Theory and Numerics of the Stepped Pressure Equilibrium Code

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collaboration between PPPL & Australian National University

→ The simplest model of approximating global, macroscopic force-balance in toroidal plasma confinement with arbitrary geometry is magnetohydrodynamics (MHD).

→ Non-axisymmetric magnetic fields generally ***do not*** have a nested family of smooth flux surfaces, ***unless*** ideal surface currents are allowed at the rational surfaces.

→ If the field is non-integrable (i.e. chaotic, with a fractal phase space), then any ***continuous*** pressure that satisfies ***B***·∇p=0 must have an ***infinitely discontinuous gradient,*** ∇p.

→ Instead, solutions with stepped-pressure profiles are guaranteed to exist. A partially-relaxed, topologically-constrained, MHD energy principle is described.

→ Equilibrium solutions are calculated numerically. Results demonstrating convergence tests, benchmarks, and non-trivial solutions are presented.

→ The constraints of ideal MHD may be applied at the rational surfaces, in which case surface currents prevent the formation of islands. Or, these constraints may be relaxed in the vicinity of the rational surfaces, in which case magnetic islands will open if resonant perturbations are applied.

An ideal equilibrium with non-integrable (*chaotic)* field and *continuous* pressure, is *infinitely discontinous*

ideal MHD theory $= \nabla p = \mathbf{j} \times \mathbf{B}$, gives $\mathbf{B} \cdot \nabla p = 0$

→ *transport of pressure along field is "infinitely" fast*
→ *no scale length in ideal MHD*
→ *pressure adapts to fractal structure of phase space*

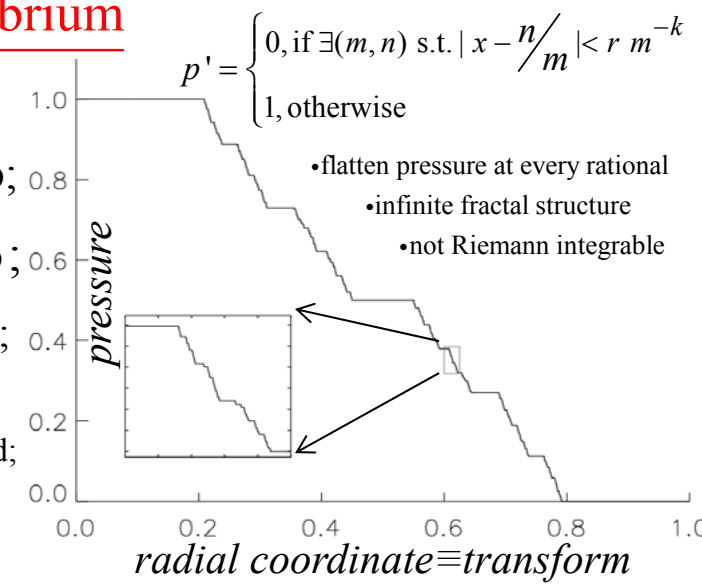chaos theory $=$ *nowhere are flux surfaces continuously nested*

*for non-symmetric systems, nested family of flux surfaces is destroyed

*islands & irregular field lines appear where transform is rational (n/m); rationals are dense in space

Poincare-Birkhoff theorem $\rightarrow$ periodic orbits, (e.g. stable and unstable) guaranteed to survive into chaos

*some irrational surfaces survive if there exists an r, $k \in \Re$ s.t. for all rationals, $|\iota - n/m| > r\, m^{-k}$

i.e. rotational-transform, ι, is *poorly approximated* by rationals,

Diophantine Condition
Kolmogorov, Arnold and Moser

ideal MHD $+$ chaos $\rightarrow$ infinitely discontinuous equilibrium

*iterative method for calculating equilibria is ill-posed;

1) $\mathbf{B}_n \cdot \nabla p = 0$ ∇p is everywhere discontinuous, or zero;

2) $\mathbf{j}_\perp = \mathbf{B}_n \times \nabla p / B_n^2$ $\mathbf{j}_\perp$ everywhere discontinuous or zero;

3) $\mathbf{B}_n \cdot \nabla \sigma = -\nabla \cdot \mathbf{j}_\perp$ $\mathbf{B} \cdot \nabla$ is *densely and irregularly* singular;

σ is single valued if and only if $\delta\sigma = -\oint_C \nabla \cdot \mathbf{j}_\perp \, dl / B = 0$

pressure must be flat across every closed field line, or parallel current is not single-valued;

4) $\nabla \times \mathbf{B}_{n+1} = \mathbf{j} \equiv \sigma\mathbf{B}_n + \mathbf{j}_\perp$ solution only if $\nabla \cdot (\sigma\mathbf{B} + \mathbf{j}_\perp) = 0$

$$p' = \begin{cases} 0, \text{if } \exists (m,n) \text{ s.t. } |x - \frac{n}{m}| < r\, m^{-k} \\ 1, \text{otherwise} \end{cases}$$

• flatten pressure at every rational
• infinite fractal structure
• not Riemann integrable

pressure vs *radial coordinate≡transform*

To have a well-posed equilibrium with chaotic $\mathbf{B}$ need to
$\rightarrow$ introduce non-ideal terms, such as resistivity, η, perpendicular diffusion, $\kappa_\perp$, [*HINT*, *M3D*, *NIMROD*,..],
$\rightarrow$ or return to an energy principle, but relax infinity of ideal MHD constraints

Instead, a multi-region, relaxed energy principle for MHD equilibria with non-trivial pressure and chaotic fields

Energy and helicity integrals (defined in nested volumes)

$$W_l = \underbrace{\int_{V_l} \left(\frac{p}{\gamma - 1} + \frac{B^2}{2} \right) dv}_{\text{energy}}, \qquad H_l = \underbrace{\int_{V_l} \left(\mathbf{A} \cdot \mathbf{B} \right) dv}_{\text{helicity}}, \qquad \text{where } \mathbf{B} = \nabla \times \mathbf{A} \text{ and } pV^{\gamma} = const.$$
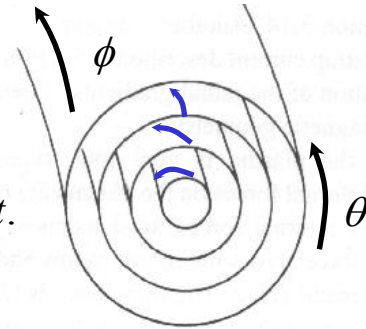
Seek minimum-energy state, subject to constraint of conserved helicity: $F = \sum_{l=1}^{N} \left(W_l - \mu_l H_l / 2 \right)$

Allow for _unconstrained_ variations $\delta\mathbf{A}$ and interface geometry, ξ,

      except ideal "topological" constraint $\delta\mathbf{B} = \nabla \times \left(\xi \times \mathbf{B} \right)$ _imposed discretely_ at interfaces

Equilibrium solutions when $\nabla \times \mathbf{B} = \mu_l \mathbf{B}$ in annuli, $[[p + B^2/2]] = 0$ across interfaces

$\rightarrow$ partial _Taylor relaxation_ allowed in each annulus; allows for topological variations/islands/chaos ;

$\rightarrow$ global relaxation prevented by ideal constraints; $\rightarrow$ <u>non-trivial stepped-pressure equilibria</u> !

$\rightarrow$ the solution to $\nabla \times \mathbf{B} = \mu_l \mathbf{B}$ depends on interface geometry; solved in parallel in each volume;

$\rightarrow$ solving force balance $\equiv$ adjusting interface geometry to satisfy $[[p + B^2/2]] = 0$;

    ideal interfaces that support pressure generally have irrational rotational-transform;

    standard numerical problem finding zero of multi-dimensional function; call NAG routine;

Existence of Three-Dimensional Toroidal MHD Equilibria with Nonconstant Pressure

OSCAR P. BRUNO
California Institute of Technology

PETER LAURENCE
Universita di Roma "La Sapienza"

We establish an existence result for the three-dimensional MHD equations

$$(\nabla \times \mathbf{B}) \times \mathbf{B} = \nabla p$$
$$\nabla \cdot \mathbf{B} = 0$$
$$\mathbf{B} \cdot n|_{\partial T} = 0$$

with $p \neq$ const in tori T *without symmetry*. More precisely, our theorems insure the existence of sharp boundary solutions for tori whose departure from axisymmetry is sufficiently small; they allow for solutions to be constructed with an arbitrary number of pressure jumps. © 1996 John Wiley & Sons, Inc.

→ *this was a strong motivation for pursuing the stepped-pressure equilibrium model*

→ *how large the "sufficiently small" departure from axisymmetry can be needs to be explored numerically*

By definition, an equilibrium code must constrain topology;

Definition: Equilibrium Code (fixed boundary)

given (1) boundary (2) pressure (3) rotational-transform $\equiv$ inverse q-profile (or current profile)
$\rightarrow$ calculate **B** that is consistent with force-balance; pressure profile *is not changed*!
c.f. "*coupled equilibrium - transport*" approach, that evolves pressure while evolving field

Cannot apriori specify pressure without apriori constraining topology of the field
$\rightarrow$ the constraint $\mathbf{B}\cdot\nabla p=0$ means the structure of **B** and p are intimately connected;

if p is given and **B** that satisfies force balance is to be constructed,
then flux surfaces must coincide with pressure gradients; (e.g. if p is smooth, **B** must have nested surfaces).

$\rightarrow$ specifying the profiles discretely is a practical means of retaining *some* control
over the profiles, whilst making minimal assumptions regarding the topology;

$\rightarrow$ pressure gradients are assumed to coincide with a set of strongly-irrational $\equiv$ "*noble*" flux surfaces

noble irrational

$\equiv$ limit of alternating path down Farey-tree

$\equiv$ Fibonacci sequence
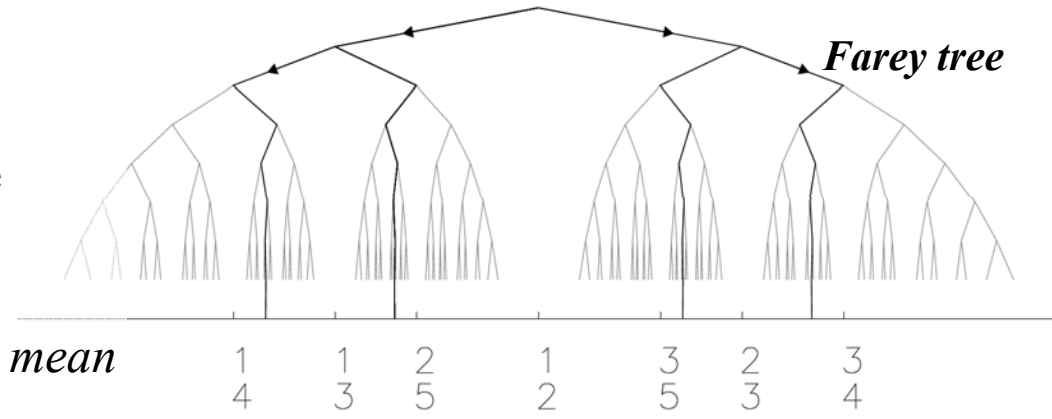
$$\frac{p_1}{q_1},\frac{p_2}{q_2},\frac{p_1+p_2}{q_1+q_2},...\rightarrow\frac{p_1+\gamma p_2}{q_1+\gamma q_2},\ \gamma=golden\ mean$$

Farey tree

$$\begin{array}{ccccccc} \frac{1}{4} & \frac{1}{3} & \frac{2}{5} & \frac{1}{2} & \frac{3}{5} & \frac{2}{3} & \frac{3}{4} \end{array}$$

Introducing the Stepped Pressure Equilibrium Code, SPEC

[Plasma Physics and Controlled Fusion, 54:014005, 2012]

The vector-potential is discretized using mixed Fourier & finite-elements

* toroidal coordinates (s, ϑ, ζ), *interface geometry $R_l = \sum_{m,n} R_{l,m,n} \cos(m\vartheta - n\zeta), Z_l = \sum_{m,n} Z_{l,m,n} \sin(m\vartheta - n\zeta)$

* exploit gauge freedom $\mathbf{A} = A_\vartheta(s, \vartheta, \zeta)\nabla\vartheta + A_\zeta(s, \vartheta, \zeta)\nabla\zeta$

* Fourier $A_\vartheta = \sum_{m,n} a_\vartheta(s) \cos(m\vartheta - n\zeta)$

* Finite-element $a_\vartheta(s) = \sum_i a_{\vartheta,i}(s)\varphi(s)$ *piecewise cubic or quintic basis polynomials*

and inserted into constrained-energy functional $F = \sum_{l=1}^{N}\left(W_l - \mu_l H_l / 2\right)$

* derivatives w.r.t. vector-potential $\rightarrow$ Beltrami field $\nabla \times \mathbf{B} = \mu\mathbf{B}$ *may be solved using (i) sparse linear solver,*
                                                                                              (ii) Newton methods   ,
* field in each annulus computed independently, distributed across multiple cpus   *or (iii) minimization   .*

* field in each annulus depends on enclosed toroidal flux (boundary condition) and

      $\rightarrow$ poloidal flux, ψ_P, and helicity,   *may adjust profiles to match (i) parallel current constraint   ,*
                                                                                  (ii) rotational-transform constraint
      $\rightarrow$ geometry of interfaces, $\xi \equiv \left\{ R_{m,n}, Z_{m,n}\right\}$ *or (iii) helicity constraint   .*

Force balance solved using multi-dimensional Newton method.

* interface geometry is adjusted to satisfy force $\mathbf{F}[\xi] \equiv \left\{[[\mathrm{p} + B^2/2]]_{m,n}\right\} = 0$

* angle freedom constrained by spectral-condensation, adjust angle freedom to minimize $\sum (m^2 + n^2)\left(R_{mn}^2 + Z_{mn}^2\right)$

* derivative matrix, $\nabla\mathbf{F}[\xi]$, computed in parallel using finite-differences   *minimal spectral width [Hirshman, VMEC]*

* call NAG routine: quadratic-convergence w.r.t. Newton iterations; robust convex-gradient method;

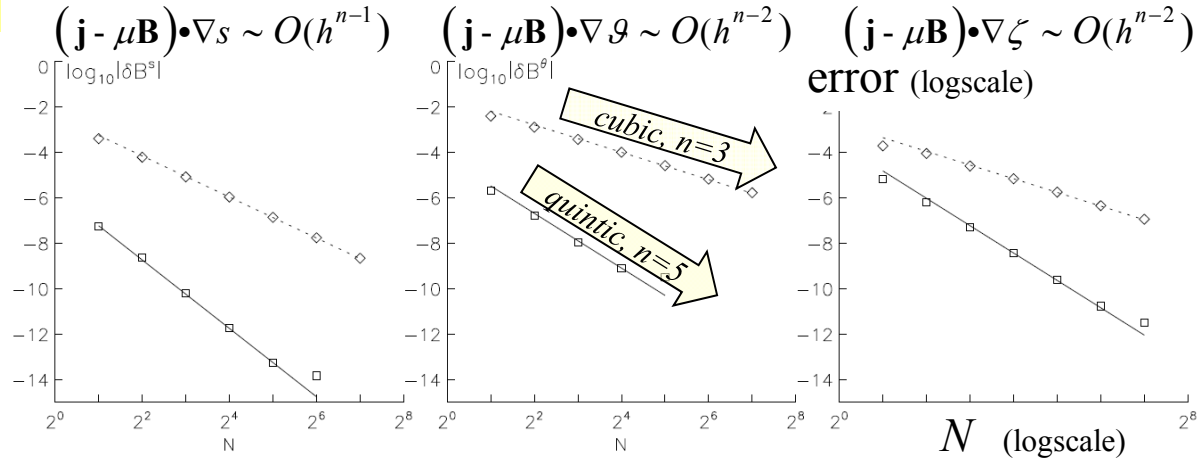# Numerical error in Beltrami field scales as expected

Scaling of numerical error with radial resolution depends on finite-element basis

$$\mathbf{A}=A_\vartheta\nabla\vartheta+A_\zeta\nabla\zeta, \quad \mathbf{B}=\nabla\times\mathbf{A}, \quad \mathbf{j}=\nabla\times\mathbf{B}, \qquad \text{need to quantify } \mathbf{error}=\mathbf{j}-\mu\mathbf{B}$$

$$A_\vartheta, A_\zeta \sim O(h^n)$$

h = radial grid size = 1 / N
n = order of polynomial

$$\sqrt{g}B^s = \partial_\vartheta A_\zeta - \partial_\zeta A_\vartheta \sim O(h^n)$$
$$\sqrt{g}B^\vartheta = \qquad\quad -\partial_s A_\zeta \sim O(h^{n-1})$$
$$\sqrt{g}B^\zeta = \partial_s A_\vartheta \qquad \sim O(h^{n-1})$$

$$\sqrt{g}j^s \sim O(h^{n-1})$$
$$\sqrt{g}j^\vartheta \sim O(h^{n-2})$$
$$\sqrt{g}j^\zeta \sim O(h^{n-2})$$

$(\mathbf{j}-\mu\mathbf{B})\cdot\nabla s \sim O(h^{n-1})$

$(\mathbf{j}-\mu\mathbf{B})\cdot\nabla\vartheta \sim O(h^{n-2})$

$(\mathbf{j}-\mu\mathbf{B})\cdot\nabla\zeta \sim O(h^{n-2})$

cubic, n=3

quintic, n=5

error (logscale)

N (logscale)

Example of chaotic Beltrami field in single given annulus;

$$R = 1.0 + r(\vartheta,\zeta)\cos\vartheta,$$
$$Z = \qquad r(\vartheta,\zeta)\sin\vartheta,$$

(m,n)=(3,1) island
+ (m,n)=(2,1) island
= chaos

inner surface
$r = 0.1$
outer interface
$r = 0.2 + \delta\left[\cos(2\vartheta - \zeta) + \cos(3\vartheta - \zeta)\right]$
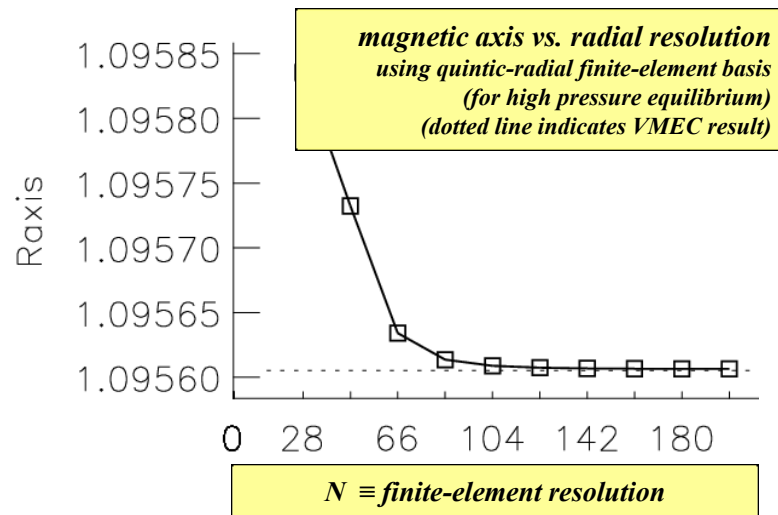
Poincaré plot, ζ=0

sub-radial grid, N=16
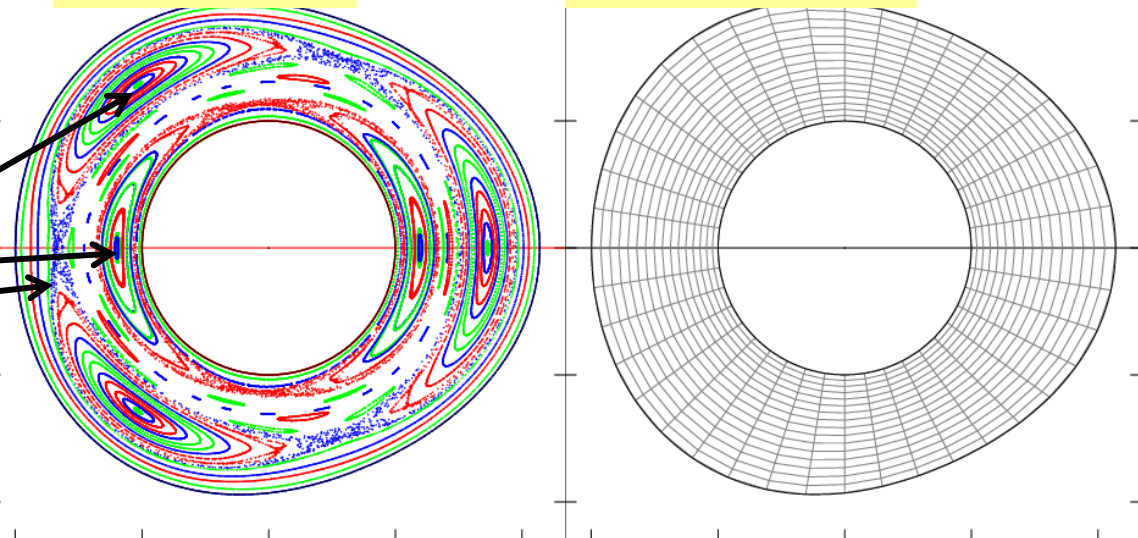
Stepped-pressure equilibria accurately approximate smooth-pressure *axisymmetric* equilibria

increasing pressure

*cylindrical Z*

upper half = SPEC & VMEC

lower half = SPEC interfaces

cylindrical Z

cylindrical R

cylindrical R

increasing pressure resolution ≡ number of interfaces

stepped-profile approximation to smooth profile

Pressure, p

toroidal flux ψ

toroidal flux ψ
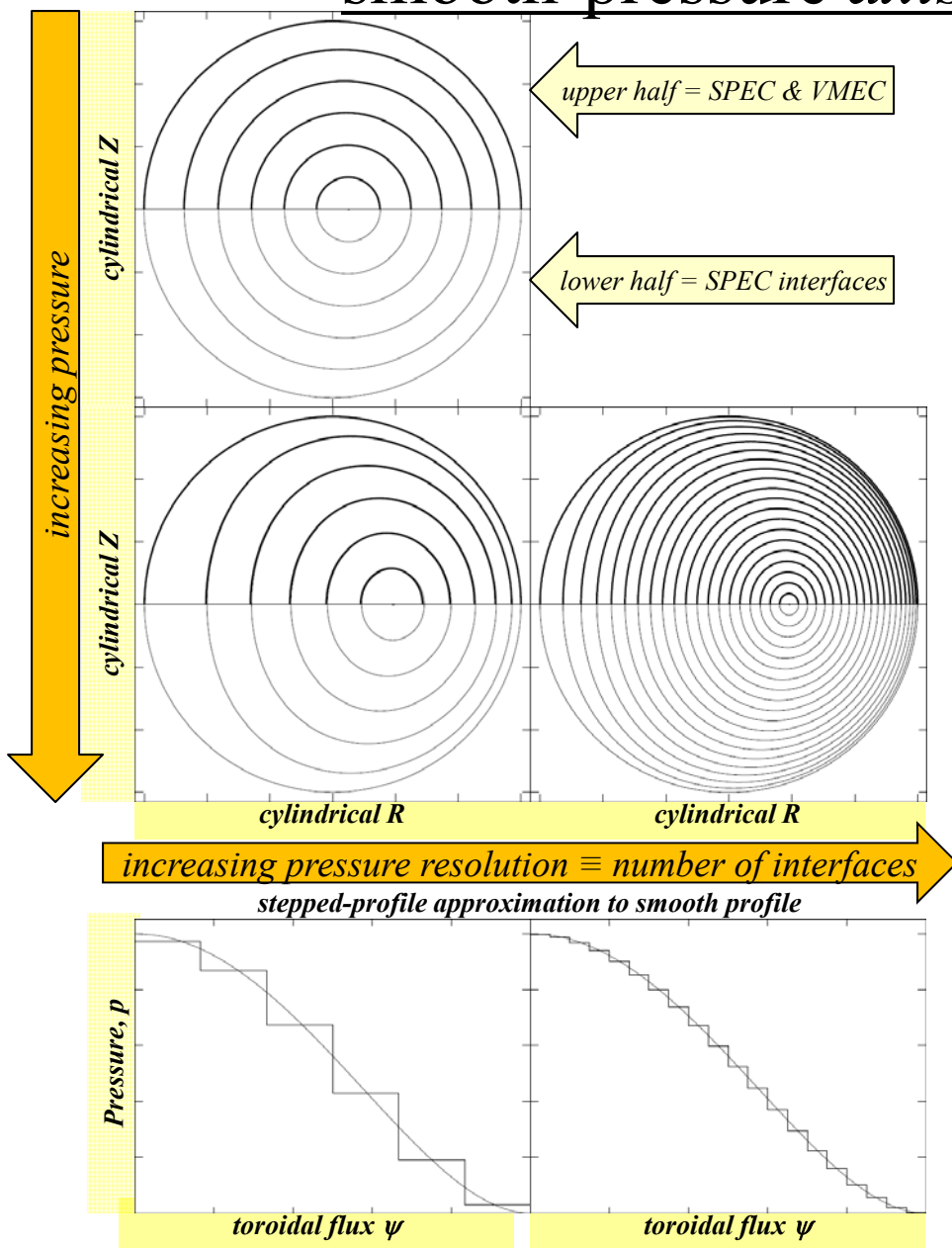
in axisymmetric geometry . . .

→ magnetic fields have family of nested flux surfaces

→ equilibria with smooth profiles exist,

→ may perform benchmarks (e.g. with VMEC)

 (arbitrarily approximate smooth-profile with stepped-profile)

→ approximation improves as number of interfaces increases

→ location of magnetic axis converges w.r.t radial resolution

magnetic axis vs. radial resolution
using quintic-radial finite-element basis
(for high pressure equilibrium)
(dotted line indicates VMEC result)

Raxis

1.09585
1.09580
1.09575
1.09570
1.09565
1.09560

0   28   66   104   142   180

N ≡ finite-element resolution

transform
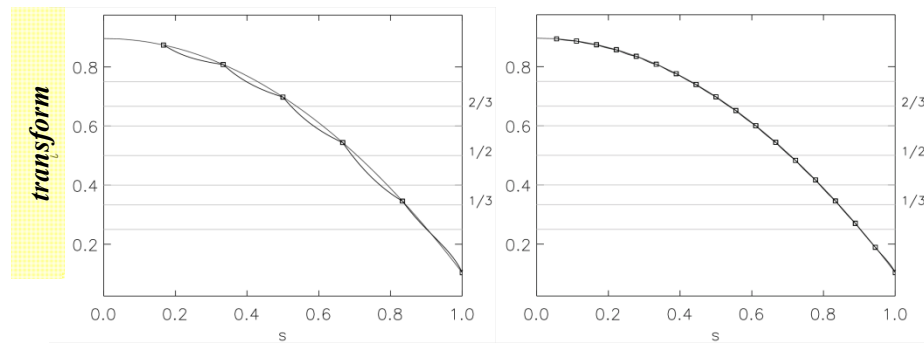
Equilibria with (i) perturbed boundary & chaotic fields, and (ii) pressure are computed .

Poincaré plot (cylindrical) β = 0%

Poincaré plot (cylindrical) β ≈ 4%
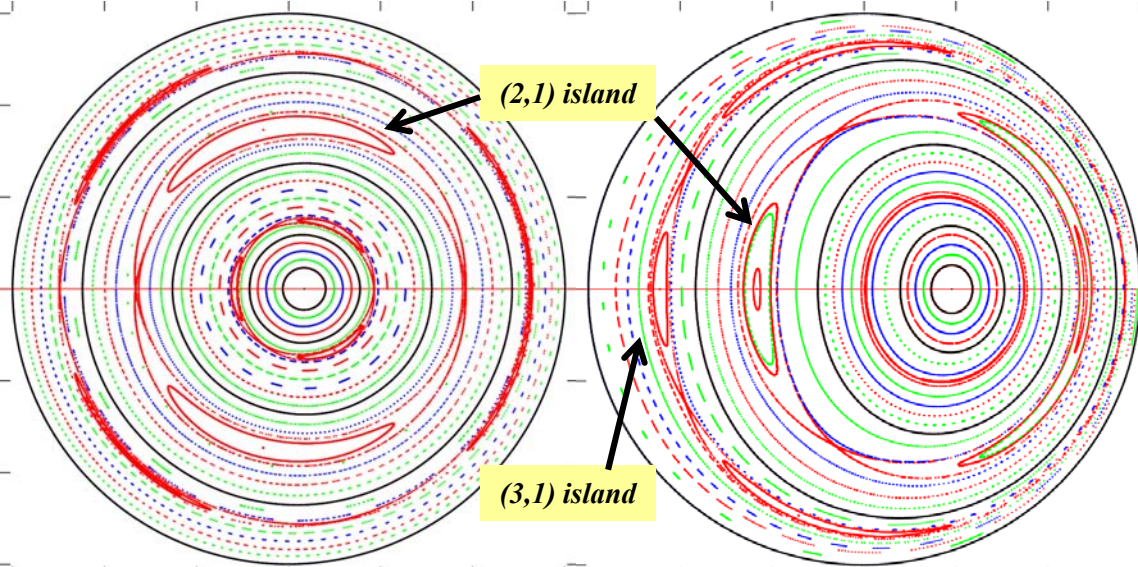
(2,1) island

(3,1) island

boundary deformation induces islands

$$R = 1.0 + r\cos\vartheta, \ Z = r\sin\vartheta$$

$$r = 0.3 + \delta\cos(2\vartheta - \phi) + \delta\cos(3\vartheta - \phi)$$

$$\delta = 10^{-4}$$

Demonstrated Convergence

of high-pressure equilibrium with islands,
with Fourier Resolution,

Poincaré plot (toroidal) β ≈ 4%

radial coordinate

← ΔW →
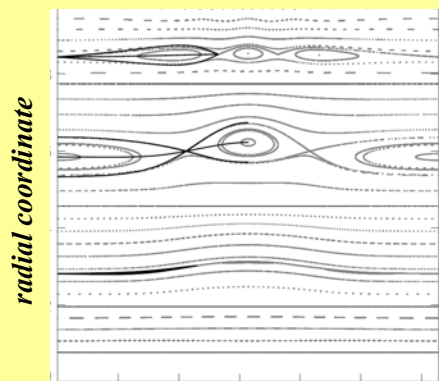
poloidal angle

Pressure profile

p

s
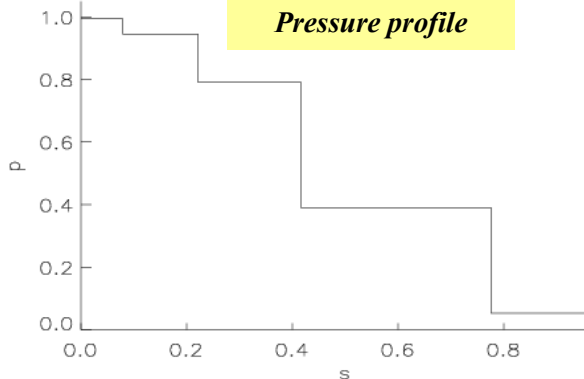
Convergence of (2,1) & (3,1) island widths .. with Fourier resolution, β ≈ 4% case
poloidal resolution   0 ≤ m ≤ M
toroidal resolution -N ≤ n ≤ N

ΔW

M
N
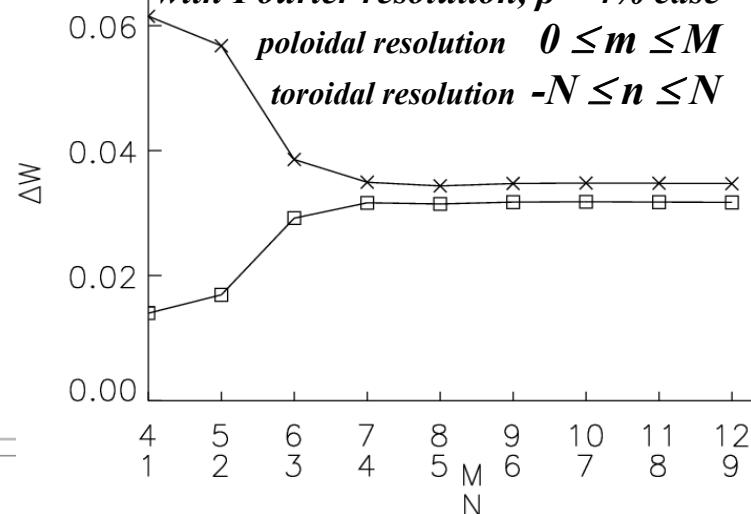
Example calculation: DIIID with N=3 applied error field

→ axisymmetric boundary & pressure profile from experiment EFIT reconstruction, $\beta \approx 1.5\%$,

(Thanks to Ed Lazarus, Sam Lazerson . . .)

→ apply 3mm, n=3 boundary deformation, with broad m spectrum

effect of RMP modelled by including (m,n)=(2,3), (3,3) & (4,3) boundary deformation,
(in spectrally condensed angle, so this corresponds to broad m spectrum in magnetic coordinates),

at present : can only treat stellarator-symmetric configurations, in fixed boundary;
for future work : include up-down asymmetry; allow free boundary;

→ strong pressure gradient near plasma edge

→ if $\mathbf{B} \cdot \nabla p \approx 0$, pressure gradients coincide with (irrational) flux surfaces

⇒ irrational intefaces chosen to coincide with pressure gradients

smooth EFIT pressure profile,
(dotted curve is smooth pressure gradient)
and stepped pressure profile approximation

pressure
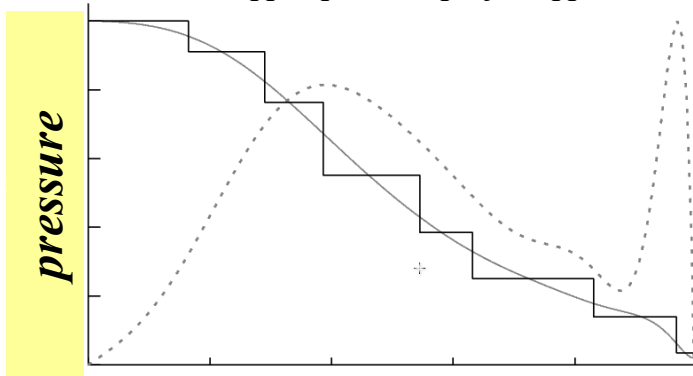
formation of magnetic islands at rational surfaces
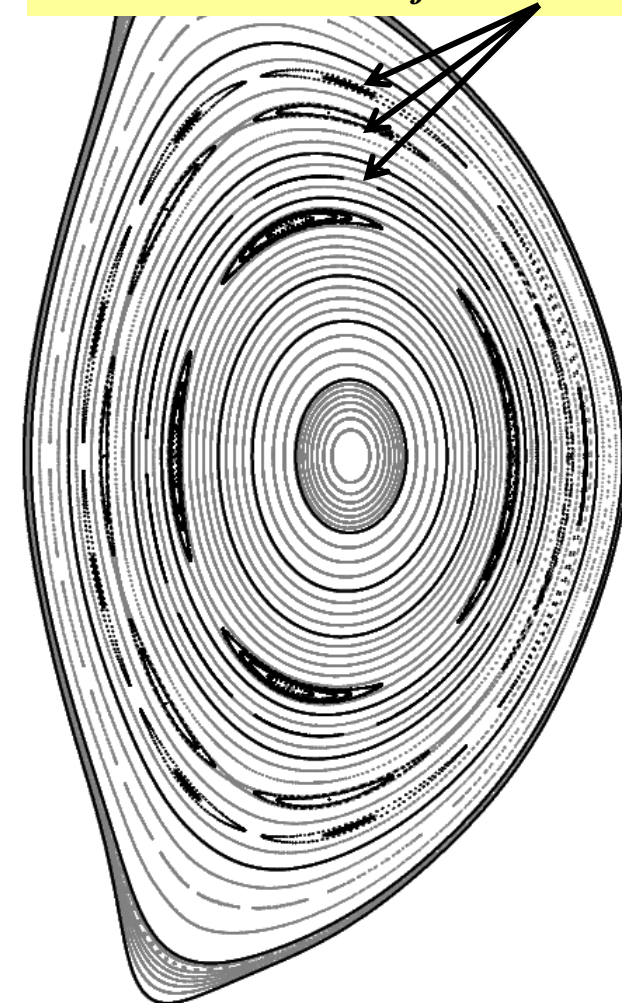
→ relaxation, reconnection (i.e. island formation) is permitted,

→ no rational "shielding currents" included in calculation.

Example of ITER relevant configuration,
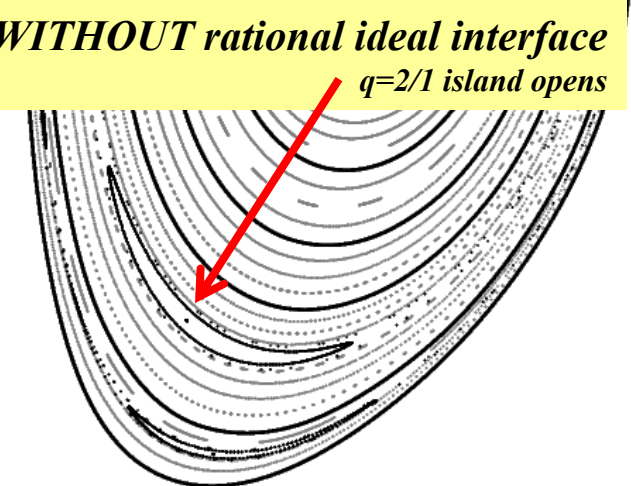## *with and without rational shielding currents*

If ideal constraint applied at rational surfaces, shielding currents prevent island formation

ITER boundary, plus perturbation

$$\delta R = \delta \cos(2\vartheta - \phi)\cos\vartheta, \quad \delta Z = \delta \cos(2\vartheta - \phi)\sin\vartheta$$

$$(\delta = 10^{-4})$$

rotational transform

Rational surface q=2/1

pressure
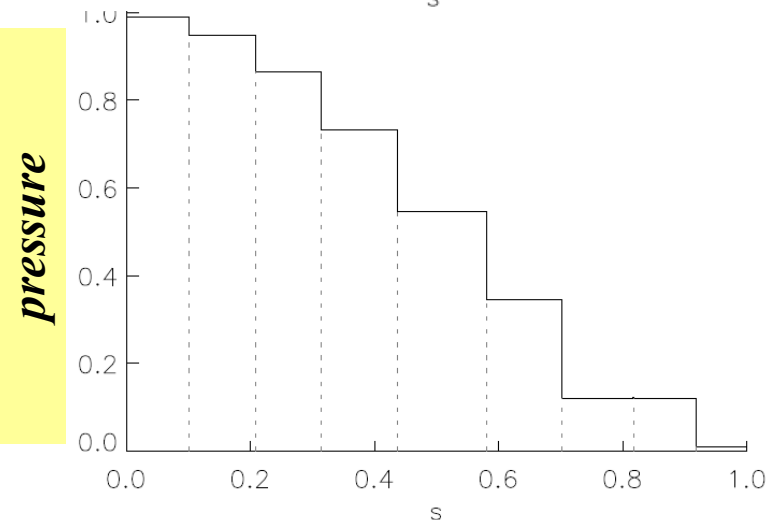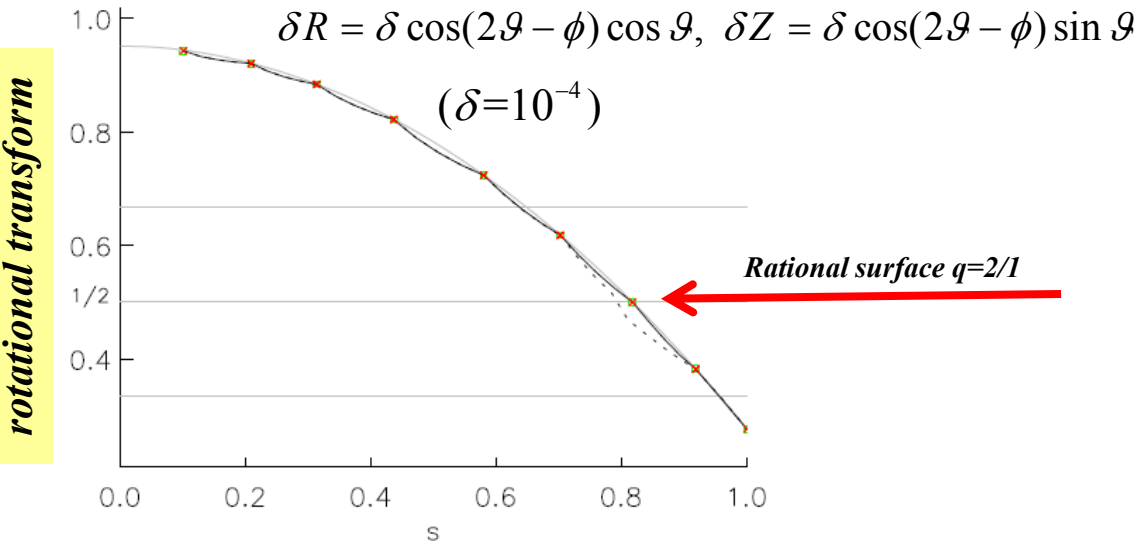
WITH rational ideal interface
no island formation
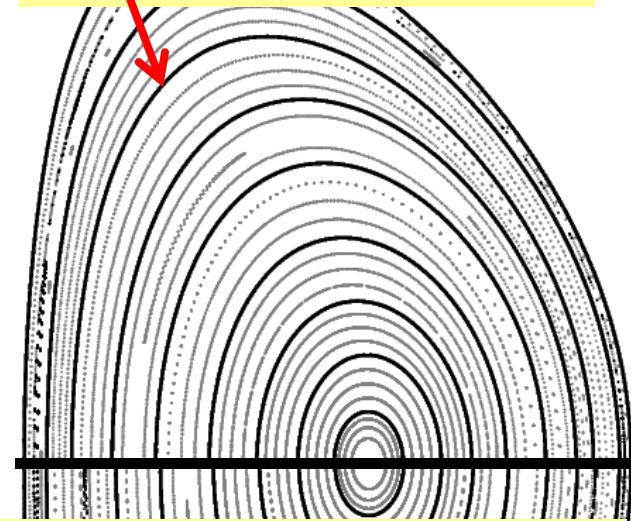
WITHOUT rational ideal interface
q=2/1 island opens

Summary

→ A partially-relaxed, topologically-constrained energy principle has been described and the equilibrium solutions constructed numerically

* using a high-order (piecewise quintic) radial discretization, and a spectrally condensed Fourier representation
* workload distrubuted across multiple cpus,
* extrema located using standard numerical methods (NAG): modified Newton's method, with quadratic-convergence
* non-axisymmetric solutions with chaotic fields and non-trivial pressure guaranteed to exist (under certain conditions)

→ Specifying the profiles discretely is a practical means of retaining some control over the profiles, while making minimal assumptions regarding the topology of the field
* it is only assumed that *some* flux surfaces exist
* pressure gradients coincide with strongly irrational flux surfaces

→ Convergence studies have been performed

* expected error scaling with radial resolution confirmed
* detailed benchmark with axisymmetric equilibria (with smooth profiles)
* demonstrated convergence of island widths with Fourier resolution

→ By enforcing the ideal constraint at the rational surfaces, the formation of magnetic islands is prohibited by the formation of surface "shielding" currents
* similar to non-linear generalization of IPEC
* relaxing ideal constraint at rational surfaces allows islands to open

Instead, a multi-region, relaxed energy principle for MHD equilibria with non-trivial pressure and chaotic fields

<u>Energy, helicity and mass integrals</u> (defined in nested volumes)
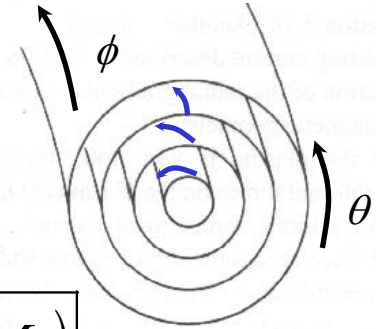
$$W_l = \int_{V_l} \left(\frac{p}{\gamma-1} + \frac{B^2}{2} \right) dv, \quad \underbrace{H_l = \int_{V_l} (\mathbf{A} \cdot \mathbf{B}) dv}_{\text{helicity}}, \quad \underbrace{M_l = \int_{V_l} p^{1/\gamma} dv}_{\text{mass}}$$

$$\underbrace{\phantom{W_l = \int_{V_l}}}_{\text{energy}}$$

Seek constrained, minimum-energy state $\boxed{F = \sum_{l=1}^{N} \left(W_l - \mu_l H_l / 2 - \nu_l M_l \right)}$

<u>1st variation due to *unconstrained* variations</u> $\delta p, \quad \delta \mathbf{A}, \quad$ and interface geometry, $\boldsymbol{\xi}$,

except ideal "topological" constraint $\delta \mathbf{B} = \nabla \times (\boldsymbol{\xi} \times \mathbf{B})$ *imposed discretely* at interfaces

$$\delta F = \sum_{l=1}^{N} \left\{ \int_{V_l} \underbrace{\left(\frac{1}{\gamma-1} - \frac{\nu_l p^{1/\gamma-1}}{\gamma} \right)}_{\substack{\nu p^{1/\gamma} = \gamma p/(\gamma-1) = const. \\ \text{in each annulus}}} \delta p \ dv + \int_{V_l} \delta \mathbf{A} \cdot \underbrace{\left(\nabla \times \mathbf{B} - \mu_l \mathbf{B} \right)}_{\nabla \times \mathbf{B} = \mu_l \mathbf{B} \text{ in each annulus}} dv - \int_{\partial V_l} \underbrace{[[p + B^2/2]]}_{\substack{\text{continuity of total pressure} \\ \text{across interfaces}}} \boldsymbol{\xi} . \mathbf{dS} \right\}$$

<u>Equilibrium solutions when $\nabla \times \mathbf{B} = \mu_l \mathbf{B}$ in annuli, $[[p+B^2/2]]=0$ across interfaces</u>

→ partial *Taylor relaxation* allowed in each annulus; allows for topological variations/islands/chaos;

→ global relaxation prevented by ideal constraints; → non-trivial *stepped − pressure* solutions;

→ the solution to $\nabla \times \mathbf{B} = \mu_l \mathbf{B}$ depends on interface geometry; solved in parallel locally in each annulus;

→ solving force balance ≡ adjusting interface geometry to satisfy $[[p+B^2/2]]=0$;

   ideal interfaces that support pressure generally have irrational rotational-transform;

   standard numerical problem finding zero of multi-dimensional function; call NAG routine;
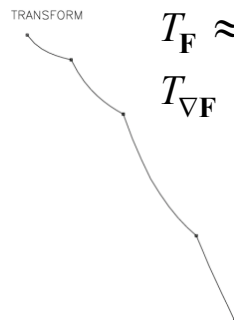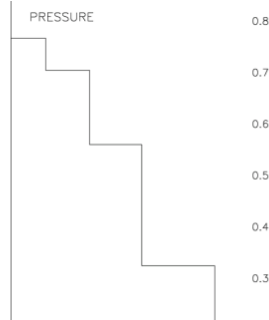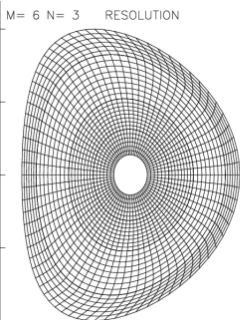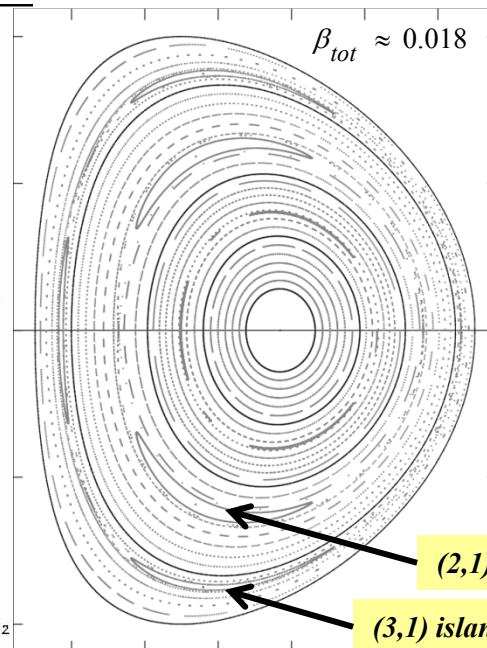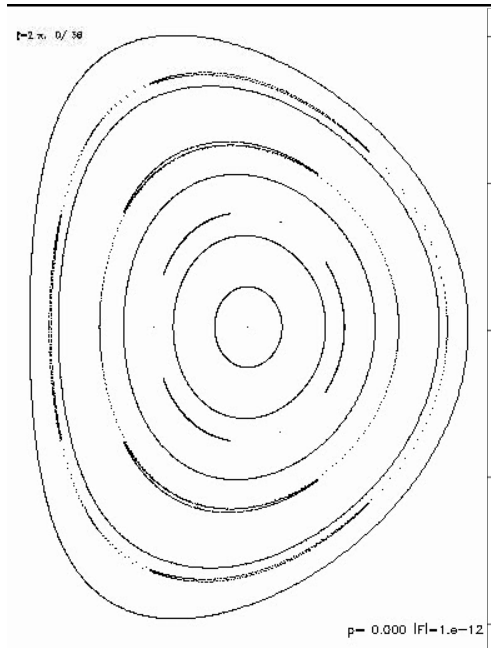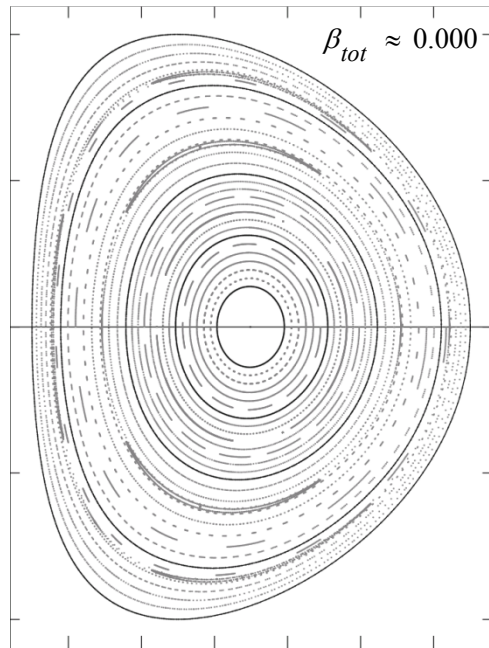
Sequence of equilibria with increasing pressure shows plasma *can* have significant response to external perturbation.

axisymmetric   plus small perturbation

$$R = 1.00 + 0.30\cos(\vartheta) + 0.05\cos(2\vartheta) + [\delta_{21}\cos(2\vartheta - \zeta) + \delta_{31}\cos(3\vartheta - \zeta)]\cos(\vartheta)$$

$$Z = 1.00 + 0.40\sin(\vartheta) + [\delta_{21}\cos(2\vartheta - \zeta) + \delta_{31}\cos(3\vartheta - \zeta)]\sin(\vartheta)$$
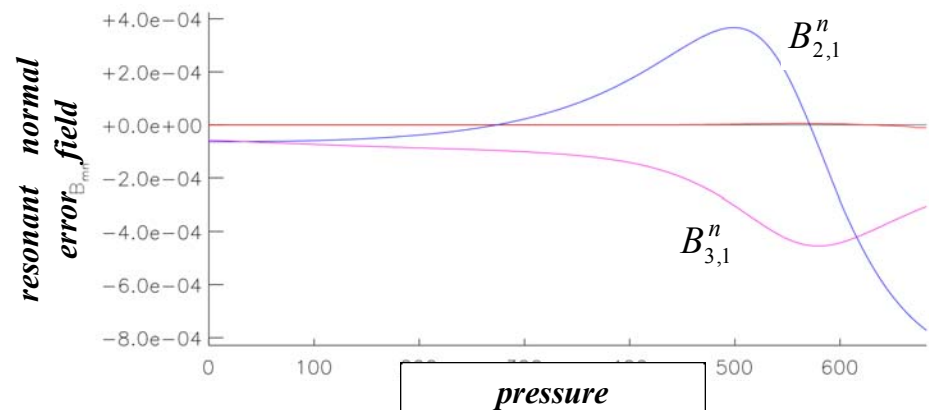

$\beta_{tot} \approx 0.000$

$\beta_{tot} \approx 0.018$

(2,1) island

(3,1) island

$$T_{VMEC} \approx 100s$$

$$T_{\mathbf{F}} \approx 30s$$

$$T_{\nabla\mathbf{F}} \approx 1.5h$$

M= 6 N= 3   RESOLUTION   PRESSURE   TRANSFORM

resonant normal error field B_{mn}

$B_{2,1}^n$

$B_{3,1}^n$

pressure

Force balance condition at interfaces gives rise to auxilliary pressure-jump Hamiltonian system.

$\rightarrow$ Beltrami condition, $\nabla \times \mathbf{B} = \mu \mathbf{B}$, and interface constraint, $\mathbf{B} \cdot \mathbf{n} = 0$, gives $\nabla \times \mathbf{B} \cdot \nabla s = 0$,

suggests surface potential, $B_\vartheta = \partial_\vartheta f$, $B_\zeta = \partial_\zeta f$, so that $\partial_\vartheta B_\zeta - \partial_\zeta B_\vartheta = 0$,

$$B^2 = (g_{\vartheta\vartheta} f_\zeta f_\zeta - 2 g_{\vartheta\zeta} f_\vartheta f_\zeta + g_{\zeta\zeta} f_\vartheta f_\vartheta)/(g_{\vartheta\vartheta} g_{\zeta\zeta} - g_{\vartheta\zeta} g_{\vartheta\zeta}), \quad \text{metric elements } g_{\alpha\beta} \equiv \partial_\alpha \mathbf{x} \cdot \partial_\beta \mathbf{x}$$

$\rightarrow$ Force balance condition, $[[p + B^2/2]] = 0$, introduce $H \equiv 2(p_1 - p_2) = B_2^2 - B_2^1 = const.$

$\rightarrow$ Let tangential field on "inner-side" of interface be given, $B_{1\vartheta} = \partial_\vartheta f$, $B_{1\zeta} = \partial_\zeta f$,

tangential field on "outer-side", $B_{2\vartheta} = p_\vartheta$, $B_{2\zeta} = p_\zeta$, determined by characteristics

$$\dot{\vartheta} = \frac{\partial H(\vartheta, \zeta, p_\vartheta, p_\zeta)}{\partial p_\vartheta}\bigg|_{\zeta, p_\vartheta, p_\zeta}, \quad \dot{p}_\vartheta = -\frac{\partial H}{\partial \vartheta}, \quad \dot{\zeta} = \frac{\partial H}{\partial p_\zeta}, \quad \dot{p}_\zeta = -\frac{\partial H}{\partial \zeta}$$

$\rightarrow$ 2 d.o.f. Hamiltonian system, and invariant surfaces only exist if "frequency" is irrational

$\Rightarrow$ ideal interfaces that support pressure must have irrational transform

Sequence of equilibria with increasing pressure shows plasma *can* have significant response to external perturbation.
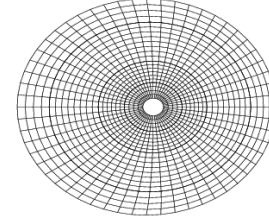
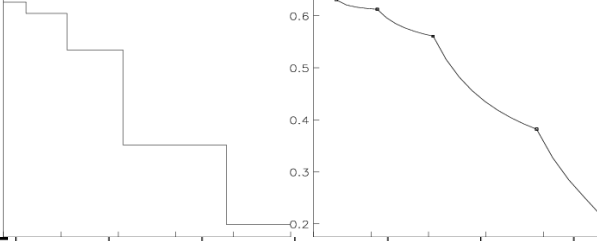axisymmetric plus perturbation $\qquad\qquad \delta_{21}=\delta_{31}=10^{-4}$

$R = 1.00 + [0.30 + \delta_{21}\cos(2\vartheta - \zeta) + \delta_{31}\cos(3\vartheta - \zeta)]\cos(\vartheta)$

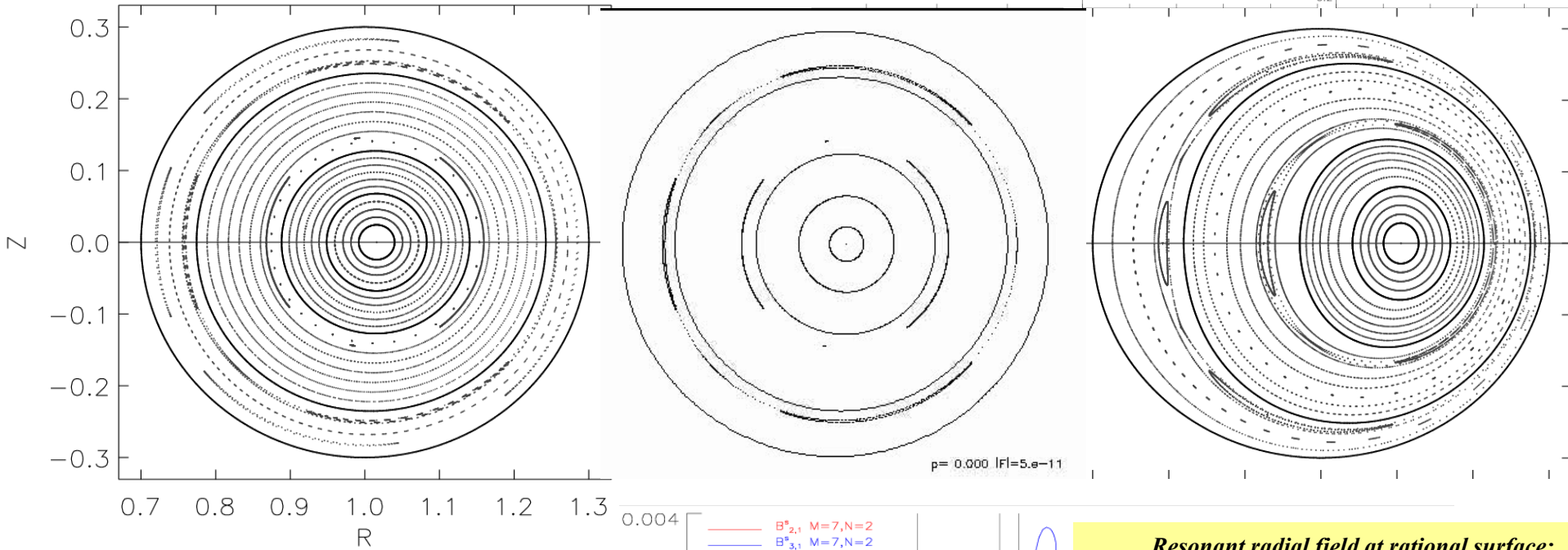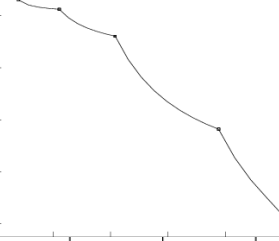$Z = 1.00 + [0.30 + \delta_{21}\cos(2\vartheta - \zeta) + \delta_{31}\cos(3\vartheta - \zeta)]\sin(\vartheta)$

Resonant radial field at rational surface; n=1,2,3 stability from PEST;