

# Theory and numerics of partially-relaxed, topologically-constrained, MHD equilibria with chaotic magnetic fields

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*20<sup>th</sup> International Toki Conference, 7-10 December 2010, Toki, Japan*

## Motivation & Outline

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

→ As toroidal magnetic fields are analogous to 1-1/2 Hamiltonians, and are generally chaotic, we need an MHD equilibrium code that allows for chaotic fields.

→ Existing ideal MHD equilibrium codes with chaotic fields fail to accommodate the fractal structure of Hamiltonian chaos. This leads to an ill-posed numerical algorithm for computing numerically-intractable, pathological equilibria.

→ A new partially-relaxed, topologically-constrained MHD equilibrium model is described and implemented numerically. Results demonstrating convergence tests, benchmarks, and non-trivial solutions are presented.

# Ideal-force-balance with *chaotic* field is pathological

## ideal MHD theory =

\*ideal-force-balance,  $\nabla p = \mathbf{j} \times \mathbf{B}$ , gives  $\mathbf{B} \cdot \nabla p = 0$

→ transport of pressure along field is “infinitely” fast  
 → no scale length in ideal MHD  
 → pressure adapts exactly to structure of phase space

## chaos theory =

\*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 → periodic orbits, (e.g. stable and unstable) guaranteed to survive into chaos

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

i.e. rotational-transform,  $\iota$ , is *poorly approximated* by rationals,

**Diophantine condition**  
 Kolmogorov, Arnold and Moser

## ideal MHD theory + chaos theory $\equiv$ pathological equilibrium

\*Spitzer iterations are ill-posed

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

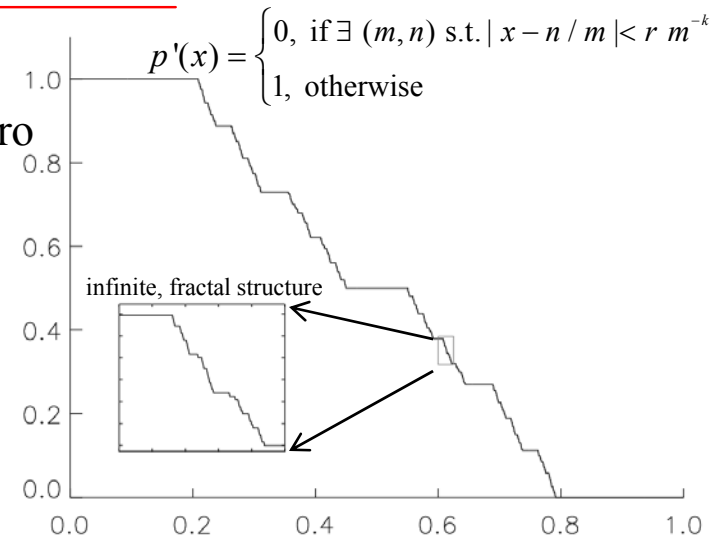
2)  $\mathbf{j}_\perp = \mathbf{B}_n \times \nabla p / B_n^2 \rightarrow \mathbf{j}_\perp$  is discontinuous or zero

3)  $\mathbf{B}_n \cdot \nabla \sigma = -\nabla \cdot \mathbf{j}_\perp \rightarrow$  cannot be inverted to obtain parallel current

$\mathbf{B} \cdot \nabla$  is *densely and irregularly singular*

condition that  $\sigma$  be single valued  $\delta\sigma = -\oint_C \nabla \cdot \mathbf{j}_\perp dl / B = 0$

4)  $\nabla \times \mathbf{B}_{n+1} = \mathbf{j} \equiv \sigma \mathbf{B}_n + \mathbf{j}_\perp$



To have a well posed equilibrium with chaotic  $\mathbf{B}$  need to extend beyond ideal MHD.

e.g. introduce non-ideal terms, such as resistivity,  $\eta$ , perpendicular diffusion,  $\kappa_\perp$ , [HINT, M3D, ..],

→ or can relax infinity of ideal MHD constraints

Taylor relaxation: a weakly resistive plasma will relax,  
subject to single constraint of conserved helicity

Taylor relaxation, [Taylor, 1974]

$$W = \underbrace{\int_V (p + B^2 / 2) dv}_{\text{plasma energy}}, \quad H = \underbrace{\int_V (\mathbf{A} \cdot \mathbf{B}) dv}_{\text{helicity, } \mathbf{B}=\nabla \times \mathbf{A}}$$

Constrained energy functional  $F = W - \mu H / 2$ ,  $\mu \equiv$  Lagrange multiplier

Euler-Lagrange equation, for *unconstrained* variations in magnetic field,  $\nabla \times \mathbf{B} = \mu \mathbf{B}$

linear force-free field  $\equiv$  Beltrami field

***But, . . . Taylor relaxed fields have no pressure gradients***

Ideal MHD equilibria and Taylor-relaxed equilibria are at opposite extremes . . . .

Ideal-MHD  $\rightarrow$  imposition of *infinity* of ideal MHD constraints  
non-trivial pressure profiles, but structure of field is *over-constrained*

Taylor relaxation  $\rightarrow$  imposition of *single* constraint of conserved global helicity  
structure of field is not-constrained, but pressure profile is trivial, i.e. *under-constrained*

**We need something in between . . .**

**. . . perhaps an equilibrium model with *finitely* many ideal constraints, and *partial* Taylor relaxation?**

# Introducing the multi-volume, partially-relaxed model of MHD equilibria with topological constraints

## Energy, helicity and mass integrals

$$\underbrace{W_l = \int_{V_l} \left( \frac{p}{\gamma-1} + \frac{B^2}{2} \right) dv}_{\text{plasma energy}}, \quad
 \underbrace{H_l = \int_{V_l} (\mathbf{A} \cdot \mathbf{B}) dv}_{\text{helicity}}, \quad
 \underbrace{M_l = \int_{V_l} p^{1/\gamma} dv}_{\text{mass}}$$

## Multi-volume, partially-relaxed energy principle

\* A set of  $N$  nested toroidal surfaces enclose  $N$  annular volumes  
 → the interfaces are assumed to be ideal,  $\delta \mathbf{B} = \nabla \times (\delta \boldsymbol{\xi} \times \mathbf{B})$

\* The multi-volume energy functional is

$$F = \sum_{l=1}^N (W_l - \mu_l H_l / 2 - \nu_l M_l)$$

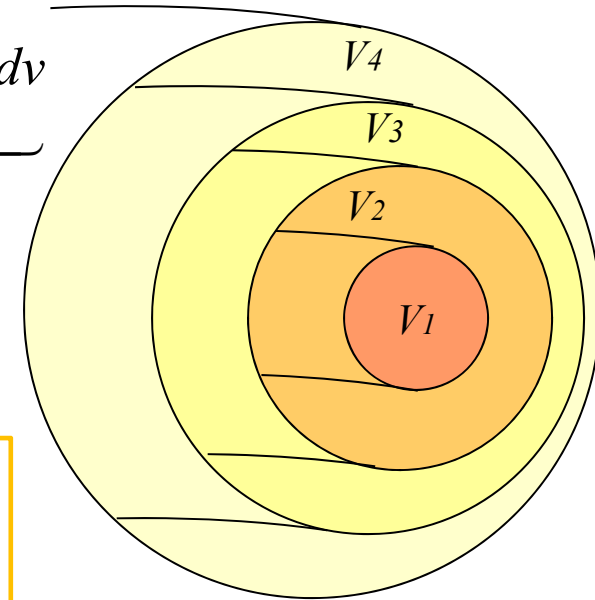
## Euler-Lagrange equation for *unconstrained* variations in $\mathbf{A}$

In each annulus, the magnetic field satisfies  $\nabla \times \mathbf{B}_l = \mu_l \mathbf{B}_l$

## Euler-Lagrange equation for variations in interface geometry

Across each interface, pressure jumps allowed, but total pressure is continuous  $[[p + B^2/2]] = 0$

→ an analysis of the force-balance condition is that the interfaces must have strongly irrational transform



→ field remains tangential to interfaces,  
 → a finite number of ideal constraints, imposed topologically!

*ideal interfaces coincide with KAM surfaces*

# Topological constraints : pressure gradients coincide with flux surfaces

## The ideal interfaces are chosen to coincide with pressure gradients

→ parallel transport dominates perpendicular transport,

→ simplest approximation is  $\mathbf{B} \cdot \nabla p = 0$

→ *structure of B and structure of the pressure are intimately connected;*

→ pressure gradients **must** coincide with KAM surfaces  $\equiv$  ideal interfaces

→ *cannot apriori specify pressure without apriori constraining structure of the field;*

A fixed boundary equilibrium is defined by :

(i) given pressure,  $p(\psi)$ , and rotational-transform profile,  $\iota(\psi)$

(ii) geometry of boundary;

(a) only stepped pressure profiles are consistent (numerically tractable) with chaos and  $\mathbf{B} \cdot \nabla p = 0$

(b) the computed equilibrium magnetic field must be consistent with the input profiles

(a) + (b) = where the pressure has gradients, the magnetic field must have flux surfaces.

# Existence of Three-Dimensional Toroidal MHD Equilibria with Nonconstant Pressure

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

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

with  $p \neq \text{const}$  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.

Communications on Pure and Applied Mathematics, Vol. XLIX, 717–764 (1996)

→ how large the “sufficiently small” departure from axisymmetry can be needs to be explored numerically . . .

# Extrema of energy functional obtained numerically; introducing the Stepped Pressure Equilibrium Code, SPEC

## The vector-potential is discretized

\* toroidal coordinates  $(s, \vartheta, \zeta)$ , \*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.

\* derivatives w.r.t. vector-potential  $\rightarrow$  linear equation for Beltrami field  $\nabla \times \mathbf{B} = \mu \mathbf{B}$

*solved using sparse linear solver*

\* field in each annulus computed independently, distributed across multiple cpus

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

$\rightarrow$  poloidal flux,  $\psi_p$ , and helicity-multiplier,  $\mu$

*adjusted so interface transform is strongly irrational*

$\rightarrow$  geometry of interfaces,  $\xi \equiv \{R_{m,n}, Z_{m,n}\}$

## Force balance solved using multi-dimensional Newton method.

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

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

\* derivative matrix,  $\nabla \mathbf{F}[\xi]$ , computed using finite-differences

*minimal spectral width [Hirshman, VMEC]*

\* quadratic-convergence w.r.t. Newton iterations

*future work . . .*

1) *approximate derivative matrix  $\sim 2^{\text{nd}}$  variation of energy functional*

2) *implement pre-conditioner*

# Numerical error in Beltrami field scales as expected

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

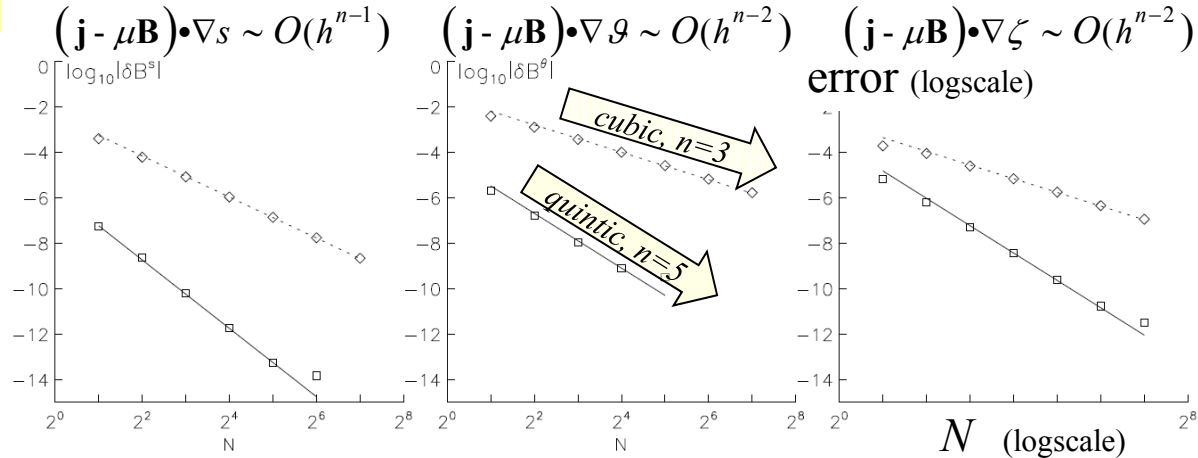
$$\mathbf{A} = A_\vartheta \nabla \vartheta + A_\zeta \nabla \zeta, \quad \mathbf{B} = \nabla \times \mathbf{A}, \quad \mathbf{j} = \nabla \times \mathbf{B}$$

need to quantify error  $\mathbf{j} - \mu \mathbf{B}$

$$A_\vartheta, A_\zeta \sim O(h^n) \quad \begin{array}{l} h = \text{radial grid size} = 1/N \\ n = \text{order of polynomial} \end{array}$$

$$\begin{aligned} \sqrt{g} B^s &= \partial_\vartheta A_\zeta - \partial_\zeta A_\vartheta \sim O(h^n) \\ \sqrt{g} B^\vartheta &= -\partial_s A_\zeta \sim O(h^{n-1}) \\ \sqrt{g} B^\zeta &= \partial_s A_\vartheta \sim O(h^{n-1}) \end{aligned}$$

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



## Example of chaotic Beltrami field

Poincaré plot,  $\zeta=0$

Poincaré plot,  $\zeta=\pi$

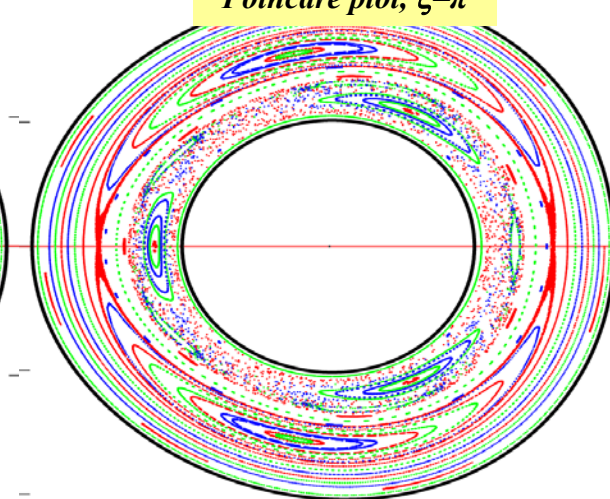
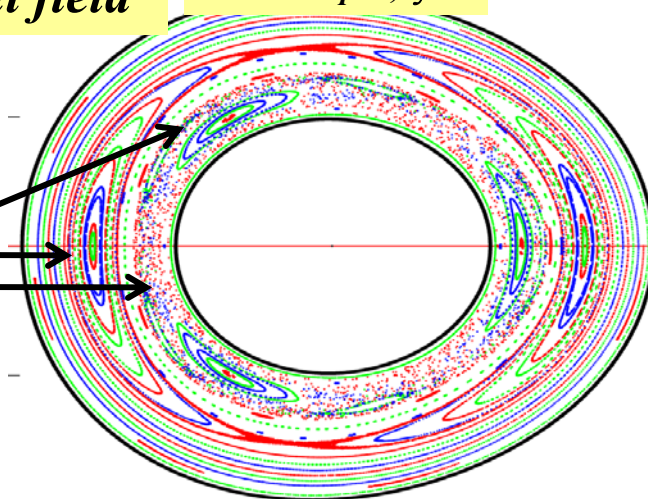
$$\begin{aligned} R &= 1.0 + r(\vartheta, \zeta) \cos \vartheta, \\ Z &= r(\vartheta, \zeta) \sin \vartheta, \end{aligned}$$

inner surface  
 $r = 0.1$

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

outer interface

$$r = 0.2 + \delta [\cos(2\vartheta - \zeta) + \cos(3\vartheta - \zeta)]$$



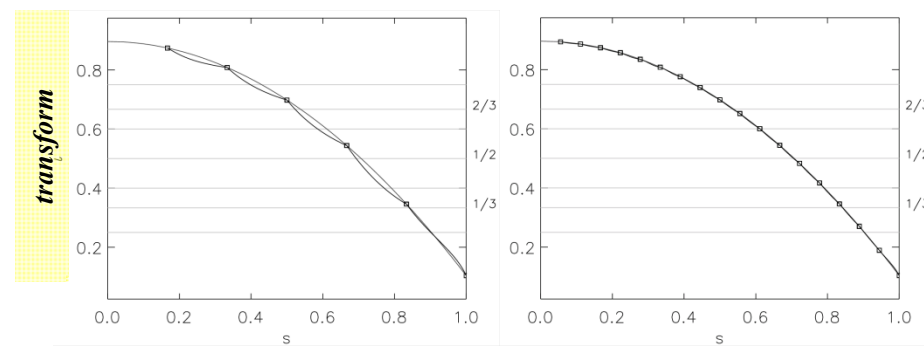
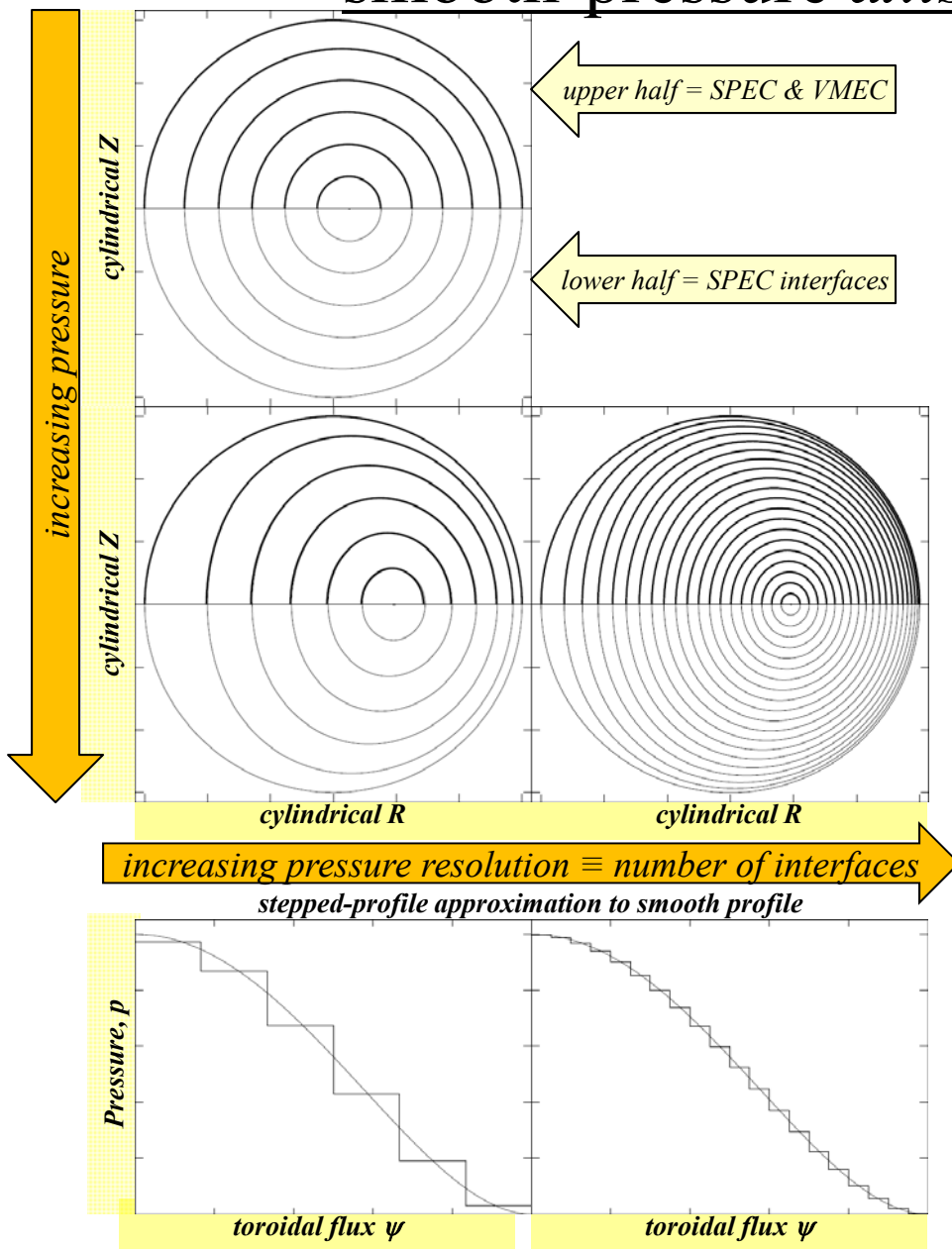
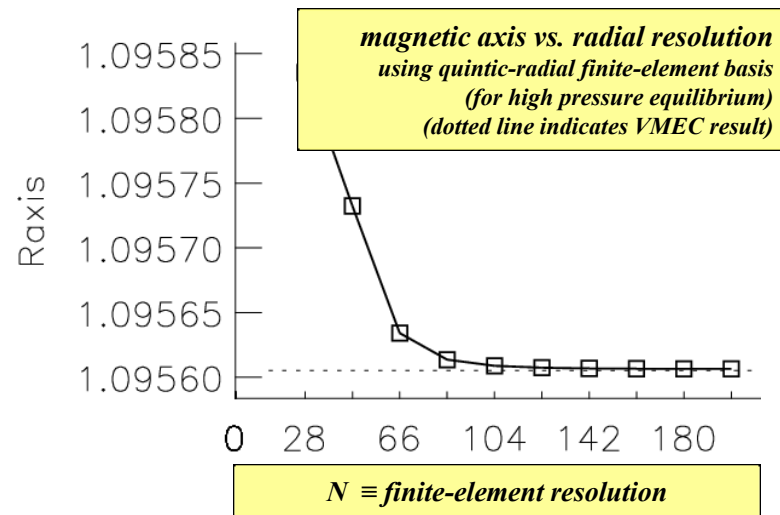


# stepped-pressure equilibria accurately approximate

## smooth-pressure *axisymmetric* equilibria

### 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



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

zero-pressure equilibrium  
 $\beta = 0\%$

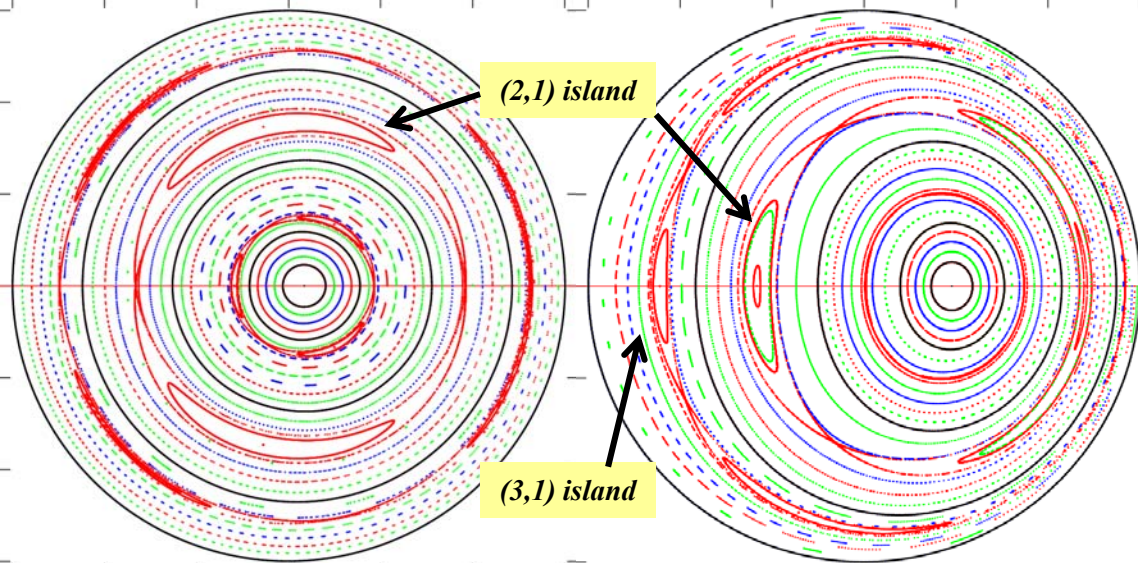
high-pressure equilibrium  
 $\beta \approx 4\%$

boundary deformation induces islands

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

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

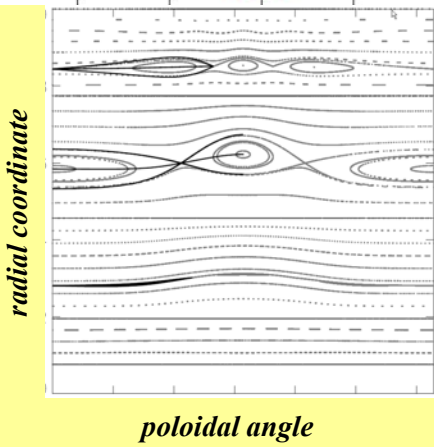
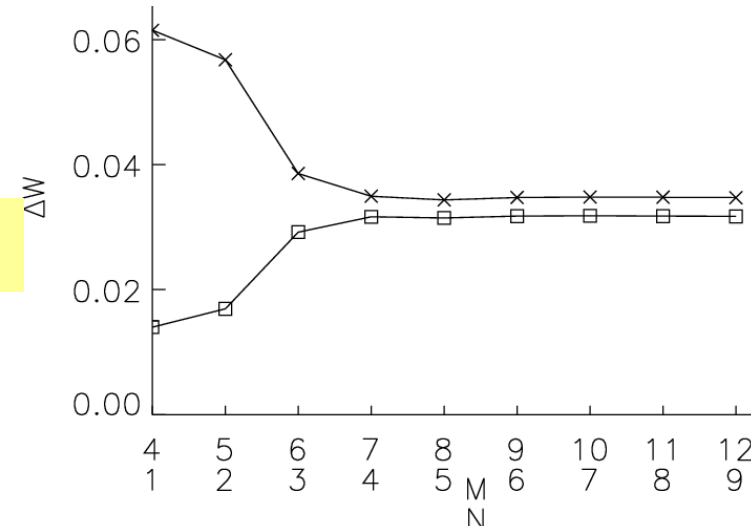
Demonstrated convergence  
with Fourier resolution



(2,1) island

(3,1) island

Convergence of (2,1) & (3,1) island widths  
with Fourier resolution for  $\beta \approx 4\%$  case



← island widths estimated by fitting quasi-rational surface through island chain

# Summary

→ A partially-relaxed, topologically-constrained energy principle has been presented for MHD equilibria with chaotic fields and non-trivial (i.e. non-constant) pressure

→ The model has been implemented numerically

- \* using a high-order (piecewise quintic) radial discretization
- \* an optimal (i.e. spectrally condensed) Fourier representation
- \* workload distributed across multiple cpus,
- \* extrema located using Newton's method with quadratic-convergence

→ Intuitively, the equilibrium model is an extension of Taylor relaxation to multiple volumes

→ The model has a sound theoretical foundation

- \* solutions guaranteed to exist (under certain conditions)

→ The numerical method is computationally tractable

- \* does not invert singular operators
- \* does not struggle to resolve fractal structure of chaos

→ Convergence studies have been performed

- \* expected error scaling with radial resolution confirmed
- \* detailed benchmark with axisymmetric equilibria (with smooth profiles)
- \* that the island widths converge with Fourier resolution has been confirmed



# Toroidal magnetic confinement depends on flux surfaces

Transport in magnetized plasma dominately parallel to  $\mathbf{B}$

→ if the field lines are not confined (e.g. by flux surfaces), then the plasma is poorly confined

Axisymmetric magnetic fields possess a continuously nested family of flux surfaces

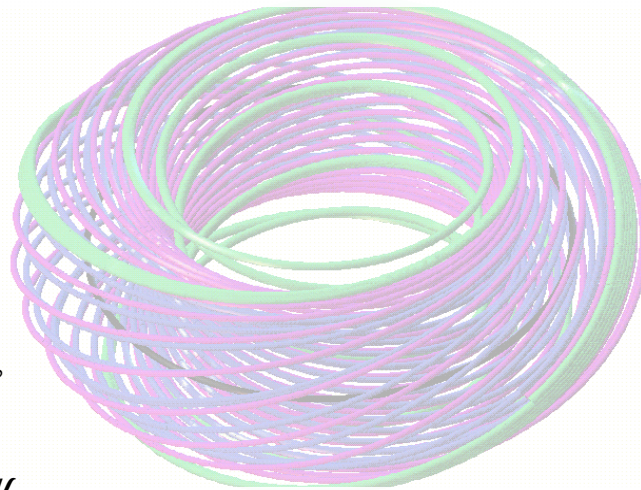
→ nested family of flux surfaces is guaranteed if the system has an ignorable coordinate

magnetic field is called integrable

→ rational field-line  $\equiv$  periodic trajectory family of periodic orbits  $\equiv$  rational flux surface

→ irrational field-lines cover *irrational* flux surface

magnetic field lines wrap around toroidal "flux" surfaces



straight-field-line flux coordinates,

$$\mathbf{B} \cdot \nabla \psi = 0$$

$$\mathbf{B} = \nabla \psi \times \nabla \vartheta + \iota(\psi) \nabla \zeta \times \nabla \psi$$

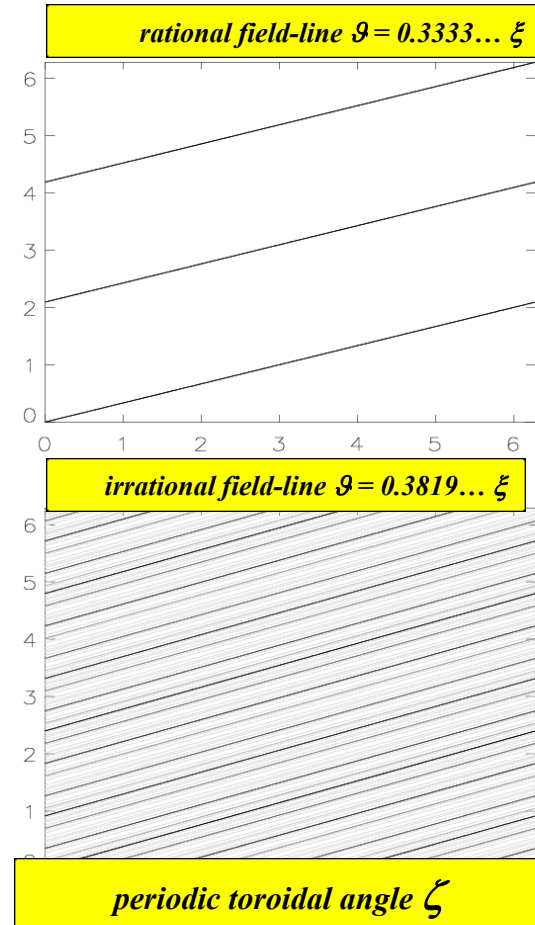
$$\sqrt{g} \mathbf{B} \cdot \nabla \equiv \partial_\zeta + \iota \partial_\vartheta$$

magnetic differential equation,  $\mathbf{B} \cdot \nabla \sigma = s$ ,

is singular at rational surfaces,  $(m \ \iota - n) \sigma_{m,n} = i(\sqrt{g} s)_{m,n}$

periodic poloidal angle  $\vartheta$

periodic poloidal angle  $\vartheta$



# Ideal MHD equilibria are extrema of energy functional

The energy functional is

$$W = \int_V (p + B^2 / 2) dv \quad \boxed{V \equiv \text{global plasma volume}}$$

ideal variations

$$\text{mass conservation} \quad \left. \vphantom{\text{mass conservation}} \right\} \partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\text{state equation} \quad \left. \vphantom{\text{state equation}} \right\} d_t (p \rho^{-\gamma}) = 0$$

$$\text{Faraday's law, ideal Ohm's law} \quad \left. \vphantom{\text{Faraday's law, ideal Ohm's law}} \right\} \delta \mathbf{B} = \nabla \times (\delta \boldsymbol{\xi} \times \mathbf{B}) \quad \rightarrow \text{ideal variations don't allow field topology to change "frozen-flux"}$$

the first variation in plasma energy is

$$\delta W = \int_V (\nabla p - \mathbf{j} \times \mathbf{B}) \cdot \delta \boldsymbol{\xi} dv \quad \begin{array}{l} \text{Euler Lagrange equation for globally ideally-constrained variations} \\ \text{ideal-force-balance} \quad \nabla p = \mathbf{j} \times \mathbf{B} \end{array}$$

→ two surface functions, e.g. the pressure,  $p(s)$ , and rotational-transform  $\equiv$  inverse-safety-factor,  $i(s)$ ,

and → a boundary surface ( $\dots$  for fixed boundary equilibria  $\dots$ ),

constitute "boundary-conditions" that must be provided to uniquely define an equilibrium solution

..... The computational task is to compute the magnetic field that is consistent with the given boundary conditions...

nested flux surface topology maintained by singular currents at rational surfaces

from  $\nabla \cdot (\sigma \mathbf{B} + \mathbf{j}_\perp) = 0$ , parallel current must satisfy  $\mathbf{B} \cdot \nabla \sigma = -\nabla \cdot \mathbf{j}_\perp$ , where  $\mathbf{j}_\perp = \mathbf{B} \times \nabla p / B^2$

$$\sigma_{m,n} = \frac{i(\sqrt{g} \nabla \cdot \mathbf{j}_\perp)_{m,n}}{(m_i - n)} + \delta(m_i - n)$$

- magnetic differential equations are singular at rational surfaces (periodic orbits)
- pressure-driven "Pfirsch-Schlüter currents" have  $1/x$  type singularity
- $\delta$ -function singular currents shield out islands

# Topological constraints : pressure gradients coincide with flux surfaces

## The ideal interfaces are chosen to coincide with pressure gradients

- parallel transport dominates perpendicular transport,
- simplest approximation is  $\mathbf{B} \cdot \nabla p = 0$
- pressure gradients **must** coincide with KAM surfaces  $\equiv$  ideal interfaces

→ *structure of B and structure of the pressure are intimately connected;*

→ *cannot a priori specify pressure without a priori constraining structure of the field;*

[next order of approximation,  $\mathbf{B} \cdot \nabla p$  is small, e.g.  $\partial_t p = \kappa_{\parallel} \nabla_{\parallel}^2 p + \kappa_{\perp} \nabla_{\perp}^2 p = 0$ , with  $\kappa_{\parallel} \gg \kappa_{\perp}$ , e.g.  $\kappa_{\perp} / \kappa_{\parallel} \sim 10^{-10}$

\*pressure gradients coincide with KAM surfaces, cantori . .

\*pressure flattened across islands, chaos with width  $> \Delta w_C \sim (\kappa_{\perp} / \kappa_{\parallel})^{1/4}$

\* anisotropic diffusion equation solved analytically,  $p' \propto 1 / (\kappa_{\parallel} \varphi_2 + \kappa_{\perp} G)$ ,  $\varphi_2$  is quadratic-flux across cantori, G is metric term]

→ *where there are significant pressure gradients, there can be no islands or chaotic regions with width  $> \Delta w_C$*

A fixed boundary equilibrium is defined by:

- given pressure,  $p(\psi)$ , and rotational-transform profile,  $\iota(\psi)$
- geometry of boundary;

(a) only stepped pressure profiles are consistent (numerically tractable) with chaos and  $\mathbf{B} \cdot \nabla p = 0$

(b) the computed equilibrium magnetic field must be consistent with the input profiles

(a) + (b) = where the pressure has gradients, the magnetic field must have flux surfaces.

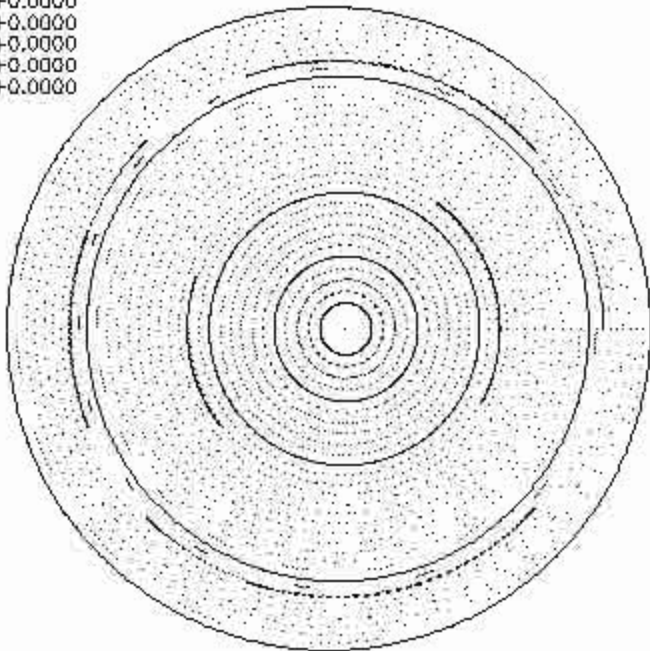
→ non-trivial stepped pressure equilibrium solutions are *guaranteed* to exist

# A sequence of equilibria with increasing pressure and perturbed boundary are computed

*movie of sequence of equilibria with increasing pressure*

$\beta = 0.0000\%$

$\omega_1 = +0.0000$   
 $\omega_2 = +0.0000$   
 $\omega_3 = +0.0000$   
 $\omega_4 = +0.0000$   
 $\omega_5 = +0.0000$



$p = 0.0000$

phase of islands flips near  $n=\infty$  stability boundary