** in `setParam` to 0 will return all the profiles interpolated into the new ψ_N grid provided in the source file, however all the profiles will be interpolated into the new ϕ_N counterpart if **nrhopsi** is set to 1, and `read_chease` function will return only the new ψ_N , ϕ_N , ρ_{ψ_N} , and ρ_{ϕ_N} grids to the calling function/script and ignore the original grids provided in the *CHEASE* file. The source of new grids are passed to the `**kwargs` input argument of the `read_chease` function as described in section(3.3.1).

The `read_chease` function returns all the profiles and equilibrium geometry encapsulated in a dictionary. The name (=key) and description of the returned profiles are listed in the following table:¹⁷

Measurement	Description
q	Safety Factor Profile
B0EXP	Toroidal B at Magnetic Axis
R0EXP	R-Coordinate at Magnetic Axis
ITEXP	Total Experimental Toroidal Current
PSIN	ψ_N
PHIN	ϕ_N (with grid source)
rhopsi	ρ_{ψ_N}
rhotor	ρ_{ϕ_N} (with grid source)
rbound	r-coordinate of magnetic boundary surface
zbound	z-coordinate of magnetic boundary surface
shear	Magnetic Shear ($\tilde{s}(\psi)$)
signeo	Neoclassical Conductivity ($\sigma_{neo}(\psi)$)
Te (Ti)	Electron (Ion) Temperature ($T_e(\psi)$ ($T_i(\psi)$))
ne (ni,nz)	Electron (Ion,impurities) Density ($n_e(\psi)$ ($n_i(\psi), n_z(\psi)$))
pprime	Total Pressure Gradient ($P'(\psi)$)
pressure	Total Pressure of All Species ($P(\psi)$)
ffprime	current flux function ($ff'(\psi)$)
Ibs	Bootstrap Current ($I_{bs}(\psi)$)
Jbs	Bootstrap Current Density ($J_{bs}(\psi)$)
Iprl	Parallel Current ($I_{ }(\psi)$)
Jprl	Parallel Current Density ($J_{ }(\psi)$)
Istr	Surface Current ($I^*(\psi)$)
Itor	Toroidal Current ($I_\phi(\psi)$)
Jtor	Toroidal Current Density ($J_\phi(\psi)$)

There are also a complete list of the magnetic coefficients (g_{ij}), Jacobian transformation matrix (J), and other parameters that can be of interested to the users.

¹⁷Due to the long list of parameters returned from the `read_chease` function after reading the *CHEASE* file, we ONLY listed here those are frequently used by *CheasePy* code. The `read_chease` function has a full list of all parameters that are read from the *CHEASE* file. This [paper](#) has a full description of the *CHEASE* parameters.

3.4 Creating Input Files

Before any iteration of *CheasePy* the **write_expntz** and **write_expeq** functions are called to create the *EXPTNZ* and *EXPEQ* files, respectively, which are used as input files to *CHEASE* code. However, if the *namelist* parameter *NEQDSK* is set to *zero*, only the **write_expntz** function is called and the *EQDSK* file is used as input to *CHEASE*.¹⁸ The user can specify the sources of each profile to be used to create the *EXPTNZ* and *EXPEQ* files in the **setParam** input argument to the **write_expntz** and **write_expeq** functions, as we explained in sections 3.4.2 and 3.4.1. After every iteration, the output files are renamed by adding a suffix *_iterxxx* to reflect the iteration number, for instance *chease_iter000.h5*, *EXPEQ_iter000.OUT*, and *EXPTNZ_iter000.OUT* for the *zeroth* iteration.

3.4.1 Creating EXPEQ File

The *EXPEQ* file has the (r,z) coordinates of the LCMS, in addition to the pressure and current profiles. *CheasePy* provides the **write_expeq(setParam,outfile,**kwargs)** function to create the *EXPEQ* file and/or return all the contents of that file as a dictionary structure with field names that follow the description in section(3.3.4). This function takes the following arguments:

Argument	Default	Description
setParam	{}	Specify the sources for different profiles.
outfile	True	Create an output EXPEQ file.
**kwargs	None	Specify the path to the source files.

The first argument, **setParam**, has a dictionary structure to specify the types and sources of the grid (**nrhmesh**), the pressure profile (**nppfun**), and current profile (**nsttp**), each of these inputs takes a list that has the structure of **[type,source]**. There are three sources accepted in **setParam** for **nrhmesh**: {0,'chease'}, {1,'eqdks'}, or {7,'imported'}, six sources for **nppfun**: {0,'chease'}, {1,'eqdks'}, {2,'expeq'}, {3,'expntz'}, {4,'profiles'}, {5,'iterdb'}, or {7,'imported'}, and four sources for **nsttp**: {0,'chease'}, {1,'eqdks'}, {2,'expeq'}, or {7,'imported'}. The path to the source files, i.e. 'chease', 'eqdsk', 'expeq', 'expntz', 'profiles', and 'iterdb', must be provided in the ****kwargs** argument. However, if the {7,'imported'} sources is chosen, a dictionary of the profiles ({name,data}) must be provided in the ****kwargs** argument, e.g. {'pressure',[list of pressure data]}. All the returned profiles are projected (interpolated) into the grid provided in the **nrhmesh** source by setting the grid source in the **setParam** in the read function to the common grid source.

On the other hand, the type of the grid (**nrhmesh**) is either {0,'rhopsi'} or {1,'rhoto'}, the type of the pressure profile (**nppfun**) is either {4,'pprime'} or {8,'pressure'}, and the type of the current profile (**nsttp**) is either {1,'ffprime'}, {2,'istr'}, {3,'iprl'}, or {4,'jprl'}. The *CheasePy* user has to ensure that the source file has the requested profile. For example, the *EQDSK* file has a single current profile, i.e. *ffprime* and both pressure profiles, i.e. *pressure* and *pprime*. The current profile in the *EXPEQ* file depends on the value of *NPROPT* parameter in the input *chease_namelist* file. However, the *CHEASE* source has all types of profiles. Finally, the user should remember that all quantities in the *EXPEQ* source are normalized, which is not the case in other sources.

If the **setParam** is empty dictionary, the types are set to their default values, i.e. **nrhmesh** = 0, **nppfun** = 8, and **nsttp** = 1. Hence, any provided source in the ****kwargs** will be used to create the new *EXPEQ* file, otherwise, *CheasePy* will search for the *EQDSK* and use it as a source for the profiles. In a similar way, the source for the (r,z) coordinates of the LCMS is taken to be the same source for the **nrhmesh** grid.

The second input argument (outfile) takes *True* if the user wants to create the *EXPEQ* file and receive a return dictionary with the content of the *EXPEQ* file, or *False* if the user wants only that returned dictionary without creating the *EXPEQ* file.

¹⁸ *CheasePy* renames *EQDSK* file to *EXPEQ* to be recognized by *CHEASE* code.

3.4.2 Creating EXPTNZ File

The *EXPTNZ* file contains the density and temperature profiles for electrons and ions, and the effective atomic number. *CheasePy* provides the `write.exptnz(setParam,outfile,**kwargs)` function to create the *EXPTNZ* file and/or return all the contents of that file as a dictionary structure with field names that follow the description in section(3.3.2). This function takes the following arguments:

Argument	Default	Description
setParam	{}	Specify the sources for different profiles.
outfile	True	Create an output EXPEQ file.
**kwargs	None	Specify the path to the source files.

The first argument, `setParam`, has a dictionary structure to specify the types and sources of the grid (`nrhomesh`), the electron density and temperature profiles (`eprofiles`), and ion density and temperature profiles (`iprofiles`). There are three sources accepted in `setParam` for `nrhomesh`: {0,'chease'}, {1,'eqdks'}, or {7,'imported'}, four sources for `eprofiles` and `iprofiles`: {0,'chease'}, {3,'exptnz'}, {4,'profiles'}, {5,'iterdb'}, and/or {7,'imported'}. The path to the source files, i.e. 'chease', 'eqdsk', 'exptnz', 'profiles', and 'iterdb', must be provided in the `**kwargs` argument. However, if the {7,'imported'} sources is chosen, a dictionary of the profiles ({name,data}) must be provided in the `**kwargs` argument, e.g. {'pressure',[list of pressure data]}. All the returned profiles are projected (interpolated) into the grid provided in the `nrhomesh` source by setting the grid source in the `setParam` in the read function to the common grid source. On the other hand, the type of the grid (`nrhomesh`) is either {0,'rhopsi'} or {1,'rhoto'}.

If the `setParam` is empty dictionary, the type of the grid is set to its default value, i.e. `nrhomesh = 0`. Hence, any provided source will be used to create the *EXPTNZ* file, otherwise, the *EXPTNZ* will be the source of the profiles and grid. Finally, the user should remember that all quantities in the *EXPTNZ* source are in SI units.

The second input argument (`outfile`) takes *True* if the user wants to create the *EXPTNZ* file and receive a return dictionary with the content of the *EXPTNZ* file, or *False* if the user wants only that returned dictionary without creating the *EXPTNZ* file.

3.5 Running CheesePy

A user can run *CheasePy* code in a directory that has *CHEASE* code executable named *chease_hdf5* and *runchease.py* by typing this command in a terminal window:

```
python runchease.py
```

This command calls the **cheasepy** function to prepare the required input files and run *CHEASE* code. The **cheasepy** function takes *four* input arguments, i.e. **srcVals**, **namelistVals**, **cheaseVals**, and **importedVals**, that set the sources of density, temperature, and pressure profiles, geometry parameters, the list of *CHEASE* namelist parameters, and the *CheasePy* mode of operation. Details for these input arguments are described below.

3.5.1 Profiles and Geometry Sources

In the *runchease.py* script a dictionary variable named **srcVals** is initialized, and then the sources are specified for each type. The temperature and density profiles for the ions, electrons, and impurities can be taken from different sources, such as *profiles*, *exptnz*, *iterdb*, or *chease* files, with the source for electrons and ions+impurities profiles can be different. The density and temperature of electrons, ions, and impurities (if any) taken from any combinations of the previous sources can also be used to calculate the total pressure. Otherwise, the total pressure, the current, and equilibrium geometry are taken directly from *eqdsk*, *expeq*, or *chease* files.

With These different sources, each source is identified by its name or a number as shown in the table below:

Number	0	1	2	3	4	5	7
Source	chase	eqdsk	expeq	exptnz	profiles	iterdb	imported

Example 3.1. If the sources for electron profile, ion profile, pressure, and current are *exptnz*, *profiles*, *eqdsk*, and *expeq* files, respectively. Also, all the profiles will be interpolated on the ρ_{ϕ_N} defined in *eqdsk* file. Hence, **srcVals** variable will be defined as follow:

```
srcVals = {}
srcVals['iprofiles.src'] = 'profiles'
srcVals['eprofiles.src'] = 'exptnz'
srcVals['pressure.src'] = 'eqdsk'
srcVals['current.src'] = 'expeq'
srcVals['rhomesh.src'] = 'eqdsk'
```

Example 3.2. If the sources for electron and ion profiles are taken from the *profiles* file, however, the pressure and current profiles are taken from the *eqdsk* file. The ρ_{ϕ_N} grid is taken from the common source of each related profile, i.e. the ρ_{ϕ_N} grid used in the generated *exptnz* file is the same as that in the *profiles* file, and the ρ_{ϕ_N} grid used in the generated *expeq* is the same as that in the *eqdsk* file. Hence, **srcVals** variable will be defined as follow:

```
srcVals = {}
srcVals['iprofiles.src'] = 'profiles'
srcVals['eprofiles.src'] = 'profiles'
srcVals['pressure.src'] = 'eqdsk'
srcVals['current.src'] = 'eqdsk'
srcVals['rhomesh.src'] = None
```

In addition to the profiles and grid sources defined in the **srcVals** variable, there is another variable also defined in the **srcVals** which is not a source of any profile but a method of how to treat the last closed magnetic surface (LCMS). This variable is called **boundary_type**, and it takes **0** or **'asis'**

in case the LCMS will be written as it is read from the source file without any massaging or processing of its coordinates. However, if `boundary_type` receives `1` or `'interp'` the coordinates taken from the source file will be interpolated to have the LCMS defined at a specific length of ρ_{ψ_N} . This interpolation is needed when the LCMS has an x-point (i.e. singular point) which makes *CHEASE* either crashes or gives irrelevant/incorrect results in case the *TENSBND* parameter wasn't set to the right value, i.e. -1.¹⁹

The interpolation function `magsurf.solvflines` is defined in the *efittools.py* python package, and it returns the (r,z) coordinates of the LCMS after solving the magnetic field lines equations using a fifth-order Rung-Kutta method. The `magsurf.solvflines` function receives the path to the *eqdsk* file in the `eqdskfpath` argument, a cutoff ψ_N value for the LCMS in the `psi`, and a tolerance value for the desired accuracy in the `eps` argument. When the *NEQDSK* in *chease.namelist* parameter is set to `0`, the function `magsurf.solvflines` is called with `psi 0.999`.²⁰

In the table of profile and grid sources above we referred to a source for the profiles called `imported`. This source type is useful when *CheasePy* user wants to import a profile for any quantity from an external source, or the user wants to do some processing on any profile's data before include it as an input to *CHEASE* code. All imported profiles which are passed to `cheasepy` function through the `importedVals` argument must be accompanied with the ρ_{ψ_N} and ρ_{ϕ_N} grids. Passing the imported profiles along with their corresponding grid is required because these grids are used for interpolating those profiles onto the common grid on each input file to *CHEASE* code, i.e. *exptnz* and *expeq*. This means if the user has profiles from several external sources, all of these profiles have to be projected onto the same grids before passing them to the `cheasepy` function.

Example 3.3. A file, *externalSource.dat*, has four columns for ρ_{ψ_N} , ρ_{ϕ_N} , n_e , and T_e profiles, and a user need to use these profiles as input to *CHEASE*. The steps the user has to follow to use these profiles from that external source to *CHEASE* are as follow:

```
import numpy as npy
eprofiles = npy.loadtxt(externalSource.dat)

importedVals = {}
importedVals['rhotor'] = npy.array(eprofiles[:,0])
importedVals['rhopsi'] = npy.array(eprofiles[:,1])
importedVals['Te'] = npy.array(eprofiles[:,2])*1.0e3
importedVals['ne'] = npy.array(eprofiles[:,3])*1.0e19

srcVals = {}
srcVals['iprofiles_src'] = 'exptnz'
srcVals['eprofiles_src'] = 'imported'
srcVals['pressure_src'] = 'eqdsk'
srcVals['current_src'] = 'expeq'
srcVals['rhomesh_src'] = 'eqdsk'
```

In example(3.3) the electron density and temperature profiles, and the ρ_{ψ_N} and ρ_{ϕ_N} grids are assigned to different keys in the `importedVals` dictionary. Then, the `'eprofiles_src'` item in the `srcVals` dictionary is set to `'imported'`. Hence, all the electron profiles will be taken from the `'imported'` profiles. However, if the user wants to take only the electron temperature from the

¹⁹Although *TENSBND* is a very good tool provided by *CHEASE* to interpolate around the x-point, the code user doesn't have any control on how close the new LCMS will be close to the original one. However, using the `'interp'` attribute with `boundary_type` allows the user to set a cutoff value for ρ_{ψ_N} that defines the LCMS.

²⁰The value of `psi` in the call to the `magsurf.solvflines` can be increased or decreased by *CheasePy* user. However, with a `psi` value that is very close to `1.0` the magnetic field lines solver might return (r,z) coordinates of an open field surface (outside the separatrix), which causes *CHEASE* code to crash. So the *CheasePy* user has to verify that a closed surface is returned from `magsurf.solvflines` function by using a suitable `psi` value.

external source and take the electron density from the *profiles* file, the user can import only the electron temperature from the external source, and keep the **'eprofiles_src'** item in the **srcVals** assigned to **'profiles'**, as shown in example(3.4) below.

Example 3.4. A user wants to import only the temperature profile from an external source and take the electron density and ion profiles from the *profiles* file.

```
import numpy as npy
eprofiles = npy.loadtxt(externalSource.dat)

importedVals = {}
importedVals['rhotor'] = npy.array(eprofiles[:,0])
importedVals['rhopsi'] = npy.array(eprofiles[:,1])
importedVals['Te'] = npy.array(eprofiles[:,2])*1.0e3

srcVals = {}
srcVals['iprofiles_src'] = 'profiles'
srcVals['eprofiles_src'] = 'profiles'
srcVals['pressure_src'] = 'eqdsk'
srcVals['current_src'] = 'expeq'
srcVals['rhomesh_src'] = 'eqdsk'
```

The question that might be arisen now is: How will *CheasePy* use the **'imported'** electron temperature if the user didn't pass it to the **srcVals** dictionary? The answer to this question is simple: When **importedVals** dictionary is passed to **cheasepy** function as an input argument, it, in turn, passes it to **write_exptnz** and **write_expeq** functions. When any of these functions receives the content of **importedVals** dictionary, they inspect that content and enforce any imported profile to override the corresponding profile provided in the **srcVals** dictionary. Therefore, the **'imported'** electron temperature profile provided in **importedVals** overrides the same profile provided in **srcVals**. This takes place for any profile used to construct *EXPTNZ* and *EXPEQ* files.

As we explained earlier, the pressure profile is compromised of (at least) two components from ions and electrons, where $P_T = n_e T_e + n_i T_i$. In addition, there might be contributions from the impurities and fast ions with the total pressure given by: $P_T = n_e T_e + n_i T_i + n_z T_z + n_b T_b$, where n_b and T_b are the density and temperature of fast ions. A common mistake is done in examples 3.3 and 3.4 when the pressure profile is taken directly from the *EQDSK* file without considering the changes in one of its components which is the electron density and/or temperature profiles. Therefore, the total pressure has to be recalculated using the contribution of the imported profiles of the electron density and/or temperature. The following example explains how to calculate the new total pressure using the new electron profile.

Example 3.5. A user has two *iterdb* files, *basecase.iterdb* which has the original profiles of the electrons, ions, and impurities, and *modTeProf.iterdb* which has a modified electron temperature (T_e) profile. The following code shows how to include the contribution of the modified electron temperature into the pressure profile.

```
import cheasepy

inParam = {nrhomesh:0}

baseITERDB = cheasepy.read_iterdb(iterdbfpath='basecase.iterdb',
                                   setParam=inParam,eqdsk='EQDSK')
modITERDB = cheasepy.read_iterdb(iterdbfpath='modTeProf.iterdb',
                                   setParam=inParam,eqdsk='EQDSK')
```

```

importedVals = {}
importedVals['rhotor'] = modITERDB['rhotor']
importedVals['rhopsi'] = modITERDB['rhopsi']
importedVals['Te'] = modITERDB['Te']

eqdskdata = cheesePy.read_eqdsk(eqdskfpath='EQDSK')

importedVals['pressure'] = eqdskdata['pressure']-baseITERDB['pressure']
                                + modITERDB['pressure']

srcVals = {}
srcVals['iprofiles_src'] = 'iterdb'
srcVals['eprofiles_src'] = 'iterdb'
srcVals['pressure_src'] = 'eqdsk'
srcVals['current_src'] = 'expeq'
srcVals['rhomesh_src'] = 'eqdsk'

```

In example(3.5), although the **'pressure_src'** is set to **'eqdsk'**, the imported value of the total pressure will override the sourced profile in the **write_expeq** functions. Similarly, the imported electron temperature profile will override the sourced profile in the **write_exptnz** functions.

All the profiles that can be externally imported into *CheasePy* an override sourced profiles are listed in the following table:²¹

Profile	Description	Profile	Description
rhopsi	Poloidal Grid	rhotor	Toroidal Grid
ne	Electron Density	Te	Electron Temperature
ni	Ion Density	Ti	Ion Temperature
nz	Impurity Density	Tz	Impurity Temperature
Iprl	Parallel Current	Jprl	Parallel Current Density
ffprime	Current Flux Density	Istr	Surface Current
pressure	Total Pressure	pprime	Pressure Gradient
Zeff	Effective Atomic Number		

All the examples and discussions above consider only the sources for input profiles for the zeroth iteration in *CheasePy* which reconstruct the MHD equilibrium depending on the input profiles and equilibrium geometry. If *CheasePy* code runs for several iterations it will keep using the same profiles given in the source files, but ignoring the imported profiles after the zeroth iteration. Hence, another source of the profiles and equilibrium geometry sometimes required to track the changes made in the zeroth iteration by the imported profiles. *CheasePy* allows the user to change the source of each profile from one iteration to another by providing these sources in a Python *list*. For every profile the user needs to change its source, this source has to be of type list and of length equals the number of source that the user needs to switch between them. *CheasePy* code will keep using the last source in the list for the rest of iterations in case the length of the source list is less than the number of iterations. Usually the generated *EXPTNZ*, *EXPEQ*, *EQDSK*, and *CHEASE* files after each iteration have updated profiles and equilibrium geometry.

If the user needs to do several iteration for the study case in example(3.5), the second source of **'eprofile_src'** need to be taken from *EXPTNZ* or *CHEASE* files, however, the **'pressure_src'** need to be taken from *EXPEQ*, *EQDSK*, or *CHEASE* files to consider the imported profiles that was enforced in the zeroth iteration. Hence, example(3.5) can be rewritten as follow:

²¹This list can be extended to include other imported profiles by considering them in the **write_expeq** and **write_exptnz** functions.

Example 3.6. A user has two *iterdb* files, *basecase.iterdb* which has the original profiles of the electrons, ions, and impurities, and *modTeProf.iterdb* which has a modified electron temperature (T_e) profile. The following code shows how to include the contribution of the modified electron temperature into the pressure profile, and how to consider these variations in further iterations. Also, the user needs to change the source of the grid after the zeroth iteration to be taken from the *CHEASE* source file.

```
import cheasepy

inParam = {nrhomesh:0}

baseITERDB = cheasepy.read_iterdb(iterdbfpath='basecase.iterdb',
setParam=inParam,eqdsk='EQDSK')
modITERDB = cheasepy.read_iterdb(iterdbfpath='modTeProf.iterdb',
setParam=inParam,eqdsk='EQDSK')

importedVals = {}
importedVals['rhotor'] = modITERDB['rhotor']
importedVals['rhopsi'] = modITERDB['rhopsi']
importedVals['Te'] = modITERDB['Te']

eqdskdata = cheasepy.read_eqdsk(eqdskfpath='EQDSK')

importedVals['pressure'] = eqdskdata['pressure']-baseITERDB['pressure']

srcVals = {}
srcVals['iprofiles_src'] = 'iterdb'
srcVals['eprofiles_src'] = ['iterdb','exptnz']
srcVals['pressure_src'] = ['eqdsk','expeq']
srcVals['current_src'] = 'expeq'
srcVals['rhomesh_src'] = ['eqdsk','chease']
```

3.5.2 CHEASE Namelist Parameters

A list of *namelist parameters* is provided in section(3.2). These *namelist parameters* are required for *CHEASE* code to run properly and give relevant results to the case under study. *CheasePy* code has a default value for each parameter in the *namelist*, but the user can change any of them depending on several factors, such as the input profiles, input sources, and desired resolution. *CheasePy* provides a dictionary-type variable called **namelistVals** that you can use to assign a new value for any of the parameter in the *namelist*. Then, this **namelistVals** is passed as an input argument to the **cheasepy** function to create the *chease.namelist* file using the user-defined and default values for each parameter.²²

If the *CheasePy* user runs multiple iterations of the *CHEASE* code and needs to change any of the input parameters from one iteration to another, an equal length list of these parameter values need to be assigned to each item in the **namelistVals** input argument, even if the values of these parameters don't change from one iteration to another. In other words, if a user needs to change the type of couple of *namelist parameters* from **int** or **float** to **list** without changing all the type of other *namelist parameters* an error will be raised by *CheasePy* as it expects all parameters in the *namelist* of the same type, i.e *single-valued* or *list*.

²²The *CheasePy* user can revise the list of parameters required by *CHEASE* code in the table in section(3.2).

Example 3.7. A user needs to run *CHEASE* code using pressure and current profiles from the *EQDSK* for the zeroth iteration and from *EXPEQ* for other iterations. Also, *CHEASE* code should expect ff' in the zeroth iteration, and $I_{||}$ for other iterations.

```

namelistVals = {}
namelistVals['NS'] = [128, 128]
namelistVals['NT'] = [128, 128]
namelistVals['NISO'] = [128, 128]
namelistVals['NPSI'] = [512, 512]
namelistVals['NCHI'] = [512, 512]
namelistVals['RELAX'] = [0.0, 0.0]
namelistVals['NEQDSK'] = [1, 0]
namelistVals['TENSBNBND'] = [0, 0]
namelistVals['TENS PROF'] = [0, 0]
namelistVals['NRHOMESH'] = [0, 0]
namelistVals['cocos.in'] = [1, 1]
namelistVals['cocos.out'] = [11, 11]

namelistVals['NSTTP'] = [1, 3]
namelistVals['NPROPT'] = [3, 3]
namelistVals['NPPFUN'] = [8, 8]

```

It worth reminding the user that there are many other parameters those are set to their default values, and out-of-all the most two important parameters are *NRBOX* and *NZBOX* which specify the resolution of the profiles and equilibrium geometry in the output *EQDSK*.²³ So, if the user wants to use or have an *EQDSK* file of higher resolution their values need to be changed from the default, i.e. 60, and go higher in value, e.g. 513.

CheasePy code will call the `create_namelist` function and pass the list of parameters which will in turn create the *chease_namelist* file required by *CHEASE* code.

3.5.3 Modes for CheesePy Running

There are several options for a user who runs *CheasePy* that can be accessed by setting the value of `runmode` in `cheaseVals` dictionary variable:

Option 1: To setup the environment for *CHEASE* code to run by creating the required files, i.e. *EXPEQ*, *EXPTNZ*, and *chease_namelist*, and start send the right command to the system to run the *chease.hdf5* executable file in the terminal to establish the MHD equilibrium for the current input data. At the end of each successful run, *CheasePy* code will generate several plots to compare the input and output profiles in the *cheaseresults.pdf* file by calling `plot_chease` function.

Option 2: In case of unsuccessful run that doesn't produce *cheaseresults.pdf* file, the second option that `runmode` can take instruct *CheasePy* code to search for the output HDF5 files from *CHEASE* code and plot their contents against the input profiles.

Option 3: This option instructs *CheasePy* to search for all the available input and output files from any previous *CHEASE* run and remove all of these files. Hence, the current folder will contains only *chease.hdf5* and *runchease.py*. This option is helpful when a user wants to start a new *CHEASE* run, because when *CheasePy* starts running it searches first for any files from a previous run and automatically continue from where that previous run stopped.

²³The output *EQDSK* file overwrites the old version of the *EQDSK* file, in case the user wants to use the latest output *EQDSK* file as as source for profiles or equilibrium geometry for a new iteration.

When a user selects **option 1** for the **runmode** in **cheaseVals** which instructs *CheasePy* to run *CHEASE* code, the user can setup the environment using **removeinputs** and **removeoutputs** options before the run starts, and the user have three other options:

Option 1: If the user sets both **removeinputs** and **removeoutputs** options to *yes*, *CheasePy* will remove all the input and output files related any previous run before running *CHEASE* code. This requires a path to the shot files to be provided by the user for *CheasePy* to copy them into the current folder before starting a new run.

Option 2: If the user sets **removeinputs** to *no* and **removeoutputs** to *yes*, the *CheasePy* code will keep the input files and remove all the output files from any previous run, then *CheasePy* code will start an new run using the available input files in the current directory without any need to copy these files from their source directory.

Options 3: If the user sets both **removeinputs** and **removeoutputs** options to *no*, *CheasePy* will keep all the input and output files from any previous run and use the simulation data of the last iteration from that previous run as the initial condition of the current run and starts the simulation from there. This option is helpful when a previous run crashes or reaches the maximum wall time before the end of the simulation, so *CheasePy* can restarted from where it left.

The next option the user need to set in the **cheaseVals** dictionary is the path to the folder/directory of the shot measurements to copy these profile and equilibrium geometry files to the current directory. This step is required if the input and output files from a previous run were removed. The *CheasePy* user needs to remember that the filename of profile and equilibrium geometry files needs to start with folder name followed by an ‘underscore’ then the type of the data files. For example, for a shot folder named *DIID_174082*, the profiles and equilibrium geometry files should be named: *DIID_174082_EXPTNZ*, *DIID_174082_EXPEQ*, *DIID_174082_CHEASE*, *DIID_174082_EQDSK*, or *DIID_174082_PROFILES*.

The last option the *CheasePy* user has to set before calling the **cheasepy** function is the **cheasemode** entity in the **cheaseVals** dictionary which can be set to any of the following options:

Option 1: Setting **cheasemode** to ‘1’ tells *CheasePy* to reconstruct the MHD equilibrium using *CHEASE* code using the input profiles and equilibrium geometry. If the **iterTotal** entity in **srcVals** is set to a number ‘n’, *CHEASE* will rerun for ‘n’ iterations, and the source files may change depending on the length of profile’s sources list.

Option 2: Setting **cheasemode** to ‘2’ tells *CheasePy* to reconstruct the MHD equilibrium from the input profiles and equilibrium geometry using *CHEASE* code. Then, *CheasePy* will use the error in estimating the total toroidal current to correct the parallel current ($I_{||}$ or $J_{||}$), and use this corrected quantity as input to the *CHEASE* next iteration. *CheasePy* will estimate that correction in every iteration until the error is small enough to stop the simulation.

Option 3: Setting **cheasemode** to ‘3’ tells *CheasePy* to reconstruct the MHD equilibrium from the input profiles and equilibrium geometry using *CHEASE* code. Then, *CheasePy* will use the error in estimating the total toroidal current to correct the pressure component (P or P'), and use this corrected quantity as input to the *CHEASE* next iteration. *CheasePy* will estimate that correction in every iteration until the error is small enough to stop the simulation.

The **current_correction** and **pressure_correction** functions in the *cheasepy.py* are called automatically every time a correction in *parallel current* (option 2) or *pressure* (option 3), respectively,

needs to be done. The *CheasePy* user is free to do any modifications to these functions to handle the correction in a more suitable way for the case under study. But it is recommended that the user treat these functions as a template and do not change the variable name of the returned values for the *CheasePy* to run properly and give relevant results.

3.6 Plotting the Outputs

When *CheasePy* code completes the current run it plots some fields such as the density and temperature profiles, the current flux profile, the magnetic field, the toroidal current, etc., with all figures packed together in a single PDF file.²⁴ The user can plot the fields in the outputs of a previous run of *CheasePy* directly without rerun the code by calling the `plot_chease(OSPATH, skipfigs)` function which takes the path to the HDF5 files as the first arguments (`OSPATH`), and the number of skipped figures as the second argument (`skipfigs`). The number of skipped figures is useful when the *CHEASE* does large number of iterations and the user need to plot only few of them, so the user can set `skipfigs` to a number of figures that will be skipped between the plotted ones. When passing a path to a folder as the first argument to the `plot_chease` function, it searches for all files named *chease_iterxxx.h5*, parse them one by one, extract all the fields and coordinates, and then plot the selected fields. However, if you passed the path to a specific HDF5 file, it plots only the fields in this single file.

4 Future Plans

CHEASEPY code is under continuous development to add new features to the code. However, this version of the code is stable and supposed to give no issues. In case the user has any concern or need to add more features to the code you may contact Ehab Hassan at ehab@utexas.edu. Otherwise, users can add these features themselves but they supposed to inform the original developers with these added features.

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6 References

- Lütjens, Hinrich, Anders Bondeson, and Olivier Sauter. "The CHEASE code for toroidal MHD equilibria." *Computer physics communications* 97.3 (1996): 219-260.
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²⁴It is easy to add plots for other fields those are not plotted by copying the chunk of code used to plot another field and replace the name of the existing field with the new field name. You need also to rename the figure object and add it to the PDF file.