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Xujing Li and Leonid E. Zakharov

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Equilibrium Spline Interface (ESI) for magnetic confinement codes

Xujing Li[1], Leonid E. Zakharov[2]
[1]*Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science,Chinese Academy of Sciences, P.O. Box 2719, Beijing 100190, China*
[2]*Princeton Plasma Physics Laboratory Princeton, P.O. Box 451, Princeton NJ, 08543, USA*

A compact and comprehensive interface between magneto-hydrodynamic (MHD) equilibrium codes and gyro-kinetic, particle orbit, MHD stability, and transport codes is presented. Its irreducible set of equilibrium data consists of three (in 2-D case with occasionally one extra in 3-D case) functions of coordinates and four 1-D radial profiles together with their first and mixed derivatives. The C reconstruction routines, accessible also from FORTRAN, allow the calculation of basis functions and their first derivatives at any position inside the plasma and in its vicinity. After this all vector fields and geometric coefficients, required for the above mentioned types of codes, can be calculated using only algebraic operations with no further interpolation or differentiation.

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I. INTRODUCTION

In plasma simulations, which deal with highly anisotropic equations, the equilibrium codes play a fundamental role in supplying the information about magnetic configuration. For different more sophisticated plasma problems: stability, transport, particle orbit or gyro-kinetics, this information is needed in flux coordinates related to the geometry of the magnetic field.

Initially, the "equilibrium solvers" worked as a set of subroutines inside other codes. We do not consider this practical anymore. The requirements to equilibrium codes has grown considerably from primitive calculations of "fix-boundary" cases for theory purposes to the real time control of plasma equilibrium in operational devices and real time magnetic reconstruction [1]. These tasks require sophisticated interaction with numerous control systems and diagnostics. Recently, the possibility of performing the real time sensitivity analysis has emerge for generation of the best possible equilibrium reconstruction data [2]. It became almost impossible to maintain an equilibrium code updated as a subroutine inside another code which are designed for other objectives.

The practical approach is to run the codes as separate processes interacting with each other using the inter-process communications. This approach makes the maintenance of different codes independent and focused on their own specific objectives. The interface between the equilibrium and "client" codes can be provided by an intermediate layer, which requires standard information on equilibrium code and conveys it to the client code. This paper describes a universal format and a set of routines, called `ESI`, as a buffer between equilibrium and other codes. `ESI` makes the user side independent of the specific code, which generates the equilibrium data.

While the equilibrium configurations depend essentially only on two radial profiles and the shape of the plasma boundary, the request of other codes may contain numerous 2- or 3-dimensional functions representing components of the metric tensor, magnetic fields, current density, curvature of the field lines, or the magnitude of the magnetic field and its derivatives. All these functions are inter-related and many can be calculated in a different manner, potentially generating inconsistencies due to finite accuracy of the equilibrium codes. Because of this, it is important to determine what should be taken as the output data from the equilibrium codes and what can be calculated inside the "client" codes in a self-consistent manner.

At present, there are two extreme approaches to make a choice of output data from numerical equilibria. One of them requires all functions, necessary for the client code, at all necessary positions to be supplied by the equilibrium codes. An example was the initial interface of ASTRA code [3] and ESC (Equilibrium and Stability Code) [4], when the data on equilibrium configuration were supplied from ESC for both transport simulations and for modeling radio-frequency wave propagation in ASTRA. This approach works only for closely related pairs of codes, making them highly dependent on each other. It requires excessive storage capacities because the required data (e.g., some combinations of metric coefficients) may not be very smooth. This approach is not-suitable also for the situation when the client codes (like particle motion codes) need physics variables at unpredictable positions inside the plasma.

The other extreme approach uses only primitive information from the equilibrium codes, such as coordinates of grid points and a few radial profiles in the form of so-called "g-, a-files" of EFIT [5–7] or "eqdsk" of JSOLVER [8–10]. Then, the client codes, e.g., the PEST [11, 12] stability code, or ORBITS [13] for particle orbits, or transport simulation codes [14, 15] use their own mappers to generate all the necessary functions from equilibrium data.

The problem here is in interpolation and, especially, in calculation of space derivatives, entering into many physics variables. With no universal mathematical rules of doing numerical differentiation, this approach unavoidably intro-

duces its own inaccuracies and causes potential convergence problems in interaction with equilibrium codes.

The idea of Equilibrium Spline Interface (ESI), implemented in ASTRA-ESC code system in 2005, is to have a universal buffer between an equilibrium code and the user codes, as it is shown in Fig. 1. ESI possesses comprehensive information about magnetic configuration and is able to provide it to magnetic confinement codes in a ready to use form. In fact, the design of ESI includes the possibility of representing confinement magnetic fields with ergodic magnetic structures and only approximate magneto-hydrodynamical force balance.

Technically, the proposed ESI consists of (a) a data set (file, or a segment of the shared memory, or interprocess communication channel), which should be provided by an equilibrium code, and (b) of a C-source file (esiXZ.c), which contains with C- or FORTRAN- callable initialization and reconstruction routines (see Fig. 1). This paper and other documentation on the current state of ESI can be found in esiXZ.c.d documentation file.

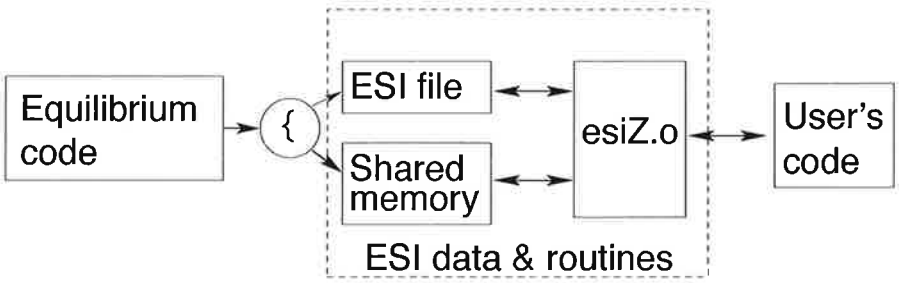


FIG. 1: Data generating equilibrium code, ESI, and the user's code

The source code esiXZ.c is self-contained and can be compiled by a simple command

```
cc -c -o esiXZ.o esiXZ.c
```

From the equilibrium codes the interface requires a standard and easy to generate set of data, specified and explained in this paper, together with the ID (defined later) of coordinates and representations. In its turn, the user side may optionally provide its own ID information during initiation of the interface. After this the interface routines can generate all necessary data for magnetic confinement codes at any point in the calculation area.

The interface is compact and comprehensive. For equilibrium configurations it includes a set of basis functions, i.e., four radial profiles and three 2-D functions of space coordinates for axisymmetric configurations (e.g., tokamaks) or 3-D functions (for stellarators). ESI data provide a Hermit polynomial representation of these well behaved functions in terms of their values, first and mixed derivatives on a mesh.

The reconstruction routines can calculate basis functions and their first derivatives at any point inside the plasma. Then, the client code can calculate the necessary vector or scalar field variables *by algebraic operations without numerical differentiation*, as it is described in this paper.

Sect. 2 introduces notations and basis of ESI functions and their relations with the physics variables and plasma profiles. Sec. 3 describes initialization of ESI and a call of main reconstruction routine at the user side. Sec. 4 contains basic geometrical relationships, while Sec. 5 provides the self consistent recipes for calculating parameters of magnetic configurations.

Sect. 6 outlines the use of ESI for tracing field lines and particle orbits. The Hamiltonian canonical coordinates are introduced for guiding center motion in 3-D nested configurations. Boozer coordinates are not canonical, as is often mistakenly believed. Sect. 7 shows sufficiency of ESI for MHD stability codes.

Finally, Sect. 8 and Sect. 9 describes the data storage structure, file formats and a set of ESI routines.

II. THE BASIS FUNCTIONS OF ESI, REFERENCE MAGNETIC COORDINATES

The curvilinear coordinates a, θ, ζ for describing magnetic configurations for plasma confinement (see, e.g., [16]) can be represented parametrically by equations

$$r = r(a, \theta, \zeta), \quad z = z(a, \theta, \zeta), \quad \varphi = \varphi(a, \theta, \zeta), \tag{1}$$

where r, φ, z are laboratory cylindrical coordinates. The typical choice of $\zeta = \varphi$ eliminates the need of the third equation. The curvilinear coordinates are assumed to be nested and their Jacobian J

$$J \equiv \frac{1}{(\nabla a \times \nabla \theta) \cdot \nabla \zeta} \tag{2}$$

is not vanishing.

In the ideal situation, the magnetic surfaces are also nested and it is possible to consider the so-called "flux" coordinates, when

$$\vec{B} \cdot \nabla a = 0. \tag{3}$$

The vector potential $\vec{A}$ of the magnetic field $\vec{B} = (\nabla \times \vec{A})$ has the following general covariant representation

$$\vec{A} = -\bar{\Phi}'\eta\nabla a + \bar{\Phi}\nabla\theta + \bar{\Psi}\nabla\zeta. \tag{4}$$

In nested coordinates the dependencies on angles θ, ζ in function $\bar{\Phi}$ can be eliminated by adding ∇u to the vector potential, thus, making it a function of (a, ζ): $\bar{\Phi} = \bar{\Phi}_{00}(a) + \widetilde{\Phi}(a, \zeta)$, where $\widetilde{\Phi}(a, \zeta)$ is an oscillatory function. Then, by massaging the radial coordinate $a = a + \xi(a, \zeta)$, using, e.g., an iterative procedure $\xi^{n+1} = -\widetilde{\Phi}^n/\bar{\Phi}'^n_{00}$, the dependence on ζ can be eliminated as well, leaving

$$\bar{\Phi} = \bar{\Phi}_{00}(a) = \bar{\Phi}(a). \tag{5}$$

After this, $\Phi(a) \equiv 2\pi\bar{\Phi}(a)$ becomes a flux of the magnetic field through the contour $a = const, \zeta = const$. (Only in the case of Field Reversed Pinches, where $\bar{\Phi}'_{00} = 0$ at the field reverse radius, this elimination may not be possible).

In the function $\bar{\Psi} = \bar{\Psi}(a, \theta, \zeta)$, it is not possible to eliminate the dependence on angle coordinates in all situations. The best representation

$$\bar{\Psi} = \bar{\Psi}_{00}(a) + \psi(a, \theta, \zeta) = \bar{\Psi}_{00}(a) + \sum_{m^*, n^*} \psi_{m^*n^*}(a) e^{im^*\theta - in^*\zeta)}, \quad \bar{\Psi}_{00}(a) \equiv \frac{1}{4\pi^2} \oint \oint \bar{\Psi} d\theta \, d\zeta \tag{6}$$

can be achieved only in a special coordinate system, called the Reference Magnetic Coordinates (RMC) [17], where only resonant Fourier harmonics $\psi_{m^*n^*}$ enter into $\bar{\Psi}$ with $m^*\bar{\Psi}'_{00} + n^*\bar{\Phi}'_{00} = 0$ at some $a = a_{m^*n^*}$. In equilibrium configurations these resonance terms determine the magnetic islands, which make the topology of the magnetic field different from the coordinate system. RMC give the most compact representation of the 3-D ergodic fields. The design of `ESI` utilizes RMC for representation of 3-D confinement magnetic fields in the form of Eq. (6).

The averaged $2\pi\bar{\Psi}_{00}$ is equal to the poloidal Ψ flux of the magnetic field through the contours $a = const, \theta = const$. For the purpose of `ESI` we consider only simple nested magnetic configurations, where

$$\bar{\Psi} = \bar{\Psi}_{00}(a) = \bar{\Psi}(a). \tag{7}$$

In the following, we will drop the subscript '00' in $\bar{\Phi}_{00}, \bar{\Psi}_{00}$ assuming representation (6) in the case of ergodic fields.

The periodic function $\eta = \eta(a, \theta, \zeta)$ is oscillatory

$$\int \eta d\theta d\zeta = 0. \tag{8}$$

For special purposes, it can be eliminated by massaging the angles

$$\theta \to \bar{\theta} = \theta + \alpha, \quad \zeta \to \bar{\zeta} + \beta, \quad \bar{\Phi}'\alpha + \bar{\Psi}'\beta = \bar{\Phi}'\eta \tag{9}$$

in order to produce the so-called "straight field line" coordinates

$$\vec{A} = \bar{\Phi}\nabla\bar{\theta} + (\bar{\Psi} + \psi)\nabla\bar{\zeta}. \tag{10}$$

"Barred" notations $a, \bar{\theta}, \bar{\zeta}$ are used for the straight field line coordinates.

In RMC, the magnetic field has the following contravariant representation

$$\vec{B} = \psi'_\theta(\nabla\theta \times \nabla\zeta) - (\bar{\Psi}' + \psi'_a + \bar{\Phi}'\eta'_\zeta)(\nabla\zeta \times \nabla a) + (\bar{\Phi}' + \bar{\Phi}'\eta'_\theta)(\nabla a \times \nabla\theta), \tag{11}$$

$$B^a \equiv \vec{B} \cdot \nabla a = \frac{\psi'_\theta}{J}, \quad B^\theta \equiv \vec{B} \cdot \nabla\theta = -\frac{\bar{\Psi}' + \psi'_a + \bar{\Phi}'\eta'_\zeta}{J}, \quad B^\zeta \equiv \vec{B} \cdot \nabla\zeta = \frac{\bar{\Phi}'(1 + \eta'_\theta)}{J}, \tag{12}$$

where ψ with resonant harmonics describes magnetic islands. In flux coordinates ($\vec{B} \cdot \nabla a = 0$, $\psi = 0$), the magnetic field $\vec{B}$ has a simpler form

$$\vec{B} = -(\bar{\Psi}' + \bar{\Phi}'\eta'_\zeta)(\nabla\zeta \times \nabla a) + (\bar{\Phi}' + \bar{\Phi}'\eta'_\theta)(\nabla a \times \nabla\theta). \tag{13}$$

The definitions (1, 13) introduce two (out of a total of four in ESI) 1-D profiles

$$\bar{\Phi}'(a), \quad \bar{\Psi}'(a) \tag{14}$$

and, together with $|\vec{B}|$, four basis functions of ESI interface

$$r = r(a,\theta,\zeta), \quad z = z(a,\theta,\zeta), \quad |\vec{B}| = B(a,\theta,\zeta), \quad \eta'_\theta \equiv \eta'_\theta(a,\theta,\zeta). \tag{15}$$

In ESI, the units of r, z are in [m], B is in [T], η is dimensionless, while fluxes Φ, Ψ are in [V·sec]. Units of a, θ, ζ are not essential.

Note, that the basic functions (14,15) represent any nested magnetic configurations, even unrelated to a static equilibrium.

In magneto-static equilibrium

$$\nabla\bar{p} = \vec{j} \times \vec{B}, \quad \vec{j} = \nabla \times \vec{B}, \quad \bar{p} \equiv \mu_0 p, \quad \vec{j} \equiv \mu_0 \vec{j}, \tag{16}$$

$$\vec{B} \cdot \nabla\bar{p} = 0, \quad \vec{j} \cdot \nabla a = 0, \tag{17}$$

where p is the plasma pressure in [MPa], $\vec{j}$ is the current density in [MA/m^2], and $\mu_0 = 0.4\pi$, one can introduce two additional 1-D profiles, i.e., $P(a), T(a)$

$$P(a) \equiv \frac{d\bar{p}}{d\bar{\Psi}}, \quad T(a) \equiv \bar{F}\frac{d\bar{F}}{d\bar{\Psi}}, \quad \bar{F} \equiv 0.2F. \tag{18}$$

Here $F = 5\bar{F}$ is the total poloidal current in [MA] through the contour $a = const, \theta = const$ (analog of magnetic flux Ψ). In axisymmetric configurations

$$\bar{F} = rB_\varphi. \tag{19}$$

ESI relies on the fact that four space coordinated functions (15) and four 1-D profiles (14), (18) together with their first derivatives contain all necessary information for transport, stability, particle motion as well as gyro-kinetic codes [18, 19]. They are called hereafter the "basis" functions. The ESI input file contains Hermit representations of r, z, ζ, B, which are well behaved and can be accurately interpolated. The function η and its derivatives are generated by ESI routines.

As a special case, ESI accepts 2-D data on a rectangular grid r, z from free boundary codes in the form of $\bar{\Psi}(r,z), \bar{\Psi}'_r, \bar{\Psi}'_z, \bar{\Psi}''_{rz}$. This is not sufficient to generate all possible information for other magnetic confinement codes. The special ESI routine can convert $r - z$ data into basis functions of flux coordinates.

ESI*reconstruction routines do not provide the second derivatives of basis functions, since the equilibrium does not give information about second derivatives.* The following sections describe the self-consistent rules of using basis function for different kinds of numerical codes without use of second derivatives.

III. MAIN RECONSTRUCTION ROUTINE OF ESI

All ESI routines are `int` C-functions, which return 0 in the case of success, and non-zero otherwise. In order to initiate ESI from a data file (which should be created by an equilibrium code), the user should use the C-code, like

```
if(File2ESI(FileName,iE)){
  printf("Failure: %s is not an ESI-file\n'',FileName);
}
```

or FORTRAN-code, like

```
external integer file2esi
if(file2esi(FileName,ie).ne.0) then
  write(*,'(aaa)')'Failure: ',FileName,' is not an ESI-file'
endif
```

The FORTRAN file name `FileName` *in* `file2esi` ***should contain*** *a space character* `' '` *at the end !.* The integer parameter $0 \leq$ `iE` < 8 activate one of instances of ESI. Several of them can be activated simultaneously.

In the case of using shared memory the corresponding function is `Shmem2ESI(int key, int iE)`, where `'key'` is a unique identification number for the memory segment, known to mutually communicating equilibrium and user codes.

`ESI` contains the main reconstruction routine `ESI2All(REAL *a,REAL *gq,int n)`, which generates the basic profiles and functions and their first derivatives in a given number `n` of points (a, θ) inside the calculation region. This routine puts the calculated values of the basis profiles and space functions into arrays, allocated in advance at the user side.

The user code should provide the storage for these arrays. The example is the following C-code

```
int N=2000;
double a[N],gq[N];
double F[N],Fa[N],gFa[N][N],gFaa[N],gYa[N],gYaa[N]
  ,T[N],Ta[N],P[N],Pa[N]
  ,r[N],ra[N],rq[N],z[N],za[N],zq[N]
  ,B[N],Ba[N],Bq[N],gh[N],gha[N],ghq[N];
int isw[N];
double gz[N],rz[N],zz[N],Bz[N],ghz[N];
```

The number N should not be less than the number of points requested in reconstruction, $n \leq N$. The last line is necessary only for the 3-D case. The FORTRAN analog of the same would be

```
      parameter (N=2000)
      double precision a(N),gq(N)
      double precision F(N),Fa(N),gFa(N),gFaa(N),gYa(N),gYaa(N)
     &      ,T(N),Ta(N),P(N),Pa(N)
     &      ,r(N),ra(N),rq(N),z(N),za(N),zq(N)
     &      ,B(N),Ba(N),Bq(N),gh(N),gha(N),ghq(N)
      integer isw(N);
      double precision gz(N),rz(N),zz(N),Bz(N),ghz(N);
      external integer link2esi,link2esi3d,esi2all,esi2all3d
```

The meaning of these arrays are specified in the Table I.

Set of output radial profiles			*Table I*
C-code	Math	C-code	Math
`F[],Fa[]`	$\bar{F}, \bar{F}'$	`isw[]`	index of the particle
`gFa[],gFaa[]`	$\bar{\Phi}', \bar{\Phi}''$	`gYa[],gYaa[]`	$\bar{\Psi}', \bar{\Psi}''$
`T[],Ta[]`	$T = \bar{F}\bar{F}'/\bar{\Psi}', T'_a$	`P[],Pa[]`	$P = \bar{p}'/\bar{\Psi}', P'_a$
Set of 2-D and 3-D output space functions			
C-code	Math	C-code	Math
`r[],ra[],rq[],rz[]`	$r, r'_a, r'_\theta, r'_\zeta$	`z[],za[],zq[],zz[]`	$z, z'_a, z'_\theta, z'_\zeta$
`B[],Ba[],Bq[],Bz[]`	$B, B'_a, B'_\theta, B'_\zeta$	`gh[],gha[],ghq[],ghz[]`	$\eta, \eta'_a, \eta'_\theta, \eta'_\zeta$

TABLE I: The list of basic profiles and 2-D functions for 2-D ESI

The addresses of these arrays should be given to `ESI`, at least once, using routine

```
i=Link2ESI(F,Fa,gFa,gFaa,gYa,gYaa,T,Ta,P,Pa
          ,r,ra,rq,z,za,zq,B,Ba,Bq,gh,gha,ghq,isw);
i=Link2ESI3d(rz,zz,Bz,ghz);
```

for C-code or for FORTRAN as

```
      i=link2esi(F,Fa,gFa,gFaa,gYa,gYaa,T,Ta,P,Pa
     &    ,r,ra,rq,z,za,zq,B,Ba,Bq,gh,gha,ghq,isw)
      i=link2esi3d_(rz,zz,Bz,ghz)
```

Again, the last line is necessary only for the 3-D case. At present, the main reconstruction routine does not use the index array `isw[i]`, which can be used as a marker of points to control some service routines.

After the addresses are given to `ESI`, the call of the main reconstruction routine is simple, as soon as the `n` $\leq$ `N` coordinates points a, θ (and ζ in 3-D case) are put into array `a[],gq[]` (and `gz[]`) by calling the routine

```
i=ESI2all(a,gq,n);
```

or for 3-D case

```
i=ESI2all3d(a,gq,gz,n);
```

The FORTRAN analog of the same is

```
i=esi2all(a,gq,n);
i=esi2all3d(a,gq,gz,n);
```

After these calls the information is placed into the mentioned arrays. In addition to the main reconstruction routine, `ESI` contains numerous service routine for calculating specialized information. Some of them are listed at the end of this paper, and their sets can be extended.

The `Link2ESI()` routines can accept `NULL` as an argument for unused variables. In this case, the reconstruction routines will not generate the corresponding data.

The next 4 sections describe how to use basic functions for calculation of physics variables.

IV. METRICS OF TOROIDAL CONFIGURATIONS

The metric tensor g_{ik} $(i = 1,2,3,\ k = 1,2,3)$ of the coordinate system $\{a,\theta,\zeta\} = \{x^1,x^2,x^3\}$ is defined by the element of length dl

$$
\begin{aligned}
&dl^2 \equiv dr^2 + dz^2 + r^2 d\varphi^2 = g_{aa}da^2 + 2g_{a\theta}da d\theta + g_{\theta\theta}d\theta^2 + 2g_{a\zeta}da d\zeta + 2g_{\theta\zeta}d\theta d\zeta + g_{\zeta\zeta}d\zeta^2, \qquad (20)\\
&g_{aa} = r'_a r'_a + z'_a z'_a + r^2\zeta'_a\zeta'_a, \quad g_{a\theta} = r'_a r'_\theta + z'_a z'_\theta + r^2\zeta'_a\zeta'_\theta,\\
&g_{\theta\theta} = r'_\theta r'_\theta + z'_\theta z'_\theta + r^2\zeta'_\theta\zeta'_\theta, \quad g_{a\zeta} = r'_a r'_\zeta + z'_a z'_\zeta + r^2\zeta'_a\zeta'_\zeta,\\
&g_{\theta\zeta} = r'_\theta r'_\zeta + z'_\theta z'_\zeta + r^2\zeta'_\theta\zeta'_\zeta, \quad g_{\zeta\zeta} = r'_\zeta r'_\zeta + z'_\zeta z'_\zeta + r^2\zeta'_\zeta\zeta'_\zeta,\\
&J = \sqrt{g}, \quad g \equiv \mathrm{Det}(g_{ik}).
\end{aligned}
$$

Gradient vectors of cylindrical and curvilinear coordinates are related with each other by a matrix of first derivatives D

$$
\begin{pmatrix} \nabla r \\ \nabla\varphi \\ \nabla z \end{pmatrix} = \mathsf{D}\cdot\begin{pmatrix} \nabla a \\ \nabla\theta \\ \nabla\zeta \end{pmatrix}, \quad \begin{pmatrix} \nabla a \\ \nabla\theta \\ \nabla\zeta \end{pmatrix} = \mathsf{D}^{-1}\cdot\begin{pmatrix} \nabla r \\ \nabla\varphi \\ \nabla z \end{pmatrix}, \quad \mathsf{D} \equiv \begin{pmatrix} r'_a & r'_\theta & r'_\zeta \\ \varphi'_a & \varphi'_\theta & \varphi'_\zeta \\ z'_a & z'_\theta & z'_\zeta \end{pmatrix}. \qquad (21)
$$

The Jacobian J of the coordinate system can be calculated as the determinant D of the matrix of first derivatives of cylindrical coordinates

$$
D = \mathrm{Det}(\mathsf{D}), \quad J = rD = \sqrt{g}, \qquad (22)
$$

In axisymmetric configurations, only $g_{aa}, g_{a\theta}, g_{\theta\theta}, g_{\varphi\varphi}$ are non-vanishing

$$
\begin{aligned}
&dl^2 \equiv dr^2 + dz^2 + r^2 d\varphi^2 = g_{aa}da^2 + 2g_{a\theta}da d\theta + g_{\theta\theta}d\theta^2 + r^2 d\varphi^2, \qquad (23)\\
&g_{aa} = r'_a r'_a + z'_a z'_a, \quad g_{\theta\theta} = r'_\theta r'_\theta + z'_\theta z'_\theta, \quad g_{\varphi\varphi} = r^2, \quad D = r'_\theta z'_a - r'_a z'_\theta. \qquad (24)
\end{aligned}
$$

`ESI` reconstruction routines provide all necessary derivatives for calculation of g_{ik}, elements of matrix D, and Jacobian J at the user side. *The derivatives of* g_{ik}, D, J *are not defined by* `ESI`.

A. Behavior near the origin $a = 0$

In configurations with a smooth current density near the axis $a = 0$, flux coordinates have a special behavior near the axis. Thus, in some coordinate systems Fourier coefficients of $r(a,\theta,\zeta), z(a,\theta,\zeta)$

$$
r = r_0 + \sum_{m=1}^{m\le M_\theta}\left[r_m e^{im\theta} + r_m^* e^{-im\theta}\right], \quad z = z_0 + \sum_{m=1}^{m\le M_\theta}\left[z_m e^{im\theta} + z_m^* e^{-im\theta}\right] \qquad (25)
$$

vanish at a certain rate when $a \to 0$. If a is proportional to the distance from the axis, then in some coordinates (ESC, Hamada, PEST, Boozer) asymptotically

$$r_0(a,\zeta) \simeq R_0(\zeta) + \frac{1}{2} r_0''(\zeta) a^2, \quad r_m(a,\zeta) \propto a^m, \quad z_0(a,\zeta) \simeq Z_0(\zeta) + \frac{1}{2} z_0''(\zeta) a^2, \quad z_m(a,\zeta) \propto a^m. \tag{26}$$

The `ESI` *data generated by the equilibrium codes in these coordinates should reflect this behavior.* All coefficients with $m = 0, m > 1$ should vanish near the axis, at least, like a^2. This would allow to resolve the details, essential for some instabilities near the magnetic axis.

In other coordinates (e.g., polar, equidistant, see Table III) all Fourier coefficients are proportional to $r_m \propto a^{m-1}$ for $m > 1$, which creates some resolution issues for `ESI` near the magnetic axis.

B. Conversion of laboratory r, φ, z into a, θ, ζ

For diagnostics on the experimental machines and other purposes, `ESI` has the ability of conversion of laboratory coordinates r, φ, z into curvilinear coordinates a, θ, ζ. This is done by a Newton iterative procedure

$$\begin{array}{lll} a^{(k+1)} & = a^{(k)} & + da^{(k)} \\ \theta^{(k+1)} & = \theta^{(k)} & + d\theta^{(k)} \\ \zeta^{(k+1)} & = \zeta^{(k)} & + d\zeta^{(k)} \end{array}, \tag{27}$$

where

$$\begin{pmatrix} da^{(k)} \\ d\theta^{(k)} \\ d\zeta^{(k)} \end{pmatrix} = \left(\mathsf{D}^{-1}\right)^{(k)} \cdot \begin{pmatrix} r - r^{(k)} \\ \varphi - \varphi^{(k)} \\ z - z^{(k)} \end{pmatrix}, \tag{28}$$

and k is the iteration counter.

V. NESTED MAGNETIC CONFIGURATIONS

The vector potential $\vec{A}$ in Eq.(4) contains integrals from the basis profiles of `ESI`

$$\Phi = 2\pi \int_0^a \bar{\Phi}'(a) da, \quad \Psi = 2\pi \int_0^a \bar{\Psi}'(a) da, \quad \eta = \int_0^\theta \eta'_\theta d\theta + \int_0^\zeta \left(\frac{1}{2\pi} \oint \eta'_\zeta d\theta \right) d\zeta. \tag{29}$$

There is a special service routine in `ESI` which calculates Ψ, Φ for the transport codes, while η and its derivatives are calculated by the main reconstruction routine.

A. Magnetic field

The contravariant representation of the magnetic field is given by Eq.(13). It can be reconstructed from `ESI` basis functions in a straightforward manner. On the other hand the derivatives of individual components of the magnetic field are not defined.

The covariant components of magnetic field B_i (integer subscript i is used to distinguish them from the physical components),

$$\vec{B} = B_1 \nabla a + B_2 \nabla \theta + B_3 \nabla \zeta, \quad B_i = g_{ik} B^k, \quad i = 1,2,3, \quad k = 1,2,3 \tag{30}$$

are useful for particle motion. Here the summation convention on repetitive indexes is assumed.

In flux coordinates (no islands) $B^1 = B^a = 0$ and only the following metric tensor combinations are present in Eq.(30)

$$K \equiv \frac{g_{\theta\theta}}{J}, \quad M \equiv \frac{g_{aa}}{J}, \quad N \equiv \frac{g_{a\theta}}{J}, \quad N_{a\zeta} \equiv \frac{g_{a\zeta}}{J}, \quad N_{\theta\zeta} \equiv \frac{g_{\theta\zeta}}{J}, \quad L \equiv \frac{J}{g_{\zeta\zeta}}. \tag{31}$$

All of them can be calculated at the user side using the relationship between co- and contra-variant components of the vector $\vec{B}$.

In the case of an "ideal" (isotropic) equilibrium, the covariant components have a special form

$$\vec{B} = (\nu + \sigma'_a)\nabla a + (\bar{I} + \sigma'_\theta)\nabla\theta + (\bar{F} + \sigma'_\zeta)\nabla\zeta \tag{32}$$

and can be calculated using

$$\nu + \sigma'_a = -N(\bar{\Psi}' + \bar{\Phi}'\eta'_\zeta) + N_{a\zeta}\bar{\Phi}'(1 + \eta'_\theta), \tag{33}$$

$$\bar{I} + \sigma'_\theta \equiv -K(\bar{\Psi}' + \bar{\Phi}'\eta'_\zeta) + N_{\theta\zeta}\bar{\Phi}'(1 + \eta'_\theta), \tag{34}$$

$$\bar{F} + \sigma'_\zeta = -N_{\theta\zeta}(\bar{\Psi}' + \bar{\Phi}'\eta'_\zeta) + \frac{1 + \eta'_\theta}{L}\bar{\Phi}'. \tag{35}$$

For the 2-D case of axisymmetry

$$\nu + \sigma'_a = -N\bar{\Psi}', \quad \bar{I} + \sigma'_\theta \equiv -K\bar{\Psi}', \quad \bar{F} = \frac{1 + \eta'_\theta}{L}\bar{\Phi}', \quad L = \frac{D}{r}. \tag{36}$$

B. Current density

In equilibrium configurations the current density $\vec{j}$ has the following contravariant form

$$\vec{j} = -(\bar{F}' - \nu'_\zeta)(\nabla\zeta \times \nabla a) + (\bar{I}' - \nu'_\theta)(\nabla a \times \nabla\theta) \quad , \tag{37}$$

where $I(a) = 5\bar{I}$ is the toroidal current through the toroidal cross-section of magnetic surfaces. Both $\bar{F}, \bar{F}'$, together with $\bar{p}, \bar{p}'$ are calculated inside `ESI` using

$$\bar{F}' = \frac{T\bar{\Psi}'}{\bar{F}}, \quad \bar{F}(a) = \sqrt{\bar{F}^2_{ref} + 2\int_{a_{ref}}^{a} T(a)\bar{\Psi}' da}, \quad \bar{p}' = P\bar{\Psi}', \quad \bar{p}(a) = \int_{a_{ref}}^{a} P\bar{\Psi}' da. \tag{38}$$

Here, a_{ref} is a reference radius, where the function $\bar{F}$ has a prescribed value, $\bar{F}(a_{ref}) = \bar{F}_{ref}$. Typically a_{ref} corresponds to the plasma boundary. The exceptional case is the RFP configurations, where a_{ref} should specify the surface with $\bar{F}(a_{ref}) = 0$. The main `ESI` reconstruction routine delivers $\bar{F}, \bar{F}'$, while $\bar{p}, \bar{p}'$ are provided by a special service routine. *For RFP case the sign of $\bar{F}$ cannot be determined from the* `ESI` *data. It is chosen using convention* $\bar{F}(0) > 0$.

The radial component of equilibrium equation (17) (the pressure balance)

$$J\bar{p}' = -(\bar{\Phi}' + \bar{\Phi}'\eta'_\theta)(\bar{F}' - \nu'_\zeta) + (\bar{\Psi}' + \bar{\Phi}'\eta'_\zeta)(\bar{I}' - \nu'_\theta) \tag{39}$$

determines $\bar{I}'(a)$ inside `ESI` from the averaged Eq.(39)

$$PJ_{00} = -\bar{\Phi}'\frac{T}{\bar{F}} + \bar{I}', \quad J_{00} \equiv \frac{1}{4\pi^2}\oint\oint J d\theta d\zeta, \quad J \equiv J_{00} + J_{\sim\sim}. \tag{40}$$

The oscillatory part of this equation, having the form of the so-called magnetic differential equation (MDE)

$$(\bar{\Phi}' + \bar{\Phi}'\eta'_\theta)\nu'_\zeta - (\bar{\Psi}' + \bar{\Phi}'\eta'_\zeta)\nu'_\theta = \bar{p}' J_{\sim\sim} + \bar{\Phi}'(\bar{F}'\eta'_\theta - \bar{I}'\eta'_\zeta) \tag{41}$$

allows one to determine the function ν. In the case of axisymmetry this is simply given by an integral

$$\bar{I}' - \nu'_\theta = TL + PJ, \quad \nu'_\theta = -TL_{\sim\sim} - PJ_{\sim\sim}, \quad \nu = -\int_0^\theta (TL_{\sim\sim} + PJ_{\sim\sim})d\theta. \tag{42}$$

In the case of 3-D equilibrium configurations, it necessary to solve MDE (41). In configurations with simple nested surfaces (with no islands), the Jacobian does not contain resonance harmonics, and MDE for ν has a nonsingular periodic solution. This is described in the next section. A special service routine of `ESI` generates ν.

Thus, all physical quantities in the equilibrium configurations can be calculated from `ESI` basis functions without using their second derivatives.

Note that the output information from ESI can appear to be inconsistent. For example, in 2-D, the third equation in (35) gives the relationship

$$\bar{\Phi}' = L_0 \bar{F}, \quad L_0 \equiv \frac{1}{2\pi} \oint \frac{D}{r} d\theta, \tag{43}$$

which gives an alternative to the Eq.(38) way of calculating $\bar{F}$. The level of discrepancy between the two calculations may be used for testing the accuracy of ESI data.

In fact, the user has no information from ESI on how to perform integration without interpolation of the integrand, which makes such comparison "illegal" within ESI rules. Instead, the main reconstruction routine of ESI provides the values of $\bar{F}, \bar{F}', \bar{\Phi}, \bar{\Phi}'$ explicitly, thus, giving L_0, L_0'. Alternatively, a specially written service routine of ESI can provide L_0, L_0', consistent with relation (43).

C. Magnetic differential equation (MDE)

For simplicity, let us assume that a, θ, ζ are straight field line coordinates with $\eta = 0$. Then, the magnetic differential equation (41)

$$\nu_\theta' + q\nu_\zeta' = -P(a) J_{\backsim}(a, \theta, \zeta) \equiv -S(a, \theta, \zeta), \quad q \equiv -\frac{\bar{\Phi}'}{\bar{\Psi}'} \tag{44}$$

has a solution

$$\nu(a, \theta, \zeta) = A(a, \zeta - q\theta) - \int_0^\theta S(a, \alpha, \zeta + q\alpha - q\theta) d\alpha, \tag{45}$$

$$A(a, \zeta) - A(a, \zeta - 2\pi q) = \int_0^{2\pi} S(a, \alpha, \zeta + q\alpha - 2\pi q) d\alpha, \tag{46}$$

where a 2-D function $A(a, \zeta)$ is added in order to provide the periodicity of ν as function of θ. The equation for A can be solved directly numerically in Fourier space

$$S(a, \theta, \zeta) \equiv \sum_n S_n(a, \theta) e^{in\zeta}, \quad A(a, \zeta) \equiv \sum_n A_n(a) e^{in\zeta}, \quad A_n(a) = \frac{e^{-in\pi q}}{2 \sin n\pi q} \int_0^{2\pi} S_n(a, \alpha) e^{inq\alpha} d\alpha. \tag{47}$$

In the general case when $\eta \neq 0$, the equation for ν (41) can be written as

$$q(1 + \eta_\theta')\nu_\zeta' + (1 - q\eta_\zeta')\nu_\theta' = -J_{\backsim} P + q(\bar{F}' \eta_\theta' - \bar{I}' \eta_\zeta') \equiv -(1 + \eta_\theta') S(a, \theta, \zeta). \tag{48}$$

A transition to a new variable $\bar{\theta} = \theta + \eta$ in $\nu(a, \theta + \eta, \zeta)$ leads to

$$q(1 + \eta_\theta')(\nu_\zeta' + \eta_\zeta' \nu_{\bar{\theta}}') + (1 - q\eta_\zeta')(\nu_\theta' + \eta_\theta' \nu_{\bar{\theta}}') = q(1 + \eta_\theta')\nu_\zeta' + (1 + \eta_\theta')\nu_{\bar{\theta}}' = -(1 + \eta_\theta') S(a, \theta, \zeta). \tag{49}$$

$$q\nu_\zeta' + \nu_{\bar{\theta}}' = -S(a, \bar{\theta} - \eta, \zeta), \tag{50}$$

whose solution is given by Eqs. (46,47).

Because of resonant denominators $nq = m$ (m, n are integers), the function ν may have a rather complicated behavior even when the MDE can be resolved. Therefore, it cannot be well represented by smooth polynomials on a finite grid, and its calculations cannot be delegated to the user. Instead, a specially designed ESI routine reconstructs ν upon the user's request.

D. Curvature of the magnetic field lines

The curvature of the magnetic field lines, essential for some instabilities,

$$\vec{k} \equiv \left(\frac{\vec{B}}{|B|} \cdot \nabla \right) \frac{\vec{B}}{|B|} = -\left(\frac{\vec{B}}{|B|} \times \left(\nabla \times \frac{\vec{B}}{|B|} \right) \right) = \frac{\bar{p}'}{|B|^2} \nabla a - \frac{((\vec{B} \cdot \nabla)|B|)}{|B|^3} \vec{B} + \frac{|B|_a'}{|B|} \nabla a + \frac{|B|_\theta'}{|B|} \nabla \theta \tag{51}$$

can be calculated at the user's side using the data from ESI reconstruction routines.

E. Evolution equation for magnetic fluxes

In evolving magnetic configurations, the electric field $\mathbf{E}$ can be written as

$$\mathbf{E} = \quad -\frac{\partial \mathbf{A}}{\partial t} - \nabla \Phi_E. \tag{52}$$

Elimination of the scalar potential $\nabla\Phi_E$ from the classical parallel Ohm's law

$$\sigma_\parallel (\vec{B} \cdot \mathbf{E}) = (\vec{B} \cdot \vec{j}) \tag{53}$$

using averaging gives the evolution equation for magnetic fluxes

$$\bar{\Phi}'_a \Psi'_t - \bar{\Psi}'_a \Phi'_t = \frac{1}{\sigma_\parallel} (\bar{F}\bar{I}' - \bar{I}\bar{F}'). \tag{54}$$

It can be rewritten as a magnetic diffusion equation

$$\Psi'_t - \frac{\bar{\Psi}'_a}{\bar{\Phi}'_a}\Phi'_t = \frac{1}{\sigma_\parallel}\left[\frac{\bar{\Phi}'\bar{F} - \bar{\Psi}'\bar{I}}{\bar{\Phi}'^2}\left(\frac{g_{\theta\theta}}{\sqrt{g}}(\Psi' + \eta'_\zeta) - \frac{g_{\theta\zeta}}{\sqrt{g}}(\Phi' + \eta'_\theta)\right)'_{00} - \frac{\bar{I}\bar{p}'}{\bar{\Phi}'^2}(\sqrt{g})_{00}\right], \tag{55}$$

$$\bar{I} = -\left(\frac{g_{\theta\theta}}{\sqrt{g}}(\Psi' + \eta'_\zeta) - \frac{g_{\theta\zeta}}{\sqrt{g}}(\Phi' + \eta'_\theta)\right)_{00}. \tag{56}$$

The averaging can be performed on the user's side, while `ESI` reconstruction provides data for all coefficients in this equation.

When the radial coordinate a represents the toroidal magnetic flux (e.g., in the ASTRA code $a = \sqrt{\frac{2\bar{\Phi}}{B_0}}$, $B_0 =$ const), the convective term in the left hand side vanishes, $\bar{\Phi}'_t = 0$.

F. Transport equations

The structure of the transport equations is given by

$$\frac{\partial}{\partial t}(Jn)_{00} + \frac{\partial}{\partial a}\left(J\vec{\Gamma}\cdot\nabla a\right)_{00} = (JS)_{00}, \quad J \equiv \sqrt{g}, \tag{57}$$

where n is a physics variable, Γ is its flux through the magnetic surface (both diffusive and convective), and S are the sources and sinks.

The `ESI` reconstruction routines provide the necessary information for calculating coefficients of the transport equations on the user's side. In contrast, the approach based on "cooking" out all the information inside the equilibrium codes is always deficient due to the unpredictable nature of plasma transport models.

G. Transition to the straight field line (SFL) coordinates

Straight field line coordinates are important for stability theory and for stellarator equilibrium calculations. `ESI` reconstruction routines provide the necessary information for making transition to the SFL coordinates $a, \bar{\theta}, \bar{\zeta}$

$$\theta = \bar{\theta} - \alpha(a,\theta,\zeta), \quad \zeta = \bar{\zeta} - \beta(a,\theta,\zeta), \tag{58}$$

$$d\theta = d\bar{\theta} - \alpha'_a da - \alpha'_\theta d\theta - \alpha'_\zeta d\zeta, \quad d\zeta = d\bar{\zeta} - \beta'_a da - \beta'_\theta d\theta - \beta'_\zeta d\zeta, \tag{59}$$

where α is an arbitrary function, determined by

$$\bar{\Phi}'\alpha + \bar{\Psi}'\beta = \bar{\Phi}'\eta. \tag{60}$$

Substitution of $d\theta, d\zeta$ (Eq. 59) into element of the length (Eq. 21) allows calculation of the metric tensor in new coordinates. With the function η, as one of the basis functions, which is calculated by the main reconstruction routine, the `ESI` interface provides information for transition into any SFL coordinates.

VI. FIELD LINES AND PARTICLE MOTION

A. Equation for magnetic field lines

In curvilinear coordinates, the magnetic field lines are determined by three ordinary differential equations

$$\frac{d\theta}{dl}=\frac{B^\theta}{|B|},\quad \frac{d\zeta}{dl}=\frac{B^\zeta}{|B|},\quad \frac{da}{dl}=\frac{B^a}{|B|}, \tag{61}$$

where B^a, B^θ, B^ζ are given by Eq.(12). In the case of of magnetic configurations with the nested surfaces, a =const, and only the two first equations are essential. `ESI` provides a special step advancing routine `ESI2mfl()` for calculating derivatives of coordinates for ODE solvers.

B. Guiding center Lagrangian equations

The guiding center Lagrangian obtained by Littlejohn has the following normalized form (see, e.g., [20])

$$L=\left(\vec{A}+\rho_\parallel\vec{B}\right)\cdot\vec{v}-H,\quad \vec{v}\equiv\frac{d\vec{r}}{d\tau},\quad \tau\equiv\Omega_0 t,\quad \Omega_0\equiv\frac{eB_0}{mc}, \tag{62}$$

$$H\equiv\rho_\parallel^2\frac{B^2}{2}+\mu B+\phi_E,\quad \mu\equiv\frac{\rho_\perp^2}{2B},\quad \phi_E\equiv\frac{mc^2\Phi_E}{e}\equiv\rho_E R_0 B_0^2,\quad \rho_E\equiv\frac{c\Phi_E}{R_0B_0\Omega_0}. \tag{63}$$

Here, $\vec{v}$ is considered as the normalized time derivative of the particle position, Ω_0 is the reference cyclotron frequency in the reference magnetic field B_0 whatever is used for normalization (e.g., for `ESI` Units, $B_0=1$ T and $\Omega_0=95.79{\cdot}10^{+6}$ sec^{-1} for protons), $\rho_\parallel,\rho_\perp$ are the ion Larmor radii calculated based on particle velocities parallel and perpendicular to the field

$$\rho_\parallel\equiv\frac{v_\parallel}{\Omega_c}=\frac{v_\parallel}{\Omega_0}\frac{B_0}{B},\quad \rho_\perp\equiv\frac{v_\perp}{\Omega_c}=\frac{v_\perp}{\Omega_0}\frac{B_0}{B}. \tag{64}$$

In the Hamiltonian H the last term ϕ_E is associated with the electric field potential Φ_E and can be expressed in terms of the Larmor radius ρ_E calculated based on drift velocity in the effective electric field Φ_E/R_0 where R_0 is some characteristic unit length (e.g., 1 m).

Written for generalized coordinates of a particle a,θ,ζ, the Lagrangian has the form

$$L=P_a\dot{a}+P_\theta\dot{\theta}+P_\zeta\dot{\zeta}-H, \tag{65}$$

$$P_a\equiv\rho_\parallel B_a,\quad P_\theta\equiv\bar{\Phi}+\int_0^a\bar{\Phi}'\eta_\theta' da+\rho_\parallel B_\theta,\quad P_\zeta\equiv\bar{\Psi}+\int_0^a\bar{\Phi}'\eta_\zeta' da+\rho_\parallel B_\zeta. \tag{66}$$

The straightforward variation of L with respect to $\rho_\parallel,a,\theta,\zeta$ leads to the following system of coupled equations of motion

$$\begin{pmatrix} 0 & B_a & B_\theta & B_\zeta \\ -B_a & 0 & J(B^\zeta+\rho_\parallel\bar{j}^\zeta) & -J(B^\theta+\rho_\parallel\bar{j}^\theta) \\ -B_\theta & -J(B^\zeta+\rho_\parallel\bar{j}^\zeta) & 0 & J(B^a+\rho_\parallel\bar{j}^a) \\ -B_\zeta & J(B^\theta+\rho_\parallel\bar{j}^\theta) & -J(B^a+\rho_\parallel\bar{j}^a) & 0 \end{pmatrix}\cdot\begin{pmatrix}\dot{\rho}_\parallel\\ \dot{a}\\ \dot{\theta}\\ \dot{\zeta}\end{pmatrix}=\begin{pmatrix}\frac{\partial H}{\partial\rho_\parallel}\\ \frac{\partial H}{\partial a}\\ \frac{\partial H}{\partial\theta}\\ \frac{\partial H}{\partial\zeta}\end{pmatrix}. \tag{67}$$

Using the matrix

$$\mathsf{A}\equiv\begin{pmatrix}a_{11}&a_{12}\\ a_{21}&a_{22}\end{pmatrix},\quad |\mathsf{A}|\equiv a_{11}a_{22}-a_{12}a_{21}=\sqrt{g}[|B|^2+\rho_\parallel(\vec{B}\cdot(\nabla\times\vec{B}))], \tag{68}$$

where

$$a_{11}\equiv B_\theta,\quad a_{12}\equiv\sqrt{g}(B^\zeta+\rho_\parallel j^\zeta),\quad a_{21}\equiv B_\zeta,\quad a_{22}\equiv-\sqrt{g}(B^\theta+\rho_\parallel j^\theta), \tag{69}$$

the equation of drift motion can be written in the explicit form

$$\begin{pmatrix} \dot{\rho}_\parallel \\ \dot{a} \\ \dot{\theta} \\ \dot{\zeta} \end{pmatrix} = \begin{pmatrix} 0 & 0 & \frac{a_{22}}{|\mathsf{A}|} & -\frac{a_{12}}{|\mathsf{A}|} \\ 0 & 0 & -\frac{a_{21}}{|\mathsf{A}|} & \frac{a_{11}}{|\mathsf{A}|} \\ -\frac{a_{22}}{|\mathsf{A}|} & \frac{a_{21}}{|\mathsf{A}|} & 0 & \frac{B_a}{|\mathsf{A}|} \\ \frac{a_{12}}{|\mathsf{A}|} & -\frac{a_{11}}{|\mathsf{A}|} & -\frac{B_a}{|\mathsf{A}|} & 0 \end{pmatrix} \cdot \begin{pmatrix} \frac{\partial H}{\partial \rho_\parallel} \\ \frac{\partial H}{\partial a} \\ \frac{\partial H}{\partial \theta} \\ \frac{\partial H}{\partial \zeta} \end{pmatrix}. \tag{70}$$

ESI allows calculation of the right hand side of the guiding center equations at any point inside the plasma without interpolations. In fact, ESI contains a guiding center motion routine which calculates the derivatives $\dot{\rho}_\parallel, \dot{a}, \dot{\theta}, \dot{\zeta}$ given $\rho_\parallel, a, \theta, \zeta$.

C. Hamiltonian equations for guiding center motion

By transformation of angle coordinates it is possible to eliminate the $B_a = \nu + \sigma_a$ term in the covariant representation of $\vec{B}$ (Eq. 32) together with the P_a term in Lagrangian. For this purpose, new, canonical coordinates $\hat{\theta}, \hat{\zeta}$ are determined by

$$\hat{\theta} = \theta + \alpha, \quad \hat{\zeta} = \zeta + \beta, \tag{71}$$

where α, β satisfy equations

$$\nu \nabla a + \nabla \sigma + \nabla(\bar{I}\alpha) + \nabla(\bar{F}\beta) - \bar{I}'\alpha \nabla a - \bar{F}'\beta \nabla a = 0, \tag{72}$$

$$\bar{I}'\alpha + \bar{F}'\beta = \nu, \quad \bar{I}\alpha + \bar{F}\beta = -\sigma, \quad \alpha = -\frac{\bar{F}\nu + \bar{F}'\sigma}{\bar{F}\bar{I}' - \bar{I}\bar{F}'}, \quad \beta = \frac{\bar{I}\nu + \bar{I}'\sigma}{\bar{F}\bar{I}' - \bar{I}\bar{F}'}. \tag{73}$$

In canonical coordinates $a, \hat{\theta}, \hat{\zeta}$ the covariant representation of the magnetic field is very simple

$$\vec{B} = \bar{I}\nabla\hat{\theta} + \bar{F}\nabla\hat{\zeta}. \tag{74}$$

The vector potential becomes

$$\vec{A} = -\bar{\Phi}'\hat{\eta}\nabla a + \bar{\Phi}\nabla\hat{\theta} + \bar{\Psi}\nabla\hat{\zeta}, \quad \bar{\Phi}'\hat{\eta} \equiv \bar{\Phi}'\eta - \bar{\Phi}'\alpha - \bar{\Psi}'\beta \tag{75}$$

Accordingly, the Lagrangian is reduced to the Hamiltonian form

$$L = P_{\hat{\theta}}\dot{\hat{\theta}} + P_{\hat{\zeta}}\dot{\hat{\zeta}} - H, \quad P_{\hat{\theta}} \equiv \bar{\Phi} + \int_0^a \bar{\Phi}'\hat{\eta}'_\theta da + \rho_\parallel \bar{I}, \quad P_{\hat{\zeta}} \equiv \bar{\Psi} + \int_0^a \bar{\Phi}'\hat{\eta}'_\zeta da + \rho_\parallel \bar{F}. \tag{76}$$

with no explicit time derivative $\dot{a}$. The equation of motion for a, θ, ζ can be now written as

$$\begin{pmatrix} 0 & 0 & \frac{\partial P_{\hat{\theta}}}{\partial \rho_\parallel} & \frac{\partial P_{\hat{\zeta}}}{\partial \rho_\parallel} \\ 0 & 0 & \frac{\partial P_{\hat{\theta}}}{\partial a} & \frac{\partial P_{\hat{\zeta}}}{\partial a} \\ \frac{\partial P_{\hat{\theta}}}{\partial \rho_\parallel} & \frac{\partial P_{\hat{\theta}}}{\partial a} & 0 & 0 \\ \frac{\partial P_{\hat{\zeta}}}{\partial \rho_\parallel} & \frac{\partial P_{\hat{\zeta}}}{\partial a} & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} \dot{\rho}_\parallel \\ \dot{a} \\ \dot{\hat{\theta}} \\ \dot{\hat{\zeta}} \end{pmatrix} = \begin{pmatrix} \frac{\partial H}{\partial \rho_\parallel} \\ \frac{\partial H}{\partial a} \\ -\frac{\partial H}{\partial \hat{\theta}} \\ -\frac{\partial H}{\partial \hat{\zeta}} \end{pmatrix}. \tag{77}$$

These equations are equivalent to Hamiltonian equations, if momenta $P_{\hat{\theta}}, P_{\hat{\zeta}}$ are used instead of $\rho_\parallel, a$

$$\dot{\theta} = \frac{\partial H}{\partial P_{\hat{\theta}}}, \quad \dot{\zeta} = \frac{\partial H}{\partial P_{\hat{\zeta}}}, \quad \dot{P}_{\hat{\theta}} = -\frac{\partial H}{\partial \hat{\theta}}, \quad \dot{P}_{\hat{\zeta}} = -\frac{\partial H}{\partial \hat{\zeta}}. \tag{78}$$

The Hamiltonian form of the equations of motion guarantees that the guiding center motion not only preserves the value of Hamiltonian H (and, in the case of symmetry, the momentum $P_{\hat{\zeta}}$), but also preserves the phase volume of an ensemble of particles in the phase space $\hat{\theta}, \hat{\zeta}, P_{\hat{\theta}}, P_{\hat{\zeta}}$.

For calculations of guiding center motion in unperturbed equilibrium configurations the Hamiltonian form does not suggest any advantage with respect to the Lagrangian form. Canonical variables are essential only for studies of perturbed particle motion, where adiabatic invariants play the key role.

Note, that there are other choices of canonic variables than Eq. (73). Indeed, in order to eliminate B_a it is sufficient to satisfy only the ∇a component in Eq. (72)

$$\nu + \sigma'_a + \bar{I}\alpha'_a + \bar{F}\beta'_a = 0, \quad \beta = -\int_0^a \frac{\nu + \sigma'_a + \bar{I}\alpha'_a}{\bar{F}} da. \tag{79}$$

The case with $\alpha = 0$ was pointed out earlier. The attempt to use the freedom for elimination of the η term in the vector potential (making SFL canonical coordinates) leads to substantial, unjustified complications in calculations. The canonic variables $a, \hat{\theta}, \hat{\zeta}$, suggested by Eq. (73) represent the best choice.

`ESI` interface is capable of providing a transition to canonical coordinates $a, \hat{\theta}, \hat{\zeta}$ and to a Hamiltonian representation of guiding center motion.

D. Hamiltonian form of the guiding center equations for axisymmetric case

Although Lagrangian written for generalized coordinates a, θ, φ of a particle conserves the particle energy $E = H$ and, in a case of symmetry, the corresponding canonical momentum, it does not have the Hamiltonian form because of the presence of $P_a\dot{a}$ term. In this section we desribe the coordinate transformation which allows to exactly eliminate this term in the case of symmetry, and to do this approximately with a rigorous small parameter in the case of 3-D configurations.

In the case of symmetry, $\partial/\partial\varphi = 0$, the Lagrangian, written for the generalized coordinates a, θ, φ of a particle

$$L = P_a\dot{a} + P_\theta\dot{\theta} + P_\varphi\dot{\varphi} - H, \tag{80}$$

$$P_a \equiv \rho_\parallel(\sigma'_a - \nu), \quad P_\theta \equiv \bar{\Phi} + \int_0^a \bar{\Phi}'\eta'_\theta da + \rho_\parallel(\bar{I} + \sigma'_\theta), \quad P_\varphi \equiv \bar{\Psi} + \int_0^a \bar{\Phi}'\eta'_\varphi da + \rho_\parallel\bar{F} \tag{81}$$

can be converted into the Hamiltonian form with no $\dot{a}$ term by a change of the ignorable variable, i.e.

$$\varphi = \zeta - \bar{\zeta}(a, \theta), \quad \dot{\varphi} = \dot{\zeta} - \bar{\zeta}'_a\dot{a} - \bar{\zeta}'_\theta\dot{\theta}, \tag{82}$$

where $\bar{\zeta}$ is a periodic function of the poloidal angle θ. With the following choice of $\bar{\zeta}$

$$\bar{\zeta} \equiv \int_0^a \frac{\sigma'_a - \nu}{\bar{F}} da = \frac{\sigma}{\bar{F}} + \tilde{\zeta}, \quad \tilde{\zeta} \equiv \int_0^a \frac{\bar{F}'\sigma - \bar{F}\nu}{\bar{F}^2} da \tag{83}$$

the covariant representation of the equilibrium magnetic field has no radial component

$$\vec{B} = (\sigma'_a - \nu)\nabla a + (\bar{I} + \sigma'_\theta)\nabla\theta + \bar{F}\nabla\varphi = (\bar{I} - \bar{F}\tilde{\zeta}'_\theta)\nabla\theta + \bar{F}\nabla\zeta. \tag{84}$$

In its turn the vector potential acquires the form

$$\vec{A} = -\bar{\Phi}'\eta\nabla a + \bar{\Phi}\nabla\theta + \bar{\Psi}\nabla\varphi = -\bar{\eta}\nabla a + \bar{\Phi}\nabla\theta + \bar{\Psi}\nabla\zeta - \nabla(\bar{\Psi}\bar{\zeta}), \tag{85}$$

$$\bar{\eta} \equiv \eta + q\bar{\zeta} = \eta + q\frac{\sigma}{\bar{F}} + q\tilde{\zeta}. \tag{86}$$

As a result, the Lagrangian takes the Hamiltonian form in variables a, θ, ζ

$$L = -\frac{d}{dt}(\bar{\Phi}'\bar{\eta}) + \bar{P}_\theta\dot{\theta} + \bar{P}_\zeta\dot{\zeta} - H, \tag{87}$$

$$\bar{P}_\theta \equiv \bar{\Phi} + \int_0^a \bar{\Phi}'\bar{\eta}_\theta da + \rho_\parallel(\bar{I} - \bar{F}\tilde{\zeta}'_\theta), \quad \bar{P}_\zeta = P_\varphi = \bar{\Psi} + \rho_\parallel\bar{F} \tag{88}$$

with no explicit time derivative $\dot{a}$. The equation of motion for a, θ, ζ can be now written as

$$\begin{pmatrix} 0 & 0 & \frac{\partial \bar{P}_\theta}{\partial \rho_\parallel} & \frac{\partial \bar{P}_\zeta}{\partial \rho_\parallel} \\ 0 & 0 & \frac{\partial \bar{P}_\theta}{\partial a} & \frac{\partial \bar{P}_\zeta}{\partial a} \\ \frac{\partial \bar{P}_\theta}{\partial \rho_\parallel} & \frac{\partial \bar{P}_\theta}{\partial a} & 0 & 0 \\ \frac{\partial \bar{P}_\zeta}{\partial \rho_\parallel} & \frac{\partial \bar{P}_\zeta}{\partial a} & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} \dot{\rho}_\parallel \\ \dot{a} \\ \dot{\theta} \\ \dot{\zeta} \end{pmatrix} = \begin{pmatrix} \frac{\partial H}{\partial \rho_\parallel} \\ \frac{\partial H}{\partial a} \\ -\frac{\partial H}{\partial \theta} \\ -\frac{\partial H}{\partial \zeta} \end{pmatrix}, \tag{89}$$

where

$$\frac{\partial \bar{P}_\theta}{\partial \rho_\parallel} = a_{11} \equiv \bar{I} - \bar{F}\bar{\zeta}'_\theta, \quad \frac{\partial \bar{P}_\theta}{\partial a} = a_{12} \equiv \bar{\Phi}'(1 + \bar{\eta}'_\theta) + \rho_\parallel[\bar{I}' - (\bar{F}\bar{\zeta}'_\theta)'_a], \tag{90}$$

$$\frac{\partial \bar{P}_\zeta}{\partial \rho_\parallel} = a_{21} \equiv \bar{F}, \quad \frac{\partial \bar{P}_\zeta}{\partial a} = a_{22} \equiv \bar{\Psi}'(1 - q\eta'_\varphi) + \rho_\parallel \bar{F}', \quad \frac{\partial H}{\partial \zeta} = 0. \tag{91}$$

The Hamiltonian form guarantees that the guiding center motion preserves the value of Hamiltonian H, the momentum $\bar{P}_\zeta = P_\varphi$, as well as preserves the phase volume of an ensemble of particles in the parameter space $\theta, \zeta, \bar{P}_\theta, \bar{P}_\zeta$. All variables in these equations are accessible through `ESI`.

E. Approximate Hamiltonian equations for 3-D configurations

In the 3-D case there is no explicit transformation to the canonical coordinates. Nevertheless, the approximate transformation can be easily performed using the fact that

$$\frac{B_a}{B_\varphi} = O\left(\frac{a_0^2}{R^2}\right) \ll 1, \tag{92}$$

where a_0, R are minor and major radii. Here, we assume that the cylindrical azimuth φ serves as a third coordinate in the curvilinear coordinate system a, θ, φ. By introducing a variable ζ

$$\varphi = \zeta - \bar{\zeta}(a, \theta, \varphi), \quad \bar{\zeta} \equiv \int_0^a \frac{\sigma'_a - \nu}{\bar{F} + \sigma'_\varphi} da, \quad \dot{\varphi} = \dot{\zeta} - \bar{\zeta}'_a \dot{a} - \bar{\zeta}'_\theta \dot{\theta} - \bar{\zeta}'_\varphi \dot{\varphi}, \tag{93}$$

the magnetic field and vector potential can be written in the form

$$\begin{aligned} \vec{B} &= [(\bar{I} + \sigma'_\theta) - (\bar{F} + \sigma'_\varphi)\bar{\zeta}'_\theta]\nabla\theta + (\bar{F} + \sigma'_\varphi)(\nabla\zeta - \bar{\zeta}'_\varphi \nabla\varphi) \\ &\simeq [(\bar{I} + \sigma'_\theta) - (\bar{F} + \sigma'_\varphi)\bar{\zeta}'_\theta]\nabla\theta + (\bar{F} + \sigma'_\varphi)(1 - \bar{\zeta}'_\varphi)\nabla\zeta, \qquad (94) \\ \vec{A} &= -\bar{\Phi}'\eta\nabla a + \bar{\Phi}\nabla\theta + \bar{\Psi}\nabla\varphi = -\bar{\Phi}'\bar{\eta}\nabla a + \bar{\Phi}\nabla\theta + \bar{\Psi}\nabla\zeta - \nabla(\bar{\Psi}\bar{\zeta}), \qquad (95) \\ \bar{\Phi}'\bar{\eta} &\equiv \bar{\Phi}'\eta + q\bar{\zeta}. \qquad (96) \end{aligned}$$

As a result, the Lagrangian acquires the Hamiltonian form

$$L = -\frac{d}{dt}(\bar{\Phi}'\bar{\eta}) + \bar{P}_\theta \dot{\theta} + \bar{P}_\zeta \dot{\zeta} - H, \tag{97}$$

$$\bar{P}_\theta \equiv \bar{\Phi} + \int_0^a \bar{\Phi}'\bar{\eta}_\theta da + \rho_\parallel[\bar{I} + \sigma'_\theta - (\bar{F} + \sigma'_\varphi)\bar{\zeta}'_\theta], \quad \bar{P}_\zeta = P_\varphi = \bar{\Psi} + \int_0^a \bar{\Phi}'\bar{\eta}_\varphi da + \rho_\parallel(\bar{F} + \sigma'_\varphi)(1 - \bar{\zeta}'_\varphi). \tag{98}$$

Addition of function $\bar{\zeta}$ into the minimal set of basic function of `ESI` allows use of the Hamiltonian form of equation of guiding center motion.

While making variation of L it is necessary to take into account that in `ESI` all functions are given as function of a, θ, φ rather than of a, θ, ζ. The difference is small and could be negligible. Otherwise, it is necessary to use relations

$$\left.\frac{\partial}{\partial a}\right|_{\theta,\zeta} = \frac{\partial}{\partial a} + \frac{\partial \varphi}{\partial a}\frac{\partial}{\partial \varphi}, \quad \left.\frac{\partial}{\partial \theta}\right|_{a,\zeta} = \frac{\partial}{\partial \theta} + \frac{\partial \varphi}{\partial \theta}\frac{\partial}{\partial \varphi}, \quad \left.\frac{\partial}{\partial \zeta}\right|_{a,\theta} = \frac{\partial \varphi}{\partial \zeta}\frac{\partial}{\partial \varphi}, \tag{99}$$

$$\frac{\partial \varphi}{\partial a} = -\frac{\bar{\zeta}'_a}{1 + \bar{\zeta}'_\varphi}, \quad \frac{\partial \varphi}{\partial \theta} = -\frac{\bar{\zeta}'_\theta}{1 + \bar{\zeta}'_\varphi}, \quad \frac{\partial \varphi}{\partial \zeta} = \frac{1}{1 + \bar{\zeta}'_\varphi} \tag{100}$$

in deriving the equation of motion from this Lagrangian.

VII. MHD ENERGY PRINCIPLE

The well-known functional of potential energy in ideal magneto-hydrodynamics (see, e.g., [?])

$$W=\frac{1}{8\pi}\int\left\{\widetilde{\vec{B}}^2+(\vec{\xi}\cdot\nabla\bar{p})(\nabla\cdot\vec{\xi})-\vec{\xi}\times(\nabla\times\vec{B})\cdot\widetilde{\vec{B}}+\gamma_0\bar{p}(\nabla\cdot\vec{\xi})^2\right\}dV,\quad \widetilde{\vec{B}}\equiv(\vec{B}\times(\nabla\times\vec{\xi})), \tag{101}$$

where $\vec{\xi}$ is the test function, does not contain anything that cannot be calculated using basis functions of `ESI`. Also, the kinetic energy term

$$K=\gamma^2\int\rho\vec{\xi}^2dV \tag{102}$$

needs only the metric tensor for its calculation.

At a deeper level, instead of three contravariant components of $\vec{\xi}$

$$\xi^{a,\theta,\zeta}\equiv\left\{\xi,\xi^\theta,\xi^\zeta\right\},\quad \xi\equiv\xi^a \tag{103}$$

another set of test functions is used, i.e, ξ,Λ,X, where

$$X\equiv(\nabla\cdot\vec{\xi}),\quad \Lambda\equiv\bar{\Phi}'\xi^\theta+\bar{\Psi}'\xi^\zeta. \tag{104}$$

In terms of ξ and Λ the perturbation of the magnetic field can be written as

$$J\widetilde{\vec{B}}=\Lambda(\nabla\theta\times\nabla\zeta)-\bar{\Phi}'\xi(\nabla\zeta\times\nabla a)-\bar{\Psi}'\xi(\nabla a\times\nabla\theta). \tag{105}$$

In new variables the potential energy has the form

$$W=\frac{1}{8\pi}\int\left\{\frac{\gamma_0\bar{p}}{\sqrt{g}}X^2+\sqrt{g}\left(\tilde{B}_a\tilde{B}^a+\tilde{B}_\theta\tilde{B}^\theta+\tilde{B}_\zeta\tilde{B}^\zeta\right)-P'\bar{\Psi}'\sqrt{g}\xi^2+[P\bar{\Psi}'\sqrt{g}\xi^2]'_a\right. \tag{106}$$

$$\left.+2(\bar{I}'-\nu'_\theta)\Lambda'_\zeta\xi-2(\bar{F}'-\nu'_\zeta)\Lambda'_\theta\xi+q'(\bar{F}'-\nu'_\zeta)\bar{\Psi}'\xi^2\right\}dad\theta d\zeta. \tag{107}$$

All functions in the integrand can be calculated by `ESI` interface.

VIII. ESI FORMAT OF THE EQUILIBRIUM DATA FILE

The source code of `ESI` is contained in the `esiXZ.c` files (available on w3.pppl.gov/~zakharov), which is complemented by the documentation file `esiXZ.c.d`. This section explains a reference data structure of the input file for `ESI`, as well as a reference layout of the shared memory as an option for communication between `ESI` and user codes. At this moment, `ESI` is operational for 2-D equilibrium configurations. Its source code and design of the data structure are extendible, thus making the `ESI` upgrade to 3-D equilibria, configurations with ergodic magnetic fields or different representations of the vacuum magnetic fields outside the plasma, etc, in a straightforward way. These updates do not affect the previous functionality. The documentation of the code is contained in the documentation file `esiXZ.c.d`, which is maintained by a special software. In fact, `esiXZ.c.d` is updated prior to or together with `esiXZ.c`, what makes it always consistent with the current state of the source `esiXZ.c` file. In particular, `esiXZ.c.d` explains routines, which are only mentioned or skipped in this paper.

All routines, mentioned below, are referenced by their `C`-names. The corresponding `FORTRAN` names are lower case version of `C`-names (in `esiXZ.c` the underscore sign '_' follows the `FORTRAN` callable names).

This section specifies the information and its format, which should be provided by the equilibrium codes in order to be used as an input for `ESI`. In examples below, the `ESC-EEC` code [4, 22] system is used as a generator of data.

A. Interface `ID`

First, we introduce the integer parameter `ID`, which reflects the basic properties of the ESI data and is composed from 5 two decimal digits `'dd'` integers (from 0 till 99), $\mathtt{ID}_a,\mathtt{ID}_\theta,\mathtt{ID}_\phi,\mathtt{ID}_v,\mathtt{ID}_{re}$ as

$$\mathtt{ID}=\mathtt{ID}_{re}*100000000+\mathtt{ID}_v*1000000+\mathtt{ID}_\phi*10000+\mathtt{ID}_\theta*100+\mathtt{ID}_a. \tag{108}$$

ID works as a sort of a 'bar-code' for recognizing data by the ESI code. First, the design of ID distinguishes between data in flux coordinates and in laboratory coordinates: $\mathtt{ID}_a, \mathtt{ID}_\theta, \mathtt{ID}_\phi$ characterize the flux coordinate data inside the plasma, which are ready for use in different plasma physics codes, and $\mathtt{ID}_v$ refers to data in the laboratory coordinates (e.g., generated by the $r-z$ codes) and to data in the vacuum region outside the plasma. Second, the ESI data may contain both the flux and laboratory coordinate output from the equilibrium codes. Otherwise, the ESI interface can generate the flux coordinate data from the laboratory coordinate data.

1. *Radial coordinate* $\mathtt{ID}_a$

The $\mathtt{ID}_a$ is designed to have the structure $\mathtt{ID}_a = 20*i+j$. The index i specifies combination of two general properties of a: $i = 0$ is for dimensional (in absolute units) ρ-like (minor radius like) coordinate a; $i = 1$ is for dimensionless (normalized) ρ-like (minor radius like) coordinate a; $i = 2$ is for dimensional V-like (volume-like) coordinate a; $i = 3$ is for normalized V-like (volume-like) a. The value $i = 4$ remains reserved.

The index $0 \le j \le 19$ determines the physics meaning of a. Some of useful cases, implemented in ESC-EEC, are specified in the Table II (e.g., vertical size, volume, magnetic fluxes, etc). The j-values $6 < j \le 19$ are reserved for unspecified choices of radial coordinate.

$\mathtt{ID}_a$ of radial coordinate a in ESI				*Table II*
$\mathtt{ID}_a$	a	$\mathtt{ID}_a$	a	Comment
0	$a = \sqrt{S}$	20	$a = \sqrt{\frac{S}{S_{boundary}}}$	S is the area of poloidal cross-section.
40	$a = S$	60	$a = \frac{S}{S_{boundary}}$	
1	$a = a_{ref}\sqrt{\frac{V}{V_{ref}}}$	21	$a = \sqrt{\frac{V}{V_{boundary}}}$	V is a volume of magnetic surface, a_{ref} [m], V_{ref} [m^3] are some dimensional reference numbers.
41	$a = V$	61	$a = \frac{V}{V_{boundary}}$	
2	$a = a_{ref}\sqrt{\frac{L}{L_{ref}}}$	22	$a = \sqrt{\frac{L}{L_{boundary}}}$	L is the inductance of the vacuum toroidal magnetic field $L \equiv \int \frac{drdz}{5r}$ inside the magnetic surface, a_{ref} [m], L [m^{-1}].
42	$a = L$	62	$a = \frac{L}{L_{boundary}}$	
3	$a = \sqrt{\frac{\Phi}{\pi B_{ref}}}$	23	$a = \sqrt{\frac{\Phi}{\Phi_{boundary}}}$	Φ is a volume of magnetic surface, B_{ref} [T] is some dimensional reference numbers (ASTRA code).
43	$a = \Phi$	63	$a = \frac{\Phi}{\Phi_{boundary}}$	
4	$a = b$	24	$a = \frac{b}{b_{boundary}}$	b is a vertical semiaxis of the cross-section of the magnetic surfaces
44	$a = b^2$	64	$a = \frac{b^2}{b^2_{boundary}}$	
5	$a = \sqrt{\frac{\Psi}{\pi B_{ref}}}$	25	$a = \sqrt{\frac{\Psi}{\Psi_{boundary}}}$	Ψ is a volume of magnetic surface, B_{ref} [T] is some dimensional reference numbers (ASTRA code).
45	$a = \Psi$	65	$a = \frac{\Psi}{\Psi_{boundary}}$	

TABLE II: Radial $\mathtt{ID}_a$ for some radial coordinates used in 2-D equilibrium codes

The use of "V"-like radial coordinates is discouraged because of possible singularities in first derivatives of space functions at the magnetic axis.

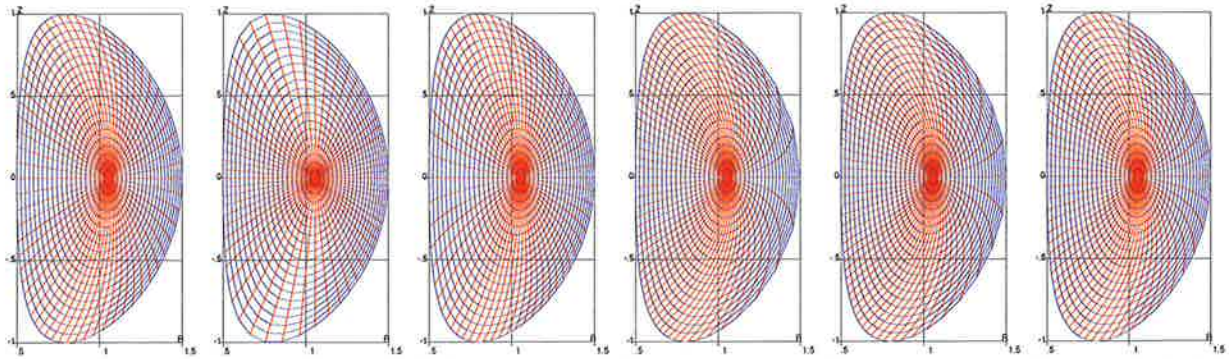
2. *Poloidal angle* $\mathtt{ID}_\theta$

The next Table III introduces the numerical identification number $0 \le \mathtt{ID}_\theta \le 99$ depending on the choice of the poloidal angle. The capital letters in the name stand for different coordinate systems and can be used for as a part of the data file names.

Fig. 2 illustrates the flux coordinates with different choices of poloial angle in an example of a spherical tokamak configuration.

$\mathtt{ID}_\theta$ **of poloidal angle** θ		*Table III*
$\mathtt{ID}_\theta$	Name	Specific property
	E-ESC	a, θ, φ, $r = r(a,\theta)$, $z = z_0(a) - b(a)\sin\theta$
1	K-KINX, polar	$r = r_0 + \rho(a,\theta,\phi)\cos\theta$,$z = z_0 + \rho(a,\theta,\phi)\sin\theta$
2	H-Hamada	$J = J(a)$
3	P-PEST	a, θ, φ, $J = f(a)r^2$
4	B-Boozer	SFL $a, \bar{\theta}, \bar{\phi}$ with $\eta = 0$ and $J = \frac{f(a)}{\lvert B\rvert^2}$
5	U-Equidistant	$g_{\theta\theta} = g_{\theta\theta}(a)$
6	V-VMEC-like	coordinates with separation of odd and even harmonics in Fourier representation of r, z in Eq.(1)
7	C-Canonical	$a, \hat{\theta}, \hat{\phi}$, Eqs.(71,73)
9	U-General	unspecified poloidal coordinates in Eq.(1)

TABLE III: Poloidal $\mathtt{ID}_\theta$ for different choices of poloial angle



(a) ID=0000000023 (b) ID=0000000123 (c) ID=0000000223 (d) ID=0000000323 (e) ID=0000000423 (f) ID=0000000723

FIG. 2: Typical coordinate systems for equilibrium configurations: a) ECS coordinates, b) KINX (polar) coordinates, c) Hamada coordinates, d) PEST coordinates, e) Boozer coordinates, f) Canonical coordinates

3. *Toroidal angle* $\mathtt{ID}_\phi$

At present, for the toroidal angle $0 \le \mathtt{ID}_\phi \le 99$ only a few values are recommended

$\mathtt{ID}_\varphi$ **of toroidal angle** ϕ		*Table IV*
$\mathtt{ID}_\phi$	ϕ	Comment
0		2D case, ϕ is ignorable coordinate
1	ϕ	cylindrical azimuth in 3-D case
2	$\bar{\zeta}$	$\bar{\theta}, \bar{\zeta}$ are straight field line angles
3	$\hat{\phi}$	$\hat{\theta}, \hat{\phi}$ canonical angles
9	$\zeta \ne \phi$	general, unspecified ζ

TABLE IV: $\mathtt{ID}_\phi$ of toroidal angle

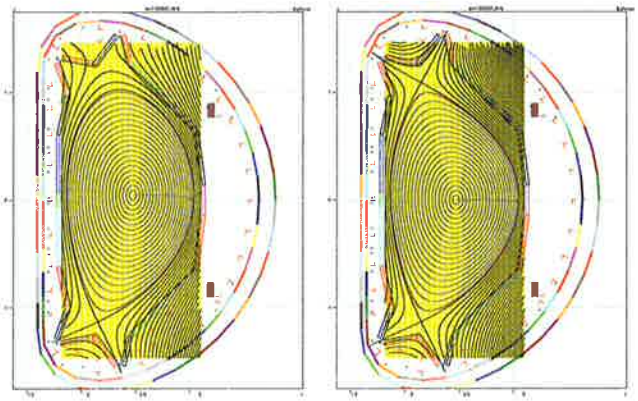
4. $\mathtt{ID}_v$ *for free boundary equilibria and vacuum fields*

Free boundary equilibrium codes are widely used for plasma control and equilibrium reconstruction in real machines, as well as for designing new devices. EFIT is a famous example. Their data are generated on $r - z$ grid, which is not

conformal to the magnetic field. The example is given in Fig. 3, where EAST equilibrium configuration is calculated by a $r-z$ routine of ESC-EEC. The ID for these data would be 1000000.

Other codes use a conformal mapping for generating a laboratory coordinate system. In both cases, a conversion into flux coordinates is necessary for using the equilibrium data in stability and transport simulation codes. In the Table V the values $1 \leq \mathtt{ID}_v \leq 9$ are reserved for this kind of data.

Because of importance for tokamak physics of the edge (pedestal) layer near the plasma boundary, it may have a special representation in flux coordinates, different from the plasma core. One example is ESC-EEC code, where the edge equilibrium code EEC uses the Hermite finite elements, while the core equilibrium code ESC used Fourier harmonics.



(a) (b)

FIG. 3: Examples of EAST free boundary equilibrium configurations with (a) single and (b) double null separatrixes calculated by ESC-EEC on $r-z$ grid.

These kind of data are represented by $10 \leq \mathtt{ID}_v \leq 19$. The values $20 \leq \mathtt{ID}_v \leq 29$ are reserved for vacuum region representations. The data on the vacuum field outside the plasma may or may not be present, and the $\mathtt{ID}_v$ reflects this.

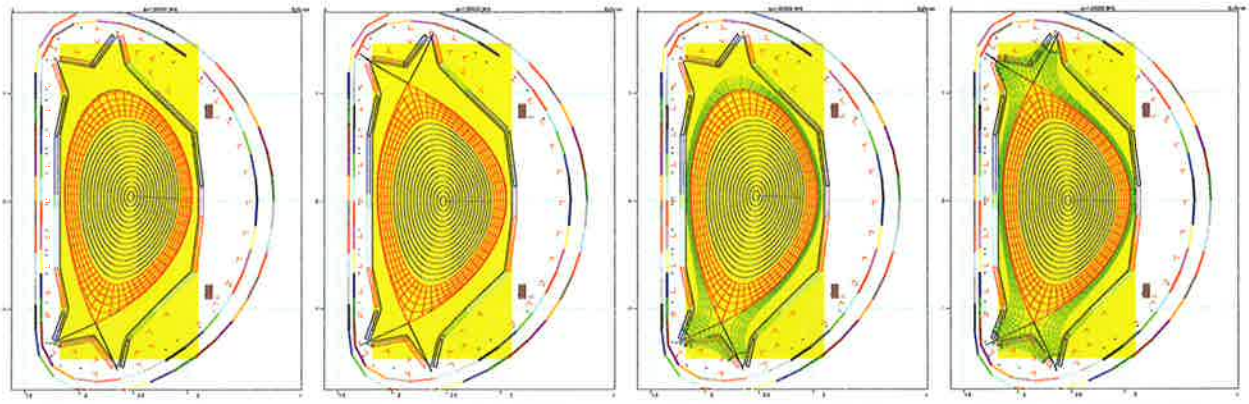
Some recommended values of $\mathtt{ID}_v$ are listed in Table V. It is expected that the presence of stochastic perturbations will be in calculations.

$\mathtt{ID}_v$ **for free boundary and vacuum data**	***Table V***
$\mathtt{ID}_v$	Comment
01	$r-z$ data (EFIT, DINA, CORSICA) in a rectangle domain
02	HELENA data in curvilinear laboratory coordinates
03-09	reserved for other laboratory coordinate data
10	2-D data for the edge layer in flux coordinates (ESC-EEC)
11-19	reserved for edge layer (Pedestal)
20	2-D data for Scrape Off Layer (SoL)in flux coordinates (ESC-EEC)
21-39	reserved for other SoL representations
40-59	reserved for both Pedestal and SoL layer representations
60-79	reserved of 3-D equilibrium perturbations
80-99	reserved for 3-D ergodic components and stochastic fields

TABLE V: $\mathtt{ID}_v$ for data on free boundary equilibrium and vacuum fields

5. $\mathtt{ID}_{re}$ *for future extensions*

The ESI interface is extensible and may include in future the data describing the evolution of the magnetic configurations or equilibrium reconstructions. These data are complimentary to the mentioned ones. For this reason a



(a) ID=00,10,00,00,23 (b) ID=00,10,00,00,23 (c) ID=00,40,00,00,23 (d) ID=00,40,00,00,23

FIG. 4: Magnetic filed lines and grid in the vacuum region outside the plasma

special $\texttt{ID}_{re}$ is reserved for their future specifications.

B. Data groups and Records in the structure of ESI data files

Both ASCII and binary files are suitable for storing the ESI data file. The human readable ASCII files contain the structural information and information on plasma parameters and radial profiles. The 2- or 3-D data can be stored in a ASCII form file, or in a stream-like binary data file. In the case of binary storage, the ASCII file specifies the name and the address of data in the stream.

The suggested names of the data files are constructed as `esiE.00` for ASCII data-file, or `esiE.00b` for binary data-file. The extension `.00` specifies the equilibrium sequence number. The binary data has `b` at the end of the extension.

Every equilibrium code of a general use should be capable of producing data and creating the ESI data files. This subsection specifies the format of the ASCII file, which should be created by individual equilibrium codes in order to be processed by ESI interface routines.

The ASCII ESI file consists of a number of groups of records. Each group starts with an identification Head-line, which has the following format

$$\texttt{<Group name>[Number of records [@address : }\underbrace{\textit{name of stream data file}}_{\text{optional}}\texttt{]](reading format)}$$

optional

Here, `<Group name>` is a predefined name of the group (listed below), then in `[...]`, the Head-line specifies the number of records, and optionally after '`@`' the starting address (in terms of bytes) of data, ending with '`:`', and then, an optional binary file name. If the file name is absent, the last opened file is assumed. The records in each group have the same data reading format, which is specified inside '`()`' parentheses.

The reading format serves two purposes: (a) it specifies the type of each data to be read, and (b) the number of items in a single record. At present, three data types are suggested: `%e` for `double`, `%d` for `int`, and `%s` for character strings. The text elements between this symbols in the format string are processed literally. The special symbol $'<'$ in the reading format indicates that the data in the records are read as a data stream. If the symbol $'<'$ is absent, the data are read according to the format per record.

The following example demonstrates the functionality of the format line:

```
(%d %d x %d %d %e 5%e %e(I.A) %s)
```

This line specifies a record, containing 2 `int` data, a character '`x`', 2 `int`, 7 `double` with last one having Units Amperes of the current, and a string data, thus, 12 data per record.

```
[65](%e <)
```

This line specifies a record read as a stream with 65 `double` data.

The comments can be freely distributed outside or between the groups of data. The single line comments with the leading '`!`' can be placed between the records.

1. Data groups for flux coordinates

Two-dimensional equilibria in flux coordinates represents a basic type of `ESI` interface. It contains several scalar data, 4 radial profile data, and 3 data sets for 2-D functions. The 3-D equilibria are represented by a complementary group of data for 3-D functions.

The first significant line in the `ESI` data file, corresponding to the first group of data, specifies the basic information on flux coordinate data. A representative example can be given by the beginning of an `ESI` ASCII file for a tokamak equilibrium calculated by `ESC-EEC` code system

```
!!! Do not edit this file
<ESI dimensions>[1](%d x %d %d %e %e %s) Date: 03/09/14 at 20:16
!Nq1 x Na1     ID  Rext  RBtor          Name |  Btor   Ipl  - this is a comment starting with !
  65 x  21 000002 2.448  2.448           ESC   1.000 1.000  - after-record comment (after Name)
<ESI [gq]>[65](%e <)
```

Here '`<ESI dimensions>`' is the predefined name of the very first group of `ESI` file, '`[1]`' means 1 as the number of records in the group. The string '`(%d x %d %d %e %e %s)`' specifies the format for reading each record (3 integers with '`x`' between the first two, two double numbers, and one string), as explained earlier. What follows the Head information (the date in the example) is a comment, ignored by the reading routine.

The following line, starting with '`!`' is also a comment. This kind of comments can also be placed between the separate records. The next line contains the data itself.

The full set of the groups names and their data are given in Tables VI-XIII.

Note, that only first 6 parameters, out of 11 listed in Table VI, are present in the example. Others are optional and are filtered out by the format line if present. They can be accepted by `ESI` if the format line will be extended for reading more data in the order specified in Table VI.

Groups 0-2: basic parameters					*Table VI*
C name	Type	Format	Math	#	Group name `<ESI dimensions>`
`Np1`	`int`	%d	$N_\theta + 1$	0	number of polodial grid points
`x`	`char`	`x`		0	separator between $N_p + 1$ and $N_a + 1$
`Na1`	`int`	%d	$N_a + 1$	0	number of radial grid points
`ID`	`int`	%d		0	`ID` of `ESI` data
`Rext`	`double`	%e	R_{ext}	0	reference major radius
`rBtor`	`double`	%e	$\bar{F}_{ref} \equiv \bar{F}(a_{ref})$	0	rB_ϕ outside the plasma
`ESI`	`char[]`	%s		0	Name of the code
`Btor`	`double`	%e	B_{tor}	0	optional
`Ipl`	`double`	%e	I_{plasma}	0	optional
`bsp1`	`double`	%e	$\bar{p}_{boundary}$	0	optional
`aref`	`double`	%e	a_{ref}	0	optional
`Vref`	`double`	%e	V_{ref}	0	optional
C name	Type	Format	Math	#	Group name `<ESI [gq]>`
`gq[Np1]`	`double`	%e	θ_j	1	grid value of poloidal angle
C name	Type	Format	Math	#	Group name `<ESI [sa]>`
`sa[Na1]`	`double`	%e	a_i	2	grid value of radial coordinate

TABLE VI: Data structure of group 0,2

In the above example the line with a record of the radial coordinate data `<ESI [gq]>[65](%e)` shows a 65 records with a single items.

The following group 3 (Table VII) is informational. These data are initialized by `ESI` after reading the set of basic data.

Group 3: Auxiliary profiles					*Table VII*
C name	Type	Format	Math	#	Group name <ESI [baF bsp gF gY]>
aF [Na1]	double	%e	$\bar{F}(a_i)$	3	Poloidal current or rB_ϕ [m·T]
bsp[Na1]	double	%e	$\bar{p}(a_i)$	3	plasma pressure $\mu_0 p$ [MPa]
gF [Na1]	double	%e	$\Phi(a_i)$	3	Toroidal flux through the magnetic surface, [Vs]
gY [Na1]	double	%e	$\Psi(a_i)$	3	Poloidal flux through the magnetic surface, [Vs]

TABLE VII: Data structure of group 3

The groups 4,5 (Table VIII) gives a list of basic radial profiles. In the case of V-like radial variable the fluxes derivatives in group 5 are represented by $\bar{\Phi}'(a), \bar{\Phi}''(a), \bar{\Psi}'(a), \bar{\Psi}''(a)$.

Groups 4,5: Basic profiles					*Table VIII*
C name	Type	Format	Math	#	Group name <ESI aT aTa aP aPa>
T [Na1]	double	%e	$T(a_i)$	4	
Ta[Na1]	double	%e	$T'(a_i)$	4	
P [Na1]	double	%e	$P(a_i)$	4	
Pa[Na1]	double	%e	$P'(a_i)$	4	
C name	Type	Format	Math	#	Group name <ESI bgFa bgFaa bgYa bgYaa>
gFa [Na1]	double	%e	$\left(\frac{\bar{\Phi}'}{a}\right)(a_i)$	5	
gFaa[Na1]	double	%e	$\left(\frac{\bar{\Phi}'}{a}\right)'_i$	5	
gYa [Na1]	double	%e	$\left(\frac{\bar{\Psi}'}{a}\right)(a_i)$	5	
gYaa[Na1]	double	%e	$\left(\frac{\bar{\Psi}'}{a}\right)'_i$	5	

TABLE VIII: Data groups 4, 5: basic profile data

```
<ESI T Ta P Pa>[21](%e %e %e %e)
!                    T                    T'_a                    P                    P'_a   #
 1.9846424244460485e+00  1.3405943022348765e-14  8.0619056626615754e-02  2.1764431728238866e-16   0
 1.9796808182902292e+00 -1.9846424571701443e-01  8.0417508981202174e-02 -8.0619057955919875e-03   1
```

The following 4 groups of records, listed in Table IX are common for 2-D and 3-D cases. Each record consists of 4 data, representing the function, its radial, poloidal and mixed derivatives as in shown in the following example

```
<ESI r ra rq raq>[1365](%e %e %e %e)
!                    r                    r'_a                   r'_gq                 r''_{a,gq}  ia  jq
  2.4808030305575612e+00  6.2827195890545617e-01 -0.0000000000000000e+00 -5.8754587638547547e-03   0   0
  2.4808030305575612e+00  6.2467076203297478e-01 -0.0000000000000000e+00 -6.7428587585144528e-02   0   1
```

Group 6-8: Basic functions of coordinates comon for 2- and 3- cases					*Table IX*
C name	Type	Format	Math	#	Group name <ESI r ra rq raq>
r [Nt1][Na1][Np1]	double	%e	$r(a_i, \theta_j, \phi_k)$	6	cylindrical radius
ra [Nt1][Na1][Np1]	double	%e	$r'_a(a_i, \theta_j, \phi_k)$	6	
rq [Nt1][Na1][Np1]	double	%e	$r'_\theta(a_i, \theta_j, \phi_k)$	6	
raq[Nt1][Na1][Np1]	double	%e	$r''_{a\theta}(a_i, \theta_j, \phi_k)$	6	
same for $z, z'_a, z'_\theta, z''_{a\theta}$				7	Group name <ESI z za zq zaq>
same for $\|B\|, \|B\|'_a, \|B\|'_\theta, \|B\|''_{a\theta}$				8	Group name <ESI B Ba Bq Baq>

TABLE IX: ESI data structure of group 6-8

Functions $\Phi, \Psi, \bar{F}, \bar{p}$ in Table VII are calculated during the initialization of ESI. Indexes i, j, k are used for the mesh points along a, θ, ϕ correspondingly

$$0 \le i \le N_a, \quad 0 \le j \le N_\theta, \quad 0 \le k \le N_\phi. \tag{109}$$

Multidimensional arrays in Tables IX are equivalent to a 1-D array referenced as `[(k*Na1+i)*Np1+j]`. In the 3-D case the following storage, listed in Table X is added for derivatives with respect to ϕ.

The 3-D case requires additional data on multidimensional functions, which are listed in Table X as groups 9-12. The record format is the same as in the previously described groups.

Group 9-12: Basic functions of coordinates specific for 3-D case					*Table X*
C name	Type	Format	Math	#	Group name<ESI [gz]>
gz [Nt1]	double	%e	ϕ_k	9	
C name	Type	Format	Math	#	Group name<ESI rz raz rqz raqz>
rz[Nt1][Na1][Np1]	double	%e	$r'_\phi(a_i, \theta_j, \phi_k)$	10	
raz[Nt1][Na1][Np1]	double	%e	$r''_{a\phi}(a_i, \theta_j, \phi_k)$	10	
rqz[Nt1][Na1][Np1]	double	%e	$r''_{\theta\phi}(a_i, \theta_j, \phi_k)$	10	
raqz[Nt1][Na1][Np1]	double	%e	$r'''_{a\theta\phi}(a_i, \theta_j, \phi_k)$	10	
same for $z'_\phi, z''_{a\phi}, z''_{\theta\phi}, z'''_{a\theta\phi}$				11	Group name <ESI zz zaz zqz zaqz>
same for $\lvert B\rvert'_\phi, \lvert B\rvert''_{a\phi}, \lvert B\rvert''_{\theta\phi}, \lvert B\rvert'''_{a\theta\phi}$				12	Group name <ESI Bz Baz Bqz Baqz>

TABLE X: ESI data structure of group 9-12: addition storage for 3-D cases

The resulting total size of ESI data for the basic groups 0-12 is

```
3*sizeof(int)+(7+13*Na1+Np1+Nt1+24*Na1*Np1*Nt1)*sizeof(double)
```

and, e.g., for `Na1=21,Np1=65,Nt1=33` this is equal to 8,651,676 bytes only, which shows the compactness of ESI.

In specific cases some groups of ESI data could be dropped or not used. A special array in the ESI code keeps addresses and sizes of these groups. It marks the absent groups by zero size.

C. Data structure for free boundary equilibria

Equilibria calculated on $r-z$ grids are widely used for controlling plasma configurations and reconstructing plasma parameters in real time. Here only a minimal set of groups for free-boundary $r-z$ equilibria is introduced leaving for future (or for other interfaces) more specifications.

D. ESI data in the plasma edge layer

The edge equilibrium code EEC was developed as an extension of ESC for representation of equilibrium configuration in flux coordinates using finite elements in the cases when a separatrix determines the plasma boundary. The edge equilibrium is interfaced with the core equilibrium from ESC at a virtual boundary whose geometry is adjusted to provide the continuity of the solution and its first derivatives across the virtual boundary. The EEC data mimic the data of the basic groups 0-8 and have the same names of the groups with a prefix EDGE.

Figs. 4a),b) show two examples of EAST plasma equilibrium configurations with one and two X-points respectively generated by ESC-EEC code in flux coordinates. The data ID = 0010000023 indicates that the data are 2-D data for the plasma edge with the radial coordinate $a = \sqrt{\frac{\Phi}{\Phi_{boundary}}}$ and the poloidal angle θ_{ESC} in the core.

In the ESI data file, the data generated by EEC code for the plasma edge follows data groups 0-8 for the plasma core. The beginnings of the first three records in this layer are shown below. These records describe the number of radial and poloidal intervals in the plasma edge.

```
<EDGE ESI dimensions>[1](%d x %d  %e %s) Date: 03/06/14
!Nq1 x nBL1    RBtor          Name |  - this is a comment starting with !
  65 x   9     6.223           EEC    - after-record comment (after Name)

<EDGE ESI [gq]>[65](%e <)
```

Groups 13-17: Equilibrium data on $r-z$					*Table XI*
C name	Type	Format	Math	#	Group name<RZ ESI dimensions>
Nr1	int	%d	N_r+1	13	number of grid points in r-direction
x	char	x		13	separator between N_r+1 and N_z+1
Nz1	int	%d	N_z+1	13	number of grid points in z-direction
ID	int	%d		13	ID of ESI data
Rext	double	%e	R_{ext}	13	Reference major radius
RBtor	double	%e	$\bar{F}_{TFC}$	13	Vacuum magnetic field outside the plasma
ESC	char[]	%s		13	name of the code
Btor	double	%e	B_{tor}	13	optional, reference toroidal field
Ipl	double	%e	I_{plasma}	13	optional, plasma current
R1	double	%e	R_1	13	optional, inner r of calculation box
Z1	double	%e	Z_1	13	optional, lower z of calculation box
R2	double	%e	R_2	13	optional, outer r of calculation box
Z2	double	%e	Z_2	13	optional, upper z of calculation box
C name	Type	Format	Math	#	Group name <RZ ESI O- B-points>
r,z,gY	double	3%e	r, z, Ψ	14	r_0, z_0, Ψ_0 of magnetic axis, r_b, z_b, Ψ_b of boundary control points
C name	Type	Format	Math	#	Group name <RZ ESI X-points>
r,z,gY	double	3%e	r, z, Ψ	15	r_X, z_X, Ψ_X of X-points, where $B_{pol}=0$
C name	Type	Format	Math	#	Group name <RZ ESI r grid>
r[Nr1]	double	%e	r_i	16	grid values of $r-$ coordinate
C name	Type	Format	Math	#	Group name <RZ ESI z grid>
z[Nz1]	double	%e	z_j	17	grid values of $z-$ coordinate
C name	Type	Format	Math	#	Group name<RZ ESI gY gYr gYz gYrz>
gY[Nr1][Nz1]	double	%e	$\Psi(r_i, z_j)$	17	Poloidal flux at the calculation grid
gYr[Nr1][Nz1]	double	%e	$\Psi'_r(r_i, z_j)$	17	Radial derivative Ψ'_r
gYz[Nr1][Nz1]	double	%e	$\Psi'_z(r_i, z_j)$	17	Vertical derivative Ψ'_z
gYrz[Nr1][Nz1]	double	%e	$\Psi''_{rz}(r_i, z_j)$	17	Mixed second derivative Ψ''_{rz}

TABLE XI: Data structure for free boundary equilibria on $r-z$ grid

```
  0.0000000000000000e+00  9.8174770424681035e-02  1.9634954084936207e-01  2.9452431127404310e-01
  3.9269908169872414e-01  4.9087385212340517e-01  5.8904862254808621e-01  6.8722339297276724e-01
        ...                     ...                     ...                     ...
<EDGE ESI [sa]>[9](%e <)
  8.0000000000000004e-01  8.2500000000000007e-01  8.5000000000000009e-01  8.7500000000000000e-01
  9.0000000000000002e-01  9.2500000000000004e-01  9.4999999999999996e-01  9.7499999999999998e-01
  1.0000000000000000e+00
```

The rest of the data on r, z, B and their derivatives follow the same format as the data for the core.

E. Flux coordinate data in vacuum region

Plasma flows in the Scrape Off Layer (SoL) outside the plasma boundary are highly anisotropic and directed predominantly along the open field lines. Accordingly, the flux coordinate representation for the vacuum magnetic fields has its value for simulation of the plasma losses and energy deposition on the plasma facing components.

The vacuum field data groups mimic the data of the basic groups 0-8 and have the same names with a prefix Vac.

Figs. 4c),d) show vacuum configurations generated by ESC-EEC code in flux coordinates for two examples of the EAST plasma equilibria. The data ID = 0040000023 indicates that the in addition to the plasma edge, the vacuum magnetic configurations is represented in flux coordinates.

The data for the SoL follow after the date in the edge region. The first record describes the number of X-points and the number of topological regions.

```
<Vac ESI dimensions>[1](%d %d %s) Date: 03/06/14 at 17:19
```

Groups 18-23: Equilibrium in the plasma edge layer					*Table XII*
C name	Type	Format	Math	#	Group name<EDGE ESI dimensions>
Nq1	int	%d	$N_\theta + 1$	18	number of grid points in θ-direction
x	char	x		18	separator between $N_r + 1$ and $N_z + 1$
nBL1	int	%d	$N_{BL} + 1$	18	number of grid points in a-direction
RBtor	double	%e	$\bar{F}_{TFC}$	18	Vacuum magnetic field outside the plasma
EEC	char[]	%s		18	name of the code
C name	Type	Format	Math	#	Group name <EDGE ESI [gq]>
gq[Nq1]	double	%e	θ_j	19	θ - poloidal angle in the boundary layer
C name	Type	Format	Math	#	Group name <EDGE ESI [sa]>
sa[nBL1]	double	%e	a_i	20	a - radial coordinate in the boundary layer
C name	Type	Format	Math	#	Group name <EDGE ESI r ra rq raq>
r[][Nq1],ra[][Nq1],rq[][Nq1],raq[][Nq1]	double	4%e	$r, r'_a, r'_q, r''_{a\theta}$	21	$r, r'_a, r'_q, r''_{a\theta}$ for grid points
C name	Type	Format	Math	#	Group name <EDGE ESI z za zq zaq>
z[][Nq1],za[][Nq1],zq[][Nq1],zaq[][Nq1]	double	4%e	$z, z'_a, z'_q, z''_{a\theta}$	22	$z, z'_a, z'_q, z''_{a\theta}$ for grid points
C name	Type	Format	Math	#	Group name <EDGE ESI B Ba Bq Baq>
B[][Nq1],Ba[][Nq1],Bq[][Nq1],Baq[][Nq1]	double	4%e	$B, B'_a, B'_q, B''_{a\theta}$	23	$B, B'_a, B'_q, B''_{a\theta}$ for grid points

TABLE XII: Data structure for the plasma edge (Pedestal)

```
! nX  nRg            Name |  - this is a comment starting with !
   1    2         ESC-EEC - after-record comment (after Name)
```

Then it is the basic information of each region, including the index of the region, the number of radial and poloidal points, and the range of radial and poloidal coordinates. Here $\texttt{gq0} \le \theta \le \texttt{gq1}$ are normalized by 2π.

```
<Vac ESI Vacuum Regions>[1](%d %d %d %e %e %e %e)
!Rg# Nq1 Na1    aX      aVac       gq0/2gp      gq1/2gp
   0  77   6  1.400  1.000        -0.060        1.060
```

The data format of r, z, B and their derivatives are the same as described in the plasma core and plasma edge layer.

In conclusion of data description, note that the ESI *format is suitable for real time inter-process communications between equilibrium and other codes, using shared memory, message passing, etc.*

IX. BASIC SET OF ESI ROUTINES

The prototypes of ESI C-routines for the user's side (some not yet available) are listed in Table XIV. The non-descriptive names of variables are constructed using the following conventions: 'g' prefixes the name of Greek math variables, 'b' prefixes "barred" variables, 'd' prefixes time derivatives, and names with 'a','q''z' after the symbol of are used for derivatives. FORTRAN-callable analogs of C-routines have the same names with capital letters replaced by lower case ones.

Except for different initialization, the use of ESI routines is independent on the storage of the data.

More complete information is given in the escXZ.c.d document file (which also contains this text as a part of it). At present ESI is functional with Equilibrium and Stability Code (ESC) for axisymmetric tokamak equilibrium configurations. ESC is interfaced with the transport simulation ASTRA code using ESI through the shared memory, and using the data files with a number of author's codes.

A. Service routines of ESI.

Some available and possible routines are listed in Table XVI. The set of service routines can be expanded with more practice.

Groups 24-29: Vacuum configuration in flux coordinates					*Table XIII*
C name	Type	Format	Math	#	Group name<Vac ESI configuration>
nX	int	%d	N_X	24	number of X-points
nReg	int	%d	N_{reg}	24	number of topological regions
EEC	char[]	%s		24	name of the code
C name	Type	Format	Math	#	Group name<Vac ESI dimensions>
iReg	int	%d	i_{Reg}	25	index of the region
Nq1	int	%d	$N_\theta + 1$	25	number of poloidal θ points
Na1	int	%d	$N_a + 1$	25	number of radial θ points
aX	double	%d	a_X	25	a-value at the plasma boundary (separatrix)
aVac	double	%d	a_{Vac}	25	a-value of the outmost field line in the region
bgq0	double	%d	$\theta_0/2\pi$	25	minimum value of θ in the region
bgq1	double	%d	$\theta_1/2\pi$	25	maximum value of θ in the region
C name	Type	Format	Math	#	Group name <Vac ESI [gq]>
gq[Nq1]	double	%e	θ_j	26	θ - poloidal angle in the vacuum region
C name	Type	Format	Math	#	Group name <Vac ESI [sa]>
sa[Na1]	double	%e	a_i	27	a - radial coordinate in the vacuum region
C name	Type	Format	Math	#	Group name <Vac ESI r ra rq raq>
r[][Nq1],ra[][Nq1],rq[][Nq1],raq[][Nq1]	double	4%e	$r, r'_a, r'_q, r''_{a\theta}$	28	$r, r'_a, r'_q, r''_{a\theta}$ for grid points
C name	Type	Format	Math	#	Group name <Vac ESI z za zq zaq>
z[][Nq1],za[][Nq1],zq[][Nq1],zaq[][Nq1]	double	4%e	$z, z'_a, z'_q, z''_{a\theta}$	29	$z, z'_a, z'_q, z''_{a\theta}$ for grid points
C name	Type	Format	Math	#	Group name <Vac ESI B Ba Bq Baq>
B[][Nq1],Ba[][Nq1],Bq[][Nq1],Baq[][Nq1]	double	4%e	$B, B'_a, B'_q, B''_{a\theta}$	30	$B, B'_a, B'_q, B''_{a\theta}$ for grid points

TABLE XIII: Data structure for the vacuum configuration

B. ESI as a structure.

In fact, the Tables VI-X show the necessary elements of a single C data-structure which is typedefined as ESIstruct. The user can work simultaneously with several of them (from 0 to 7), e.g., for comparison of different codes. But only one structure is functional at the ESI side. By default the ESI[0] is activated. Using the call

```
i=ESI2up(1);
```

one can switch between active structures.

C. ESI as a virtual machine.

In a primitive manner, ESI can mimic the "virtual machine" approach of OpenGL. A particular service, like calculation of function $|B|$, η, or graphics output can be activated any time by using

```
i=esiEnable(esiGL,NULL);
i=esiEnable(esiBASIS,ESIB);
i=esiEnable(esiBASIS,ESIgh);
```

and disabled by

```
i=esiDisable(esiGL ,NULL);
i=esi2Disable(esiBASIS,ESIB);
```

when it is not needed anymore. By default all calculations corresponding to a predefined parameter esiBASIS are activated.

The full set of possibilities is specified ESI documentation file esiXZ.c.d.

For the use of control parameters of a ESI *virtual machine the definition file, e.g.,* esiXZ.h, *(or* esiXZ.inc *for FORTRAN) should be created and included into the user source code. Its content is specified in the* ESI *source file* esiXZ.c.

Minimum set of ESI routines. Marked by * are not yet available		*Table XIV*
example of C call	*	Comment
`i=File2ESC(FNm);`		`'FNm'` is the name of the ESI data-file.
`i=FreeESI();`		frees the memory allocated for ESI by `File2ESC()`.
`i=FShM2ESC(key);`		`'key'` is the ID of the shared memory segment with ESI data
`i=Link2ESC(F,Fa ,gFa,gFaa ,gYa,gYaa ,T,Ta ,P,Pa ,r,ra,rq,z,za,zq ,B,Ba,Bq ,gh,gha,ghq,isw);`		Called once, it sends to ESI the addresses of arrays, which will contain values of the basic functions. `isw` is the integer array which could be necessary for marking the particles.
`i=ESI2all(a,gq,n);`		The main reconstruction routine, which calculates the basic functions for n particles in positions given by `a[i],q[i]`.
`i=ESI2PlP(F,Fa ,gFa,gFaa ,gYa,gYaa ,T,Ta ,P,Pa,a,n);`		Puts the values of plasma profiles $\bar{F}, \bar{F}', \bar{\Phi}', \bar{\Phi}'', \bar{\Psi}', \bar{\Psi}'', T, T', P, P'$ into arrays `F[]`, `Fa[]`, `gFa[]`, `gFaa[]`, `gYa[]`, `gYaa[]`, `T[]`, `Ta[]`, `P[]`, `Pa[]` for n points specified in `a[]`.
`i=ESI2bsp(bsp,bspa ,a,n);`		Puts the values of $\bar{p}, \bar{p}'$ into arrays `bsp[]`, `bspa[]` for n points specified in `a[]`.
`i=ESI2gFgY(gF,gY ,a,n);`		Puts the values of magnetic fluxes Φ, Ψ (un-barred) into arrays `gF[]`, `gY[]` for n points specified in `a[]`.
`i=ESIrz2agq(a,gq ,r,z,ierr,n);`		Converts n cylindrical coordinates r, z into a, θ. `ierr[i]` is the array of errors for every point with the following values: 0 - success, 1 - point $r[i], z[i]$ is out of plasma, 2 - failure in convergence to $a[i], \theta[i]$
`i=rzESI2agq(ID ,na,nq);`	*	Converts original ESI data on $r-z$ grid into ESI data in nested flux coordinates specified by the identification number `ID` with `na,nq` radial and poloidal intervals.
`i=ESI2gcm(dgr,da ,dgq,dgf ,gr,a,gq,gm,n);`	2D	Time advancing routine for guiding center motion. It calculates the time derivatives $\dot{\rho}_{\|}, \dot{a}, \dot{\theta}, \dot{\varphi}$ in Eq.(70) for n particles. `gm[]` contains magnetic moments of the particles. Integer marker `isw[]` is used behind the scene. *Only 2-D version is available.*
`i=ESI2mfl(dgqL,dgfL ,a,gq,n);`	2D	Calculates derivatives of θ_l', φ_l' in Eq.(61) with respect to length l along n magnetic field lines. *Only 2-D version is available.*

TABLE XIV: Minimum set of ESI routines

Minimum set of ESI routines for 3D. Marked by * are not yet available		*Table XV*
example of C call	*	Comment
`i=Link2ESI3d(rz,zz ,Bz,ghz);`	*	Specifies additional links for 3-D case.
`i=ESI2all3d(a,gq ,gz,n);`	*	3-D analog of `ESI2all()`.
`i=ESIrzf2agq3d(a,gq ,gz ,r,z,gf,n);`	*	3D version of `ESIrz2agq()`.

TABLE XV: Minimum set of ESI routines for 3D

X. SUMMARY

The described ESI interface has unique properties in being well organized, comprehensive, compact and independent of the computer architecture. For many plasma physics codes it can provide a uniform access to information about magnetic configurations, independent of how this information was created and by what equilibrium code.

Without changing the format of communications, ESI allows one to drop some groups of data if they are not

ESI service routines. Marked by * are not yet available		*Table XVI*
example of C call	*	Comment
`i=ESI2geom(r,ra,rq, z,za,zq, a,gq,n);`		Calculates $r, r'_a, r'_\theta, z, z'_a, z'_\theta$ for n points.
`i=ESI2rzB(r,z,B,a,n);`		Calculates $r, z, \lvert B\rvert$ for n points.
`i=rzESI2gcm(dgr,dr ,dz,dgf ,r,z,gm,n);`		Analog of ESI2gcm() with use of $r-z$ ESI data. Calculates the time derivatives $\dot{\rho}_\parallel, \dot{r}, \dot{z}, \dot{\varphi}$ for guiding center motion for n particle specified by their r, z and magnetic moment μ.

TABLE XVI: ESI service routines

necessary for a particular communication. On the other hand, within the same approach it is extendible to more general cases, e.g., anisotropic equilibria or equilibria with perturbed or ergodic magnetic configurations.

References

[1] J.R. Ferron, M.L. Walker, L.L. Lao, H.E. St. John, D.A. Humphreys and J.A. Leuer, Nucl. Fusion, **38**, p. 1055 (1998).
[2] L.E. Zakharov, J. Lewandowski, E.L. Foley, F.M. Levinton, H.Y. Yuh, V. Drozdov, D.C. McDonald, Phys. of Plasmas **15**, 092503 (2008)
[3] G.V. Pereverzev, P.N. Yushmanov, "Astra-automated system for transport analysis", IPP Garching Report IPP5/98, 1 (2002).
[4] L.E. Zakharov and A. Pletzer, Phys. of Plasmas **6**, 4693(1999)
[5] L.L. Lao, H. St. John, R.D. Stambaugh, A.G. Kellman and W. Pfeiffer, Nucl. Fusion **25** 1611 (1985)
[6] https://fusion.gat.com/theory/Efitgeqdsk
[7] https://fusion.gat.com/theory/Efitaeqdsk
[8] J. DeLucia , S. C. Jardin, A.M.M. Todd, J. Comput. Phys. **37**, 2(1980)
[9] M. Chance, S. C. Jardin, T. Stix, Phys. Rev. Lett. **51**, 1963(1983)
[10] S.C. Jardin, Computational Methods in Plasma Physics , Boca Raton, CRC Press (2010)
[11] R.C. Grimm, J. Greene, and J. L. Johnson, Meth. Comp. Physics **9**, 253(1976)
[12] R. C. Grimm, R. L. Dewar and J. Manickam J. Comp. Phys. **49**, 94(1983)
[13] R.B. White, M.S. Chance, Phys. of Fluids **27** 2455 (1984)
[14] R.J. Hawryluk, "An Empirical Approach to Tokamak Transport", in Physics of Plasmas Close to Thermonuclear Conditions, ed. by B. Coppi, et al., (CEC, Brussels, 1980), Vol. 1, pp. 19-46;
[15] J. Ongena, M. Evrard, D. McCune, "Numerical Transport Codes", in the Proceedings of the Third Carolus Magnus Summer School on Plasma Physics, (Spa, Belgium, Sept 1997), as published in Transactions of Fusion Technology, March, 1998, Vol. 33, No. 2T, pp. 181-191.
[16] L.E. Zakharov and V. D. Shafranov, Reviews of Plasma Physics (Consultants Bureau, New York, 1981), Vol. 11, p. 153
[17] X. Li, L.E. Zakharov and S.A. Galkin, (accepted by Plasma Sci. and Technology, 2014)
[18] W.X. Wang, Z. Lin, W.M. Tang, W.W. Lee, S. Ethier, J.L.V. Lewandowski, G. Rewoldt, T.S. Hahm and J. Manickam, Phys. Plasmas **13**, 092505 (2006)
[19] W.X. Wang, P.H. Diamond, T.S. Hahm, S. Ethier, G. Rewoldt and W.M. Tang, Phys. Plasmas **17**, 072511 (2010)
[20] R.B. White. "The Theory of Toroidal Confined Plasmas. Third Edition." (Imperial College Press) 345 (2014).
[21] J. P. Freidberg. "Ideal Magnetohydrodynamics", Plenum, New York, (1987)
[22] X. Li, L.E. Zakharov, Phys. of Plasmas **21**: 012505 (2014)

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Information Services
Princeton Plasma Physics Laboratory
P.O. Box 451
Princeton, NJ 08543

Phone: 609-243-2245
Fax: 609-243-2751
e-mail: pppl_info@pppl.gov
Internet Address: http://www.pppl.gov