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Equilibrium Spline Interface (ESI) for magnetic confinement codes [1]

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Abstract

A compact and comprehensive interface, called ESI, 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 four 2- or 3-D functions of coordinates and four 1-D radial profiles together with their first derivatives.

The C reconstruction routines (accessible also from Fortran), which are a part of the interface, allow the calculation of basis functions and their first derivatives at any position inside the plasma. 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.

The interface is designed for

1. ***simple nested two and three dimensional configurations***
   - ***(a) with scalar pressure,***
   - ***(b) arbitrary pressure balance (within confinement limits);***
2. ***magnetic configurations with magnetic perturbations***
   - ***(a) with scalar pressure,***
   - ***(b) arbitrary pressure balance (within confinement limits);***

Considering the simplest case of simple nested surfaces with scalar pressure as a default case, the interface specifies the the data structure, which should be generated for its input by equilibrium codes. In particular, ESI specifies what data should be provided in the ASCII (human readable form) and what is permitted to be binary.

Contents

ESI has a C-source file esiZ.c with reconstruction routines

Initiation of ESI using routines from `esiZ.c` *file from a user C-code*

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

or from FORTRAN

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

(The names of FORTRAN callable routines in ESI are the low-case version of C-names)

This step loads the information on the numerical model of magnetic configuration and makes it ready to use.

All routines are integer functions returning 0 upon success

In addition to `esiZ.c` *the full source includes the optional files:*

`esiZ.c.d,esi.h,esi.inc,esiGL.c,esiGL.c.d`

The main ESI routine provides a comprehensive set of data in a number of points inside the plasma

The second step gives adresses of user arrays to ESI

```
int n;
double a[N],gq[N];
double 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];
double gz[N],rz[N],zz[N],Bz[N],ghz[N]; /* 3-D only */

i=Link2ESI(F,Fa,gFa,gFaa,gYa,gYaa,T,Ta,P,Pa
          ,r,ra,rq,z,za,zq,B,Ba,Bq,gh,gha,ghq);
i=Link2ESI3d(rz,zz,Bz,ghz); /* 3-D only */
i=ESISetID(1,ID); /* ID of coordinate system */
```

Then, just specify coordinates `a[],q[]`*, the number of points* `n` *and call*

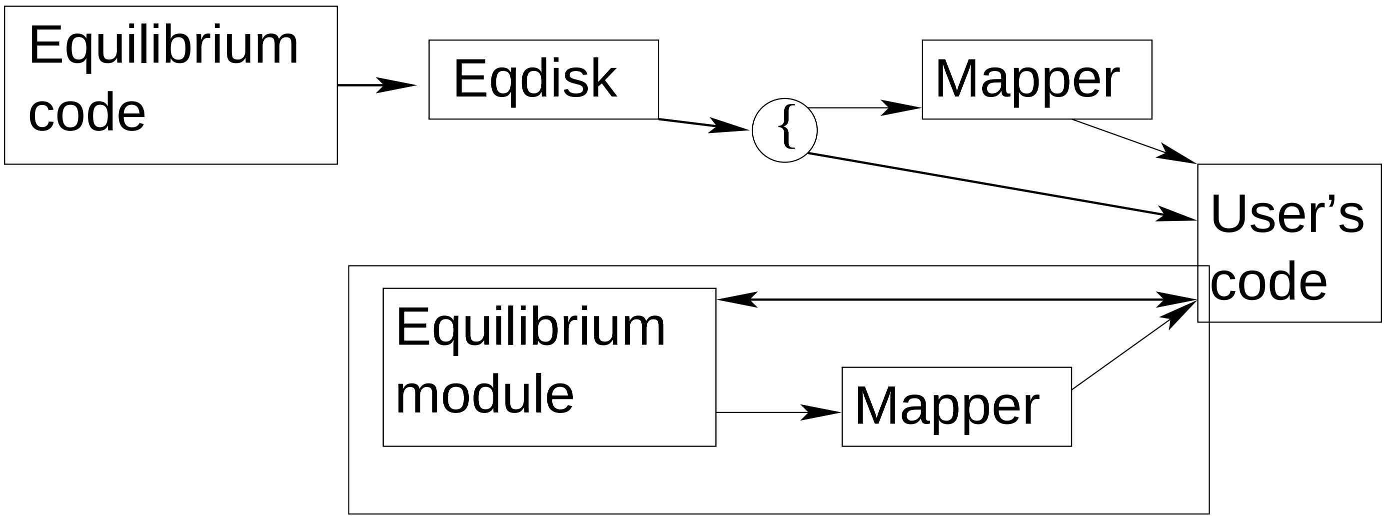
```
i=ESI2all(a,gq,n);  /*  i=ESI2all3d(a,gq,gz,n); in 3-D case */
```

as many times as necessary. The main reconstruction routine fills the user arrays with a basic, standard data set.

This is all the interface for 2-D equilibrium configurations

Numerical representation of magnetic configurations is a basic need for numerical simulations of toroidal plasmas

Even at this level there is a mess, preventing an easy and reliable code talking.



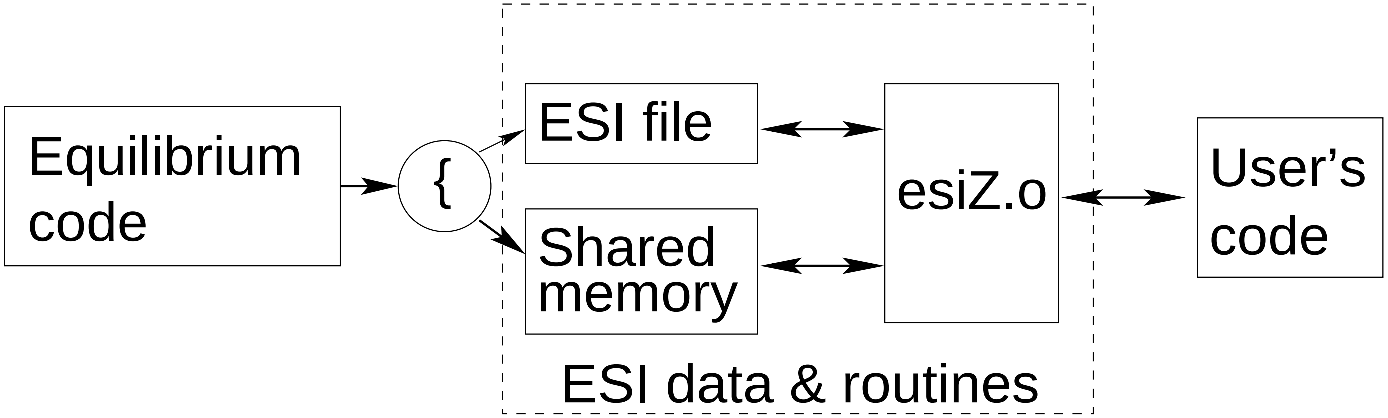
The existing approaches are serving only particular pairs of codes:

1. Eq. code prepares all the necessary data for the user code (e.g., $g_{ik}/\sqrt{g}$).
2. The user code takes only a primitive equilibrium information and generates everything necessary using an internal or external mapper.

Both approaches are common in their short sighting

ESI is introduced as a separate and self-sufficient module

As an input it takes a standard, irreducible set of data in a form sufficient for a comprehensive numerical representation of magnetic configuration.



As an output, the ESI reconstruction routines supply only a low level, standard information to the user code.

This information is sufficient for, at least, gyro-kinetic, particle orbit, MHD stability, and transport codes.

The interface is extendible to non-isotropic pressure equilibrium and perturbed configurations.

ESI addresses the entire code-talking problem by simplifying interaction with both equilibrium and the user side codes

The problem of interfacing the codes is not technical one

Sporadically created subroutines, modules, "components", formats, "server-client" models, which target the technical aspects of it, do not help.

It is necessary to distinguish between, as I called them, "complicated" and "difficult" problems

The problems of the "difficult" type are always moving towards their solution. In this sense, the "difficult" problems are not the real ones.

In contrast, the "complicated" problem is getting only worse with time.

Interfacing equilibrium codes is a simplest (but representative) example of a "complicated" problem in the stage when the mess is dominating over the technical aspects.

The physics meaning and composition of I/O data, separation of functionality, names and composition of structural elements, readability of control parameters, units, etc, all represent an intellectual, rather than the technical choice.

Even such simple interface, as ESI, requires a cross-discipline approach

By default, ESI is based on cubic polynomial representation of coordinates and physical variables in each direction.

Two types of coordinates should be covered by interface: i.e., the Laboratory cylindrical coordinates

$$r, \varphi, z, \tag{2.1}$$

and toroidal coordinates with simple nested surfaces

$$r = r(a,\theta,\zeta), \quad z = z(a,\theta,\zeta), \quad \varphi = \varphi(a,\theta,\zeta). \tag{2.2}$$

The equilibrium code should provide the values of coordinates and their first and mixed derivatives at mesh points

in 2-D case:

$$r, r'_a, r'_\theta, r''_{a\theta}, \quad z, z'_a, z'_\theta, z''_{a\theta} \tag{2.3}$$

and additionally in 3-D case:

$$\begin{gathered} r'_\zeta, r''_{a\zeta}, r''_{\theta\zeta}, r'''_{a\theta\zeta}, \quad z'_\zeta, z''_{a\zeta}, z''_{\theta\zeta}, z'''_{a\theta\zeta}, \\ \varphi, \varphi'_a, \varphi'_\theta, \varphi'_\zeta, \varphi''_{a\theta}, \varphi''_{a\zeta}, \varphi''_{\theta\zeta}, \varphi'''_{\theta\zeta}. \end{gathered} \tag{2.4}$$

In its turn, ESI can reconstruct r, φ, z and their first derivatives at any point in the plasma

Each equilibrium code is able to provide the above mentioned data

Equilibrium codes are not *required to generate the second derivatives.*

ESI does not *give an access to the second derivatives of its input functions.*

Unlike mapper, ESI is consistent with abilities of equilibrium codes and underlying physics

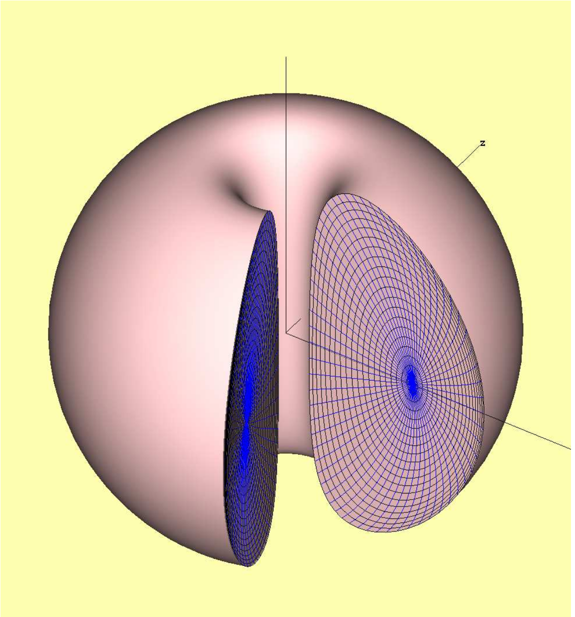
ESI restricts the equilibrium codes in choosing the radial variable

Among two types, i.e., the minor radius-like $a \propto \rho$*, and volume-like* $a \propto V$*, the second type is* not acceptable *because of singularity*

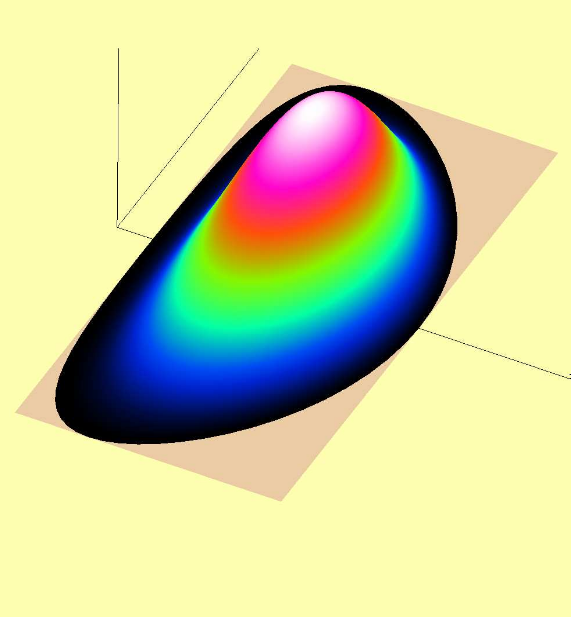
$$r'_V \simeq \left.\frac{1}{\sqrt{V}}\right|_{V \to 0} \qquad (2.5)$$

near the magnetic axis. The frequently used $a \propto \bar{\Psi}$ *generates additional singularities near the* X*-point.*

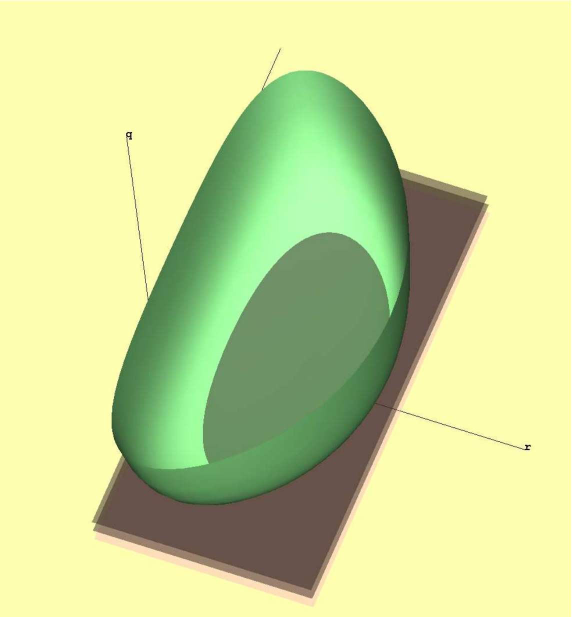
Cbesi-code has been written for inspection of interface data



NSTX equilibrium



pressure profile

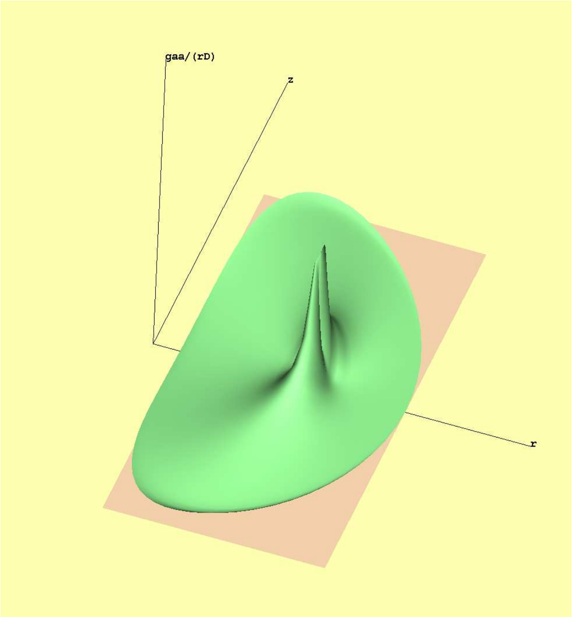


q-profile with q=1 surface

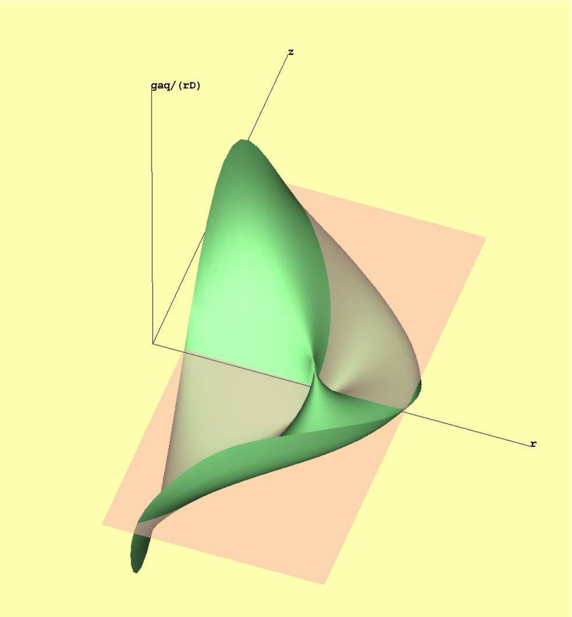
Generated by the CodeBuilder, Cbesi has a structured and formalized code control

Cbesi is equipped with both 2- and 3-D OpenGL graphics

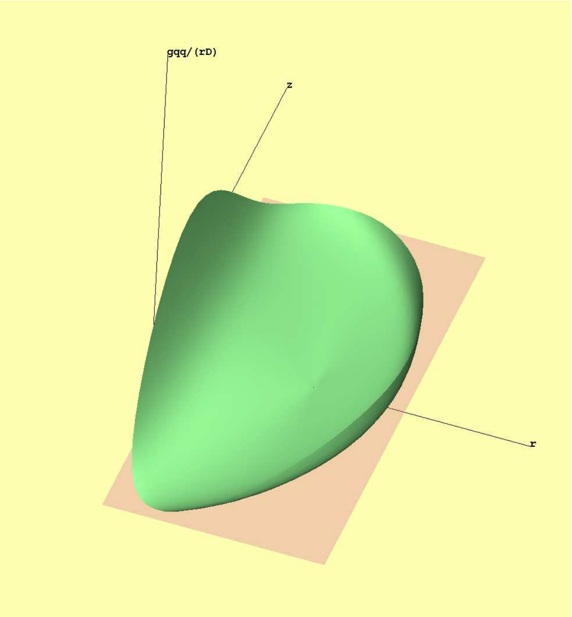
Unlike ESI, existing interfaces frequently store “unstorable”, singular data



$g_{aa}/\sqrt{g}$-*function*



$g_{a\theta}/\sqrt{g}$-*function*



$g_{\theta\theta}/\sqrt{g}$-*function*

Instead of paying attention to the content of interface plasma physicists prefer to be involved in “convergence” studies

Vector potential of magnetic field determines the physical set of functions

The covariant representation of $\mathbf{A}$, $(\mathbf{B} = \nabla \times \mathbf{A})$ *introduces three functions*

$$\mathbf{A} = -\bar{\Phi}'\eta\nabla a + \bar{\Phi}\nabla\theta + \bar{\Psi}\nabla\zeta \tag{2.6}$$

1. *The function* $\eta(a,\theta,\zeta)$ *is related to the choice of angles* θ,ζ. *In straight field line coordinates* (SFL) $\eta = 0$.

2. *In confinement configurations, using a transformation*

$$\mathbf{A} \rightarrow \mathbf{A} + \nabla u, \quad a \rightarrow a + \xi(a,\zeta) \tag{2.7}$$

the component $\bar{\Phi}(a,\theta,\zeta)$ *can always be reduced to*

$$\bar{\Phi} = \bar{\Phi}(a) \tag{2.8}$$

After this, $2\pi\bar{\Phi}(a) \equiv \Phi(a)$ *becomes the toroidal flux of the magnetic field.*

ESI requires $\bar{\Phi} = \bar{\Phi}(a)$. Only the reversed field pinches (RFP) are the exception and may have $\bar{\Phi} = \bar{\Phi}(a,\zeta)$

3. In general the $\bar\Psi(a,\theta,\zeta)$ cannot be reduced to $\bar\Psi(a)$

By massaging the shape of coordinate surfaces

$$a \to a+\xi, \quad \mathrm{B}\cdot\nabla\xi = \mathrm{B}\cdot\nabla a \tag{2.9}$$

$\bar\Psi(a,\theta,\zeta)$ *can be reduced to*

$$\bar\Psi = \bar\Psi_{00}(a) + \sum_{m,n}\hat\psi_{mn}(a,\theta,\zeta), \tag{2.10}$$

where $\hat\psi_{mn}$ *are the resonant harmonics. They determine the magnetic islands, which are topologically inconsistent with the simple nested coordinates.*

The coordinates where $\bar\Psi$ *has the form (2.10) are called the Reference Magnetic Coordinates (RMC).*

In RMC the magnetic field has the most compact representation

The input data to ESI should be given by equilibrium codes in RMC

Contravariant components of B are determined by A

$$\mathrm{B} = \hat{\psi}'_\theta(\nabla\theta \times \nabla\zeta) - (\bar{\Psi}' + \hat{\psi}'_a + \bar{\Phi}'\eta'_\zeta)(\nabla\zeta \times \nabla a) + \bar{\Phi}'(1 + \eta'_\theta)(\nabla a \times \nabla\theta). \quad (2.11)$$

For reconstruction of B the Eq. code should provide the data on

$$\eta, \hat{\psi}, \bar{\Psi}, \bar{\Phi} \quad (2.12)$$

and their first derivatives. In fact, for instead of fluxes ESI requires

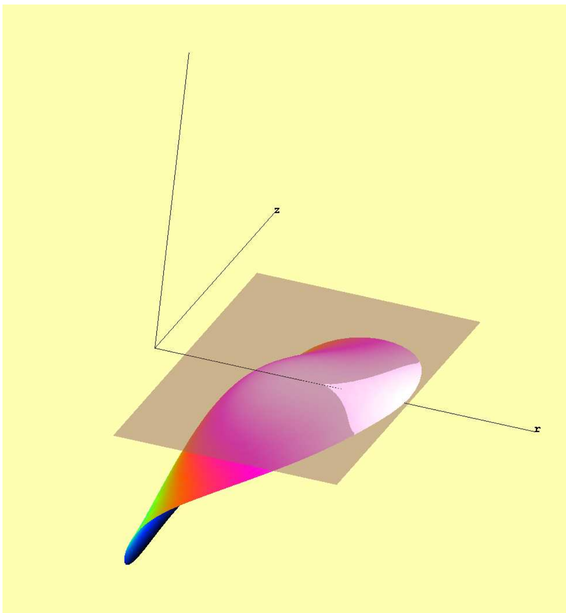
$$\bar{\Psi}', \bar{\Phi}', \bar{\Psi}'', \bar{\Phi}'' \quad (2.13)$$

The second derivatives $\bar{\Psi}'', \bar{\Phi}''$ are necessary for calculating the shear q'

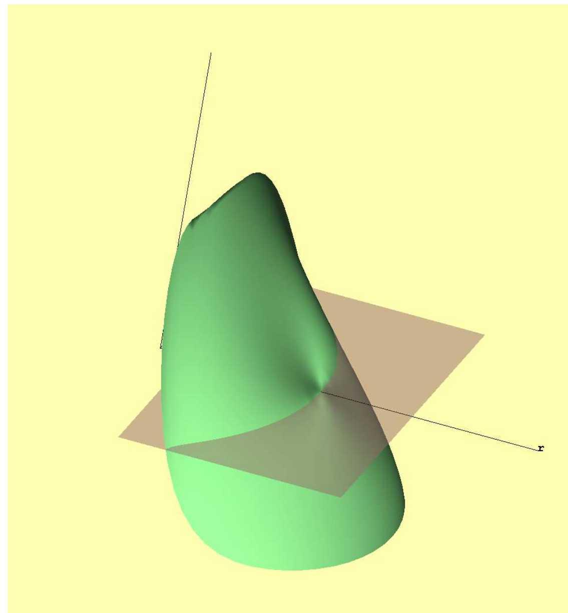
For compatibility with the guiding center codes

Eq. codes should provide $|B|$ with first and mixed derivatives at the mesh points

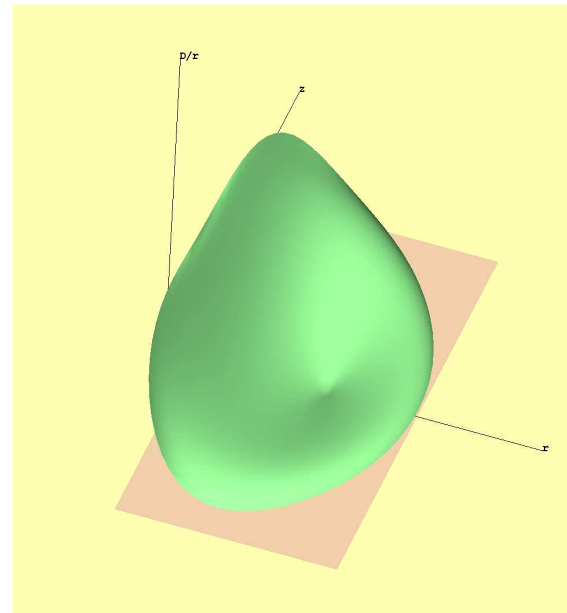
2-D functions required by ESI are all very smooth



$|\mathbf{B}| - |\mathbf{B}_{vac}|$



η *function with some defects*

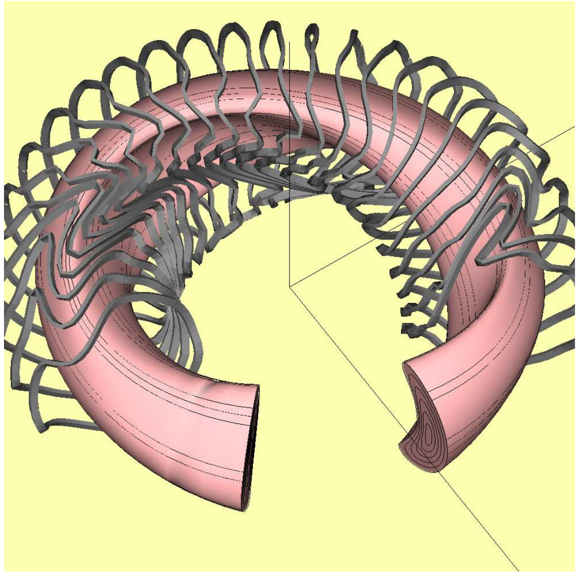


η'_θ *function*

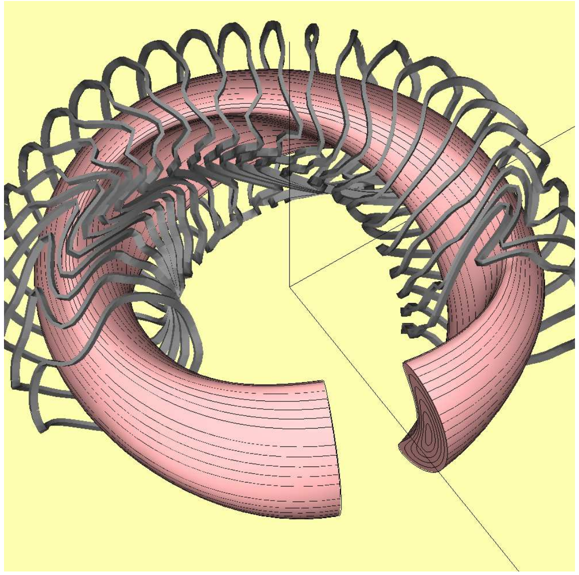
3-D OpenGL graphics makes all defects well exposed

ESI works for both "flux" and "laboratory" coordinates

Laboratory grid r, φ, z



3-D "imperfect" magnetic surfaces reconstructed with 20 turns



Same magnetic surfaces reconstructed with 40 turns

Line tracing routines are an intrisic part of ESI interface

The current density is reconstructed from the force balance

$$\nabla \bar{p} + \vec{F} = \mathrm{j} \times \mathrm{B} \tag{2.14}$$

without use of second derivatives.

For isotropic equilibrium two profiles are required from the equilibrium codes

$$P \equiv \frac{d\bar{p}}{d\bar{\Psi}}, \quad T \equiv d\bar{F}\frac{d\bar{F}}{d\bar{\Psi}} \tag{2.15}$$

Totally, for an isotropic 2-D equilibrium the equilibrium codes should provide four 2-D functions

$$r, z, \eta, |B|, \tag{2.16}$$

given on a, θ *mesh with their first and mixed derivatives, and four 1-D profiles*

$$P, T, \frac{\bar{\Psi}'}{a}, \frac{\bar{\Phi}'}{a}, \tag{2.17}$$

It is the responsibility of ESI to generate all other data about the configuration

Particle motion requires covariant components of B:

$$L = (\mathrm{A} + \rho_{||}\mathrm{B}) \cdot \mathrm{v} - H, \quad H = \rho_\perp^2 \frac{B^2}{2} + \mu B + \phi_E \tag{2.18}$$

In general

$$\mathrm{B} = \nu \nabla a + \bar{I} \nabla \theta + (\bar{F} + \tilde{F}) \nabla \zeta + \nabla \sigma \tag{2.19}$$

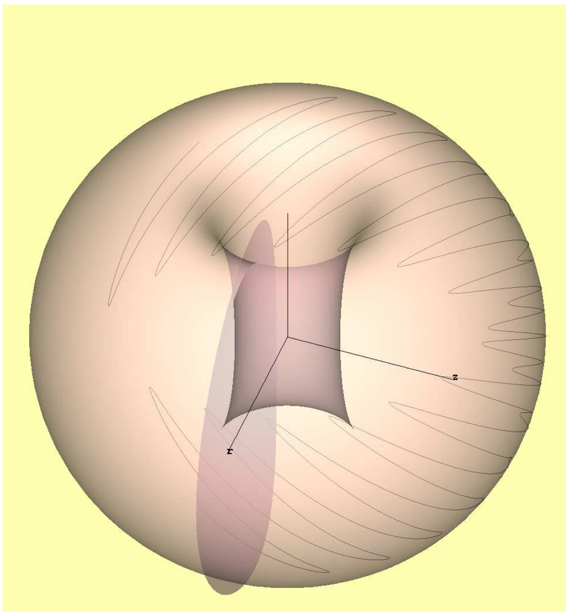
With isotropic pressure, $\tilde{F} = 0$. *Two components of* B *are determined by*

$$\begin{aligned} \bar{I} + \sigma'_\theta &\equiv -\frac{g_{\theta\theta}}{\sqrt{g}}(\bar{\Psi}' + \bar{\Phi}'\eta'_\zeta) + \frac{g_{\theta\zeta}}{\sqrt{g}}\bar{\Phi}'(1 + \eta'_\theta), \\ \bar{F} + \sigma'_\zeta &= -\frac{g_{\zeta\theta}}{\sqrt{g}}(\bar{\Psi}' + \bar{\Phi}'\eta'_\zeta) + \frac{g_{\zeta\zeta}}{\sqrt{g}}\bar{\Phi}'(1 + \eta'_\theta) \end{aligned} \tag{2.20}$$

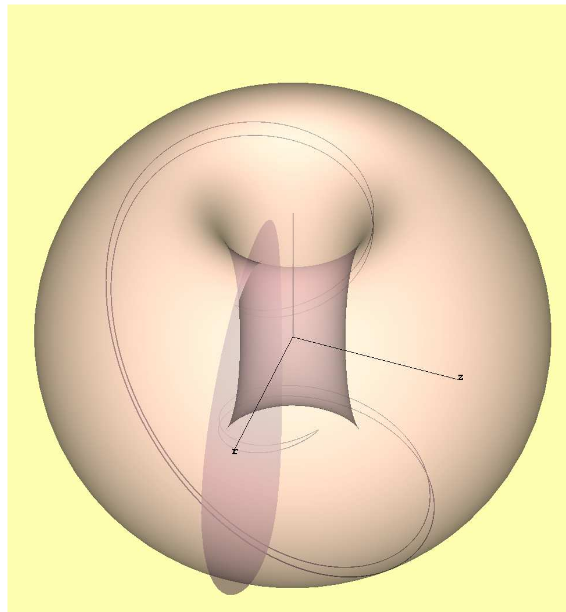
The function ν *is determined by the radial force balance*

$$\begin{aligned} &(\bar{\Phi}' + \bar{\Phi}'\eta'_\theta)\nu'_\zeta - (\bar{\Psi}' + \bar{\Phi}'\eta'_\zeta)\nu'_\theta = \\ &\bar{p}'(\sqrt{g})_\sim + \bar{\Phi}'(\bar{F}'\eta'_\theta - \bar{I}'\eta'_\zeta) \end{aligned} \tag{2.21}$$

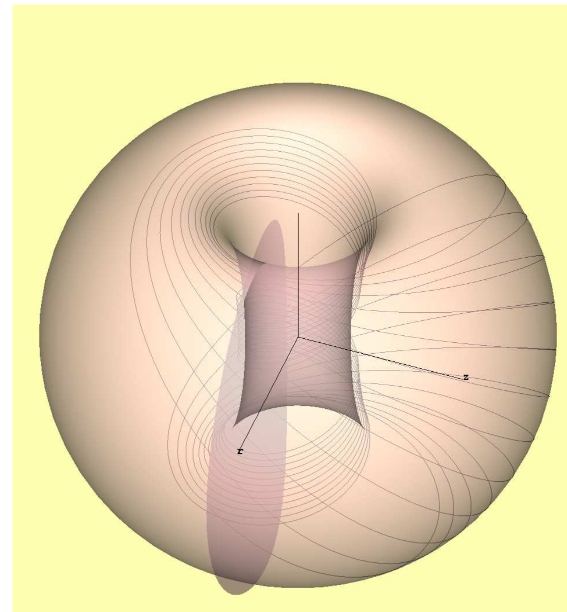
Cbesi-code is equipped with both guiding center and particle trajectory routines



5 keV D-particles in NSTX with $p_{\|} = 0.5$



Barely trapped particles, $p_{\|} = 0.87$



Barely passing particles, $p_{\|} = 0.90$

Particle motion routines are an intrinsic part of esiZ.c file

ESI calculates ν from a magnetic differential equation (MDE)

In SFL coordinates

$$\nu'_\theta + q\nu'_\zeta = P(a)(\sqrt{g})_\sim \equiv S(a,\theta,\zeta) \tag{2.22}$$

has a solution

$$\begin{aligned}\nu(a,\theta,\zeta) &= A(a,\zeta - q\theta)\\ &\quad - \int_0^\theta S(a,\alpha,\zeta + q\alpha - q\theta)d\alpha\end{aligned} \tag{2.23}$$

where

$$\begin{aligned}&S(a,\theta,\zeta) \equiv \sum_n S_n(a,\theta)e^{in\zeta}, \quad A(a,\zeta) \equiv \sum_n A_n(a)e^{in\zeta},\\ &A_n(a) = \frac{e^{-in\pi q}}{2\sin n\pi q}\int_0^{2\pi} S_n(a,\alpha)e^{inq\alpha}d\alpha.\end{aligned} \tag{2.24}$$

A service routine of ESI can generate ν

ESI provides the necessary data for making coordinate transformations. Canonical coordinates can be generated.

SFL for stability codes

$$\bar{\theta} = \theta - \alpha(a, \theta, \bar{\zeta}), \quad \bar{\zeta} = \bar{\zeta} - \beta(a, \theta, \bar{\zeta}), \\ \bar{\Phi}'\alpha + \bar{\Psi}'\beta = \bar{\Phi}'\eta, \tag{2.25}$$

where either α or β is an arbitrary function.

Hamiltonian coordinates a, θ, ζ are determines by

$$B_a = \nu + \sigma'_a = 0. \tag{2.26}$$

There are special, I called them "hat"-canonical coordinates

$$\hat{\theta} = \theta + \alpha, \quad \hat{\zeta} = \zeta + \beta, \\ \alpha = -\frac{\bar{F}\nu + \bar{F}'\sigma}{\bar{F}\bar{I}' - \bar{I}\bar{F}'}, \quad \beta = \frac{\bar{I}\nu + \bar{I}'\sigma}{\bar{F}\bar{I}' - \bar{I}\bar{F}'} \tag{2.27}$$

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

$$\mathrm{B} = \bar{I}\nabla\hat{\theta} + \bar{F}\nabla\hat{\zeta}. \tag{2.28}$$

ESI is a stuctural object acting as a virtual machine controlled by the user

All working data are enclosed into a structure, which can be cloned. The top control parameters are listed in the Table 3

ESI data structure					Table 3
C *name*	*Type*	*Size*	*Math*	#	*Group name*
Np1	int	1	$N_\theta + 1$	*0*	<ESI dimensions>
Na1	int	1	$N_a + 1$		
ID	int	1	*Type of* a, θ, ζ		
Nt1	int	1	$N_\zeta + 1$		
Lp	int	1	L_θ		
Lt	int	1	L_ζ		
rBtor	double	1	$\bar{F}_{ref} \equiv \bar{F}(a_{ref})$		
aRef	double	1	a_{ref}		
bsp1	double	1	$\bar{p}_{boundary}$		

ESI works with input files and shared memory. The ASCII files are human readable.

Compactness of interface (21x65 grid points) *allows to use ASCII files, e.g.,* `esiA.00` *for storing data, or*

as a map file, e.g., `esiA.00m`*, for storing the control parameters and pointers to a binary storage, e.g.,* `esiA.00b`

The ASCII file consists of several sections with a number of records inside

```
<ESI dimensions>[1](%d x %d %d %e %s) ESC Date:  12/17/06 at 23:05
!Np1 x Na1   ID RBtor Name
65 x  21   102 1.50  PEST Here 102 is ID of coordinate system
<ESI [gq]>[1](65%e)
```

The top of another section

```
<ESI r ra rgq raq>[1365](%e %e %e %e)
!                     r                     r'_a                    r'_q                    r"_aq
1.1189417832363331e+00  6.1752680497674650e-01 -0.0000000000000000e+00 -9.1619079100425833e-03
1.1189417832363331e+00  6.1365522061023337e-01 -0.0000000000000000e+00 -6.9646002319922323e-02
```

An example of a pointer to the same data in a binary file `esiA.00b`

```
<ESI r ra rgq raq>[1@688:esiA.00b](1365%e 1365%e 1365%e 1365%e)
```

ESI requires binary input files to be written by C-routines as a stream with no structural information

No conventions or formats hidden inside the binary files !

ESI can have up to 8 instances of a structure, called ESI

```
ESI Esi[8];
```

By default the `ESI[0]` *is activated. The user can switch between them by calling*

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

ESI design mimics the "virtual machine" approach of OpenGL

Any time a certain service, like calculation of function $|\boldsymbol{B}|$, $\boldsymbol{\eta}$, *or graphics output can be activated using*

```
i=esiEnable(esiGL,NULL);
i=esiEnable(esiBASIC,ESImodB);
i=esiEnable(esiBASIC,ESIgh);
```

and disabled by

```
i=esiDisable(esiGL ,NULL);
i=esi2Disable(esiBASIC,ESImodB);
```

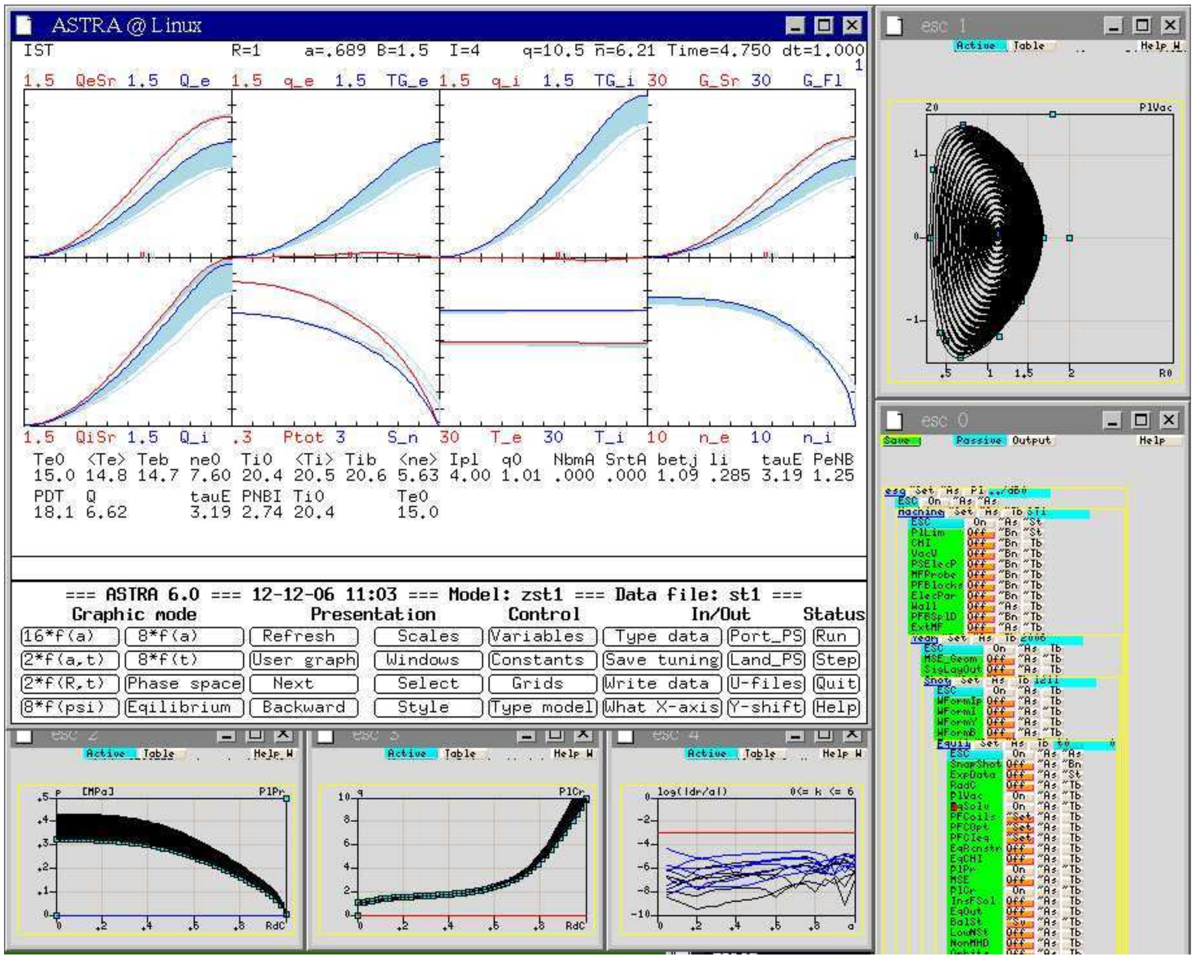
when it is not needed anymore. By default all calculations corresponding to a predefined parameter `esiBASIS` *are activated.*

The full set of possibilities is specified ESI *documentation file* `esiZ.c.d`*.*

The call of routines of deactivated service are ignored by ESI.

The virtual machine approach make, e.g., 3-D real time graphics compatible with dreams of plasma physicists of getting rid of any graphics

The interface is operational since 2002. ASTRA-ESC interact exclusively using ESI at every time step.



Hot-ion mode:

$$\beta = 0.35,$$
$$T_i = 20 \text{ [keV]},$$
$$T_e = 15 \text{ [keV]},$$
$$n_e(0) = 0.75 \cdot 10^{20},$$
$$\tau_E = 0.34 \text{ [sec]},$$
$$P_{NBI} = 2.7 \text{ [MW]},$$
$$P_{DT}^{equiv} = 18,$$
$$Q_{DT}^{equiv} = 6.6$$

ASTRA-ESC simulations of ST-1, B=1.5 T, I=4 MA, 2 MW, 80 keV NBI

At least, in describing toroidal magnetic fields it is necessary to switch finally to the science based interface.

ESI formalizes its interaction with both equilibrium and other magnetic confinement codes.

It essentially resolves the problem of “code-talking” at the basic level of plasma simulations.

The urgent need is the development of a numerical model for the separatrix boundary layer.

By its design and comprehensive approach ESI is superior to the present practice of patching the loopholes in communications