ELM control 2:

BOUT++ simulations of ELMs and RMPs

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Outline of talk

- The BOUT++ code
    - Equations solved, equilibria used, ...
- Ideal MHD simulation of ELMs
    - Linear results and comparison with ELITE
- Diamagnetic effects
    - Modification of linear growth-rates
    - Nonlinear results
- Simulation of RMPs
- Handling large delta-B / B in a field-aligned code
- Conclusions / Future work

BOUT++ Object-Oriented code

- A new C++ framework for developing plasma fluid simulation codes
- Borrows ideas and algorithms from the original 3D BOUndary Turbulence 2-fluid edge simulation code BOUT. Can simulate same set of equations.
- Aims to automate common tasks needed in a simulation code, and separate the error-prone details such as differential geometry, parallel communication and file I/O from the user-specified equations to be solved
- Collaboration with ANL on coupling to the PETSc library and developing preconditioning techniques
- BOUT++ code has been developed for:
  - 2D or 3D curvilinear geometry
  - Linear machines and tokamaks
  - Different topologies e.g. X-points
- Automatically handles parallel communication efficiently to thousands of processors

Example: Ideal MHD equations

Physics equations written in a form close to analytic expressions

$$\frac{\partial n}{\partial t} = -n\nabla\cdot\mathbf{v} - \mathbf{v}\cdot\nabla n$$

```
dndt = -n*Div(v) - V_dot_Grad(v,n)
```

$$\frac{\partial p}{\partial t} = -\mathbf{v}\cdot\nabla p - \gamma p\nabla\cdot\mathbf{v}$$

```
dpdt = -V_dot_Grad(v,p) - gamma*p*Div(v)
```

$$\frac{\partial \mathbf{v}}{\partial t} = -\mathbf{v}\cdot\nabla\mathbf{v} + \frac{1}{n}\left[(\nabla\times\mathbf{B})\times\mathbf{B} - \nabla p\right]$$

```
dvdt = -V_dot_Grad(v,v) + ((Curl(B)^B) - Grad(p))/n
```

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla\times(\mathbf{v}\times\mathbf{B})$$

```
dBdt = Curl(v^B)
```

Enables quick development of new physics models, and testing of numerical methods

ELM simulations

- Complicated models (e.g. 2-fluids) include many physical effects, but have disadvantages, including:
  - Known solutions become rare, and analytic solutions almost non-existent
  - Generating starting equilibria becomes non-trivial
  - Interpreting the results can be difficult
- Aim to develop robust simulations of ELMs, benchmarked (as far as possible) against known solutions
- Ideal MHD has been used to study the linear (and early non-linear*) behaviour of ELMs, using analytic theory and linear codes (e.g. ELITE)
  - Provides a known starting point for developing ELM simulations
- Starting by simulating (high-beta flute-) reduced MHD, for comparison with ELITE
- Simplified equilibria (limiter equilibria), currently no x-points though these can be handled.

Reduced MHD

- Start with simplest model: Reduced ideal MHD
- Solve for temperature (pressure), vorticity, and parallel vector potential. Density is a constant, flat profile
- Can be compared with ELITE / GATO

$$\frac{dp}{dt} = -\frac{1}{B_0}\mathbf{b}_0 \times \nabla\phi \cdot \nabla p$$

Pressure equation

$$\rho_0 \frac{d\omega}{dt} = B_0^2 \mathbf{b} \cdot \nabla \left(\frac{J_{||}}{B_0}\right) + 2\mathbf{b}_0 \times \kappa_0 \cdot \nabla p$$

Vorticity equation

$$\frac{\partial A_{||}}{\partial t} = -\nabla_{||}\phi$$

Magnetic potential

$$A_{||} = \mathbf{b} \cdot \mathbf{A}$$

$$\mathbf{B}_1 = \nabla A_{||} \times \mathbf{b}_0$$

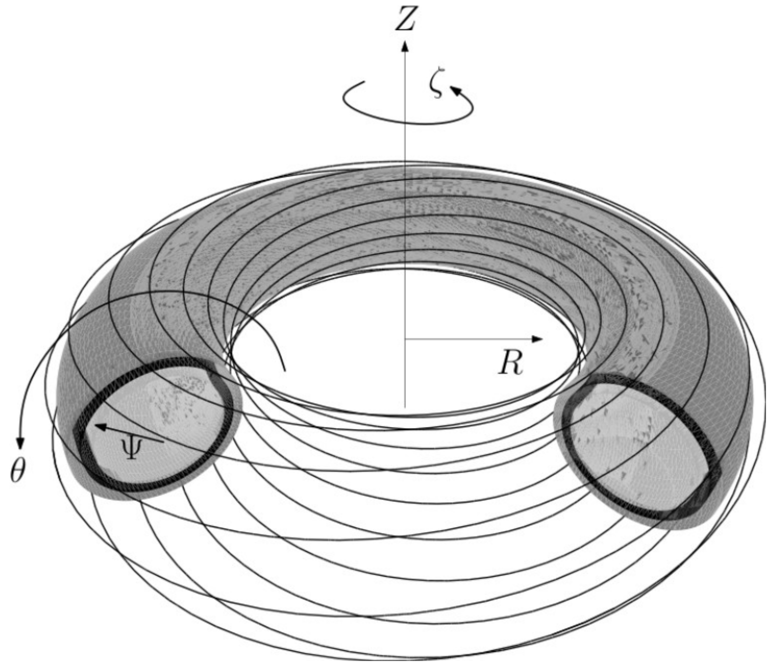
$$J_{||} = J_{||0} - \frac{1}{\mu_0}\nabla_\perp^2 A_{||}$$

Zero electric field along magnetic field-lines

Coordinate system

BOUT++ can use any (2D) metric tensor. For tokamak simulations, a field-aligned coordinate system is used

Start with standard toroidal coords

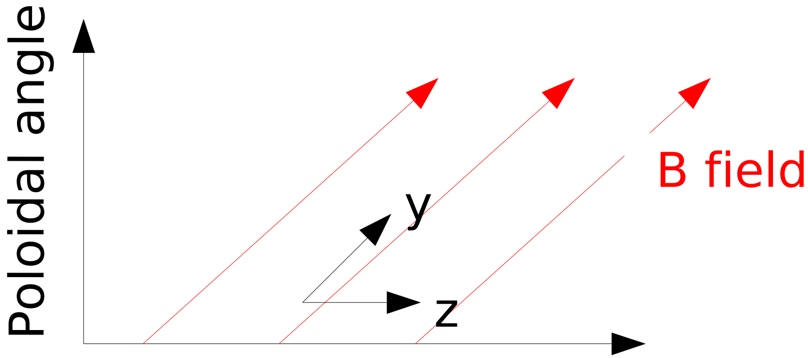


Transform into ballooning coords.

$$x = \psi - \psi_0$$
$$y = \theta$$
$$z = \zeta - \int_{\theta_0}^{\theta} \nu(\psi, \theta)\, d\theta$$

$$\nu(\psi, \theta) = \frac{\mathbf{B}\cdot\nabla\zeta}{\mathbf{B}\cdot\nabla\theta} = \frac{B_\zeta h_\theta}{B_\theta R}$$

Field-line pitch

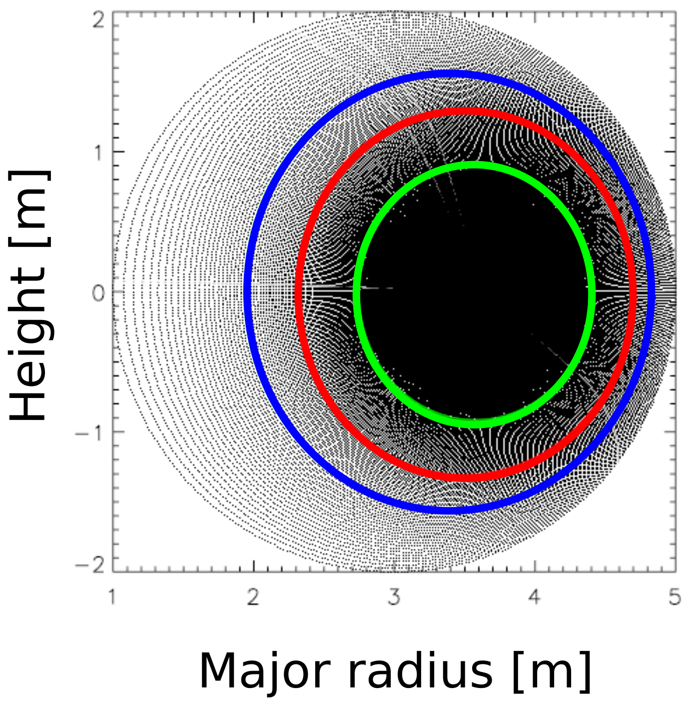


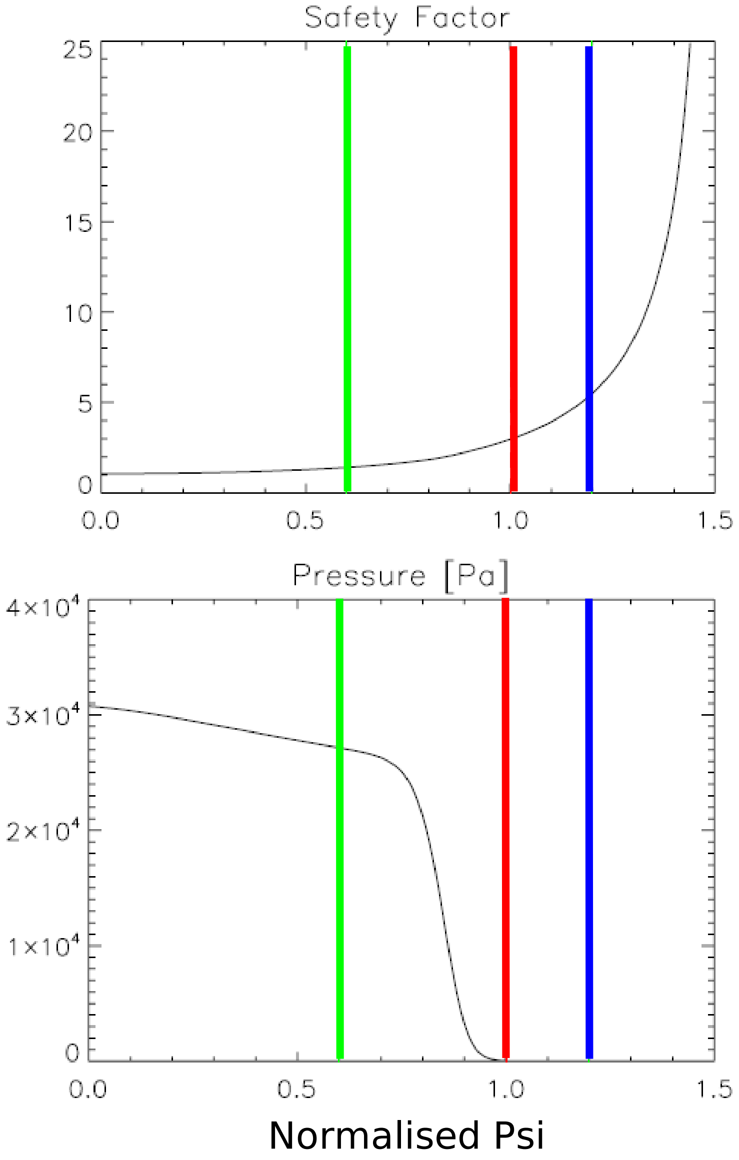
Align y coordinate with magnetic field to exploit anisotropy $k_{||} \ll k_{\perp}$

Equilibrium for ELM simulations

Starting with a simplified benchmark case

- Large aspect-ratio
- Circular cross-section
- Highly unstable equilibrium
- Strongly pressure-driven (ballooning).



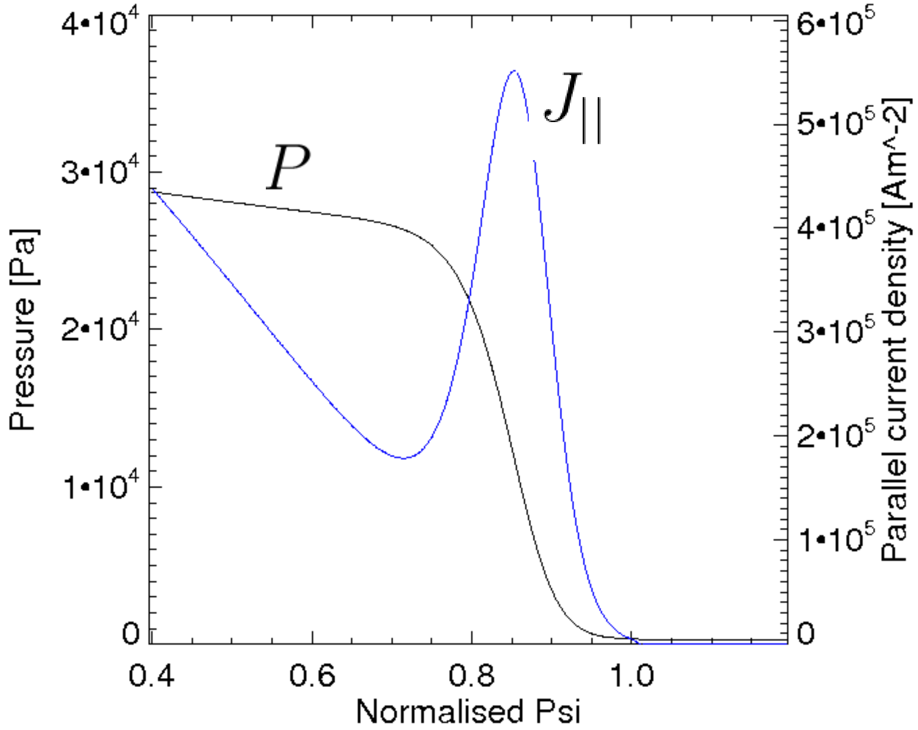


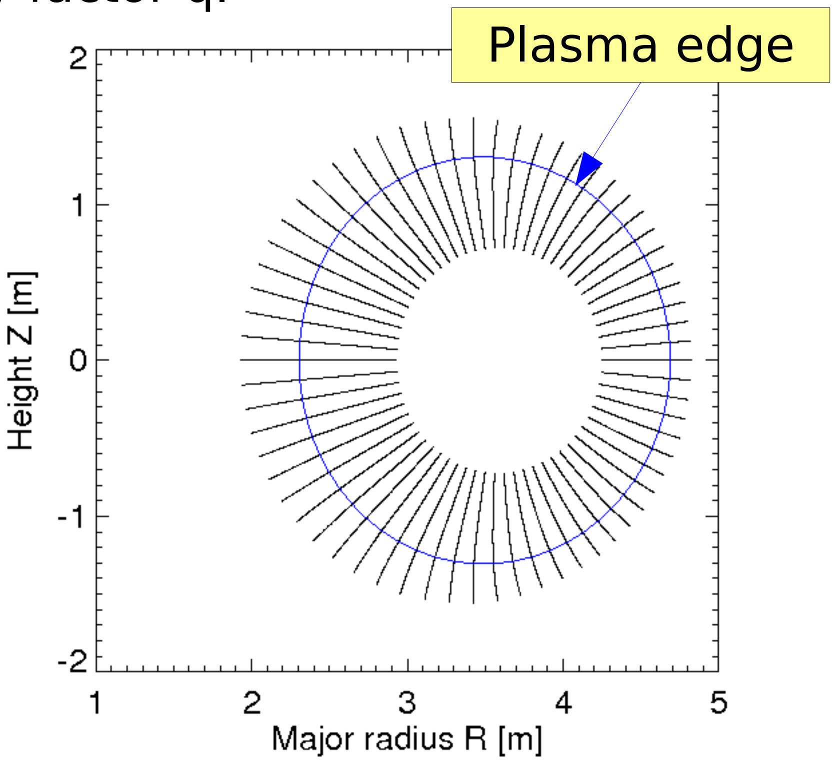
Equilibrium for ELM simulations

Grid refined in radial direction to resolve ideal modes peaked in the pedestal region

Coarsened in the poloidal direction since this is the parallel direction in this coordinate system.

Note: Poloidal resolution (slice through solution) actually ~4000 points, depending on toroidal resolution and safety factor q.

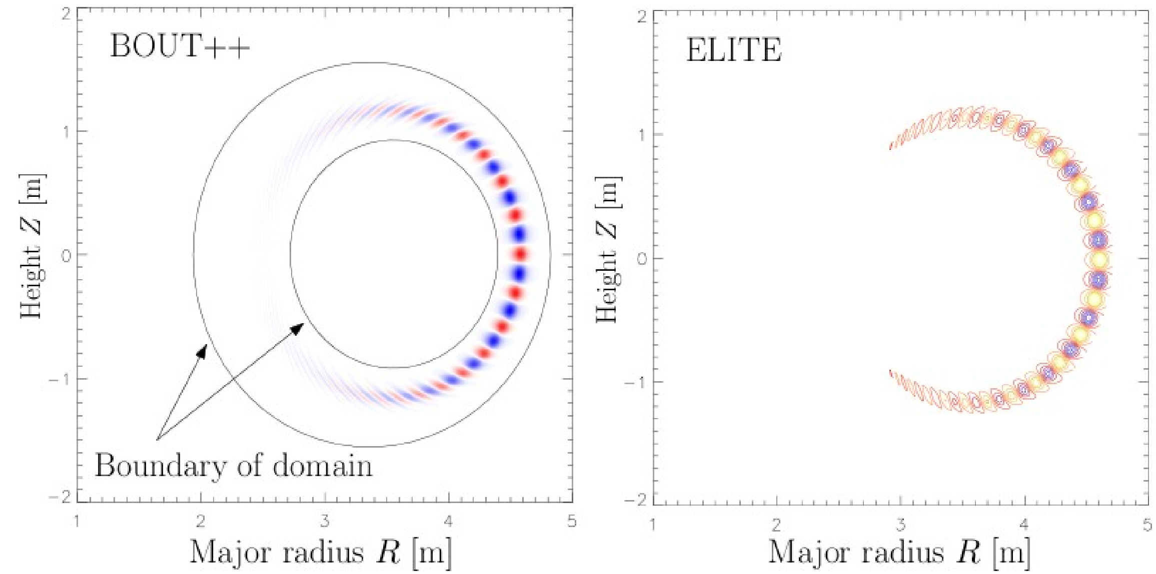




ELITE benchmarking

For linear calculations, the radial displacement can be calculated from BOUT++ using the ExB velocity

$$\gamma\xi_\psi = -\nabla\phi\times\mathbf{B}/B^2\cdot\hat{\mathbf{e}}_\psi$$



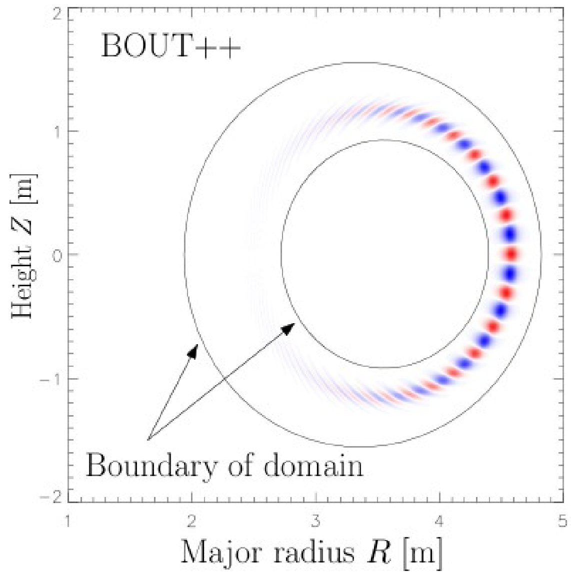
Good agreement for mode-structure

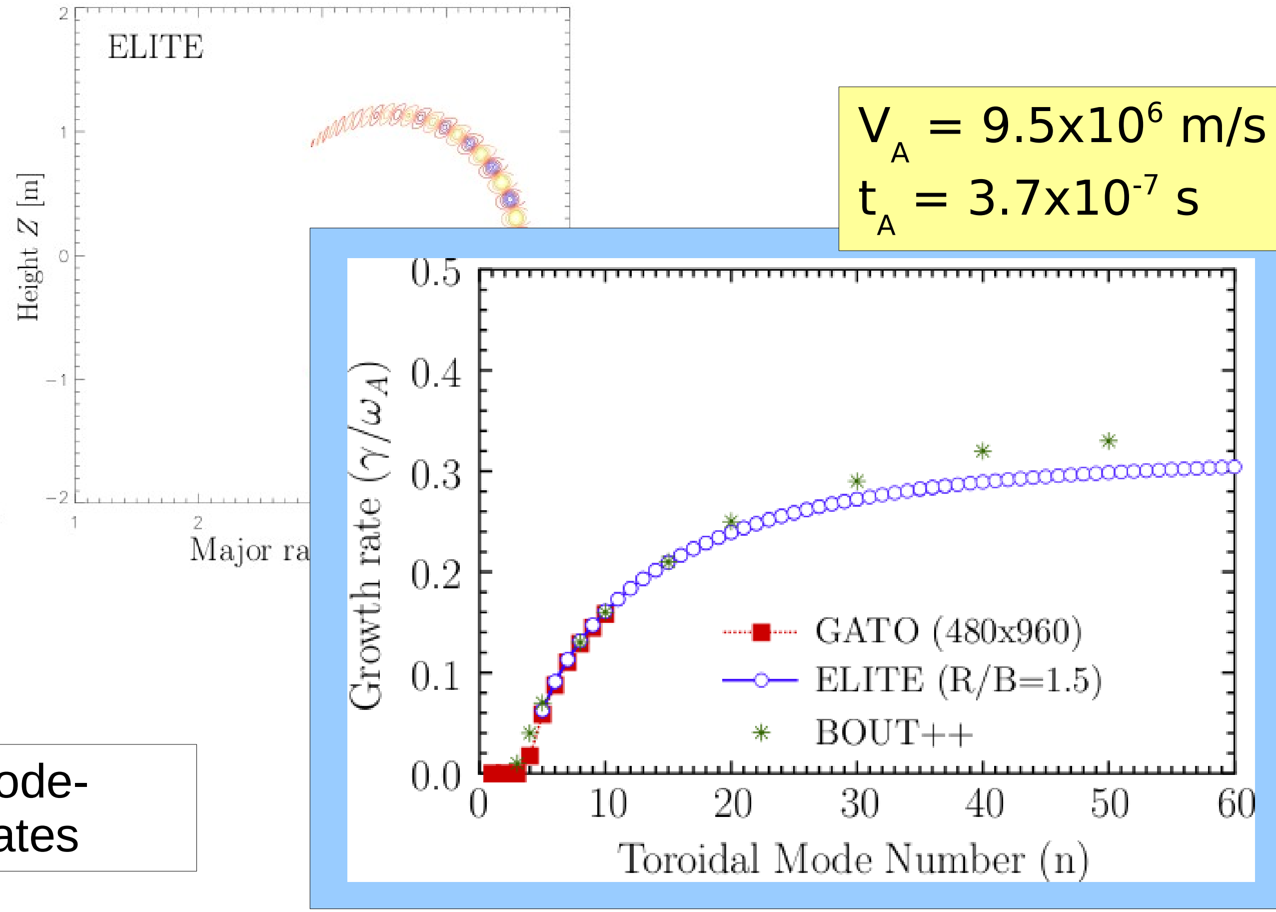
Resolution used: 256 radial, 64 parallel, 16 toroidal (1/20th of a torus)

ELITE benchmarking

For linear calculations, the radial displacement can be calculated from BOUT++ using the ExB velocity

$$\gamma \xi_\psi = -\nabla \phi \times \mathbf{B}/B^2 \cdot \hat{\mathbf{e}}_\psi$$





$V_A = 9.5 \times 10^6$ m/s
$t_A = 3.7 \times 10^{-7}$ s

Good agreement for mode-structure and growth-rates

Structure of linear modes

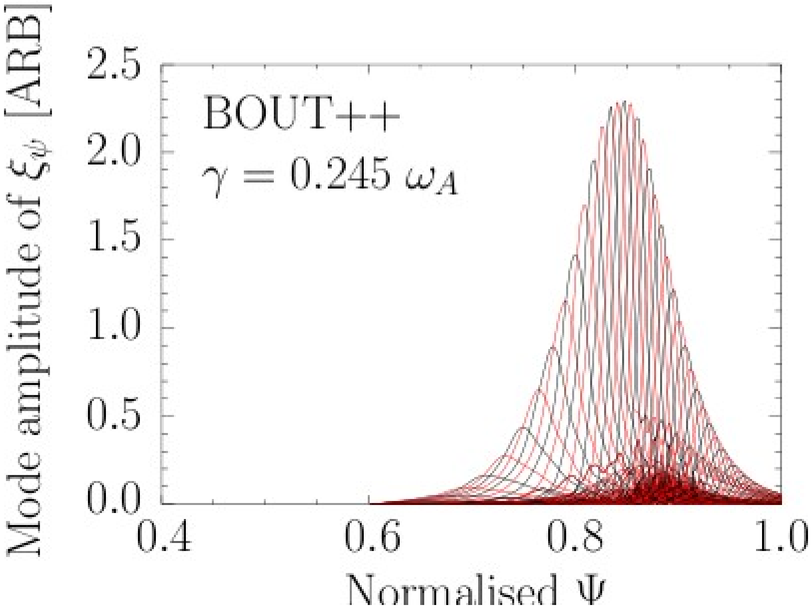
Poloidal harmonics: a more quantitative comparison of mode-structures

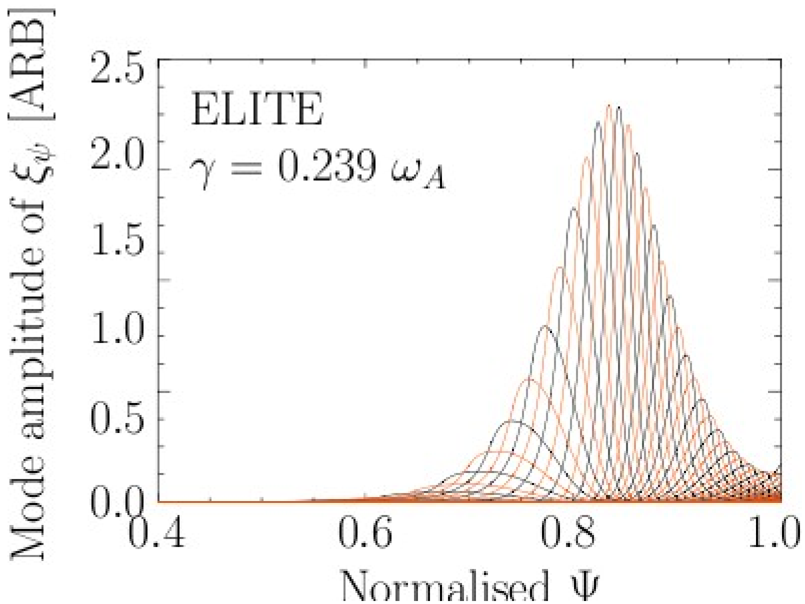
For comparison with linear MHD, calculate radial displacement

$$\gamma\xi_\psi = -\nabla\phi\times\mathbf{B}/B^2\cdot\hat{\mathbf{e}}_\psi$$

Take FFT in poloidal angle

$$\chi = \frac{1}{q}\int_{\theta_0}^{\theta}\frac{B_\zeta}{B_\theta R}\sqrt{\left(\frac{\partial R}{\partial\theta}\right)^2+\left(\frac{\partial Z}{\partial\theta}\right)^2}d\theta$$





Individual poloidal harmonics peak close to resonant surfaces

Handling of vacuum regions

- Suppression of current in “vacuum” region
- High-resistivity region
  - Results in a small time-step associated with fast diffusion
  - Current can diffuse out of plasma region into vacuum (finite transition region). This can actually increase currents in vacuum!

Handling of vacuum regions

- Suppression of current in “vacuum” region
- High-resistivity region
  - Results in a small time-step associated with fast diffusion
  - Current can diffuse out of plasma region into vacuum (finite transition region). This can actually increase currents in vacuum
- Instead, solve the magnetostatic problem in the vacuum region:

$$\nabla_\perp^2 A_{||} = 0$$

- High-resistivity region may be a more realistic model of the SOL than a perfect vacuum, but useful to keep the same model as linear codes
- In order to solve this whilst allowing a moving plasma-vacuum location, this inversion problem is turned into a time-evolution problem

Time-evolved vacuum region

In the vacuum region, solve a relaxation problem to a state with zero vacuum currents

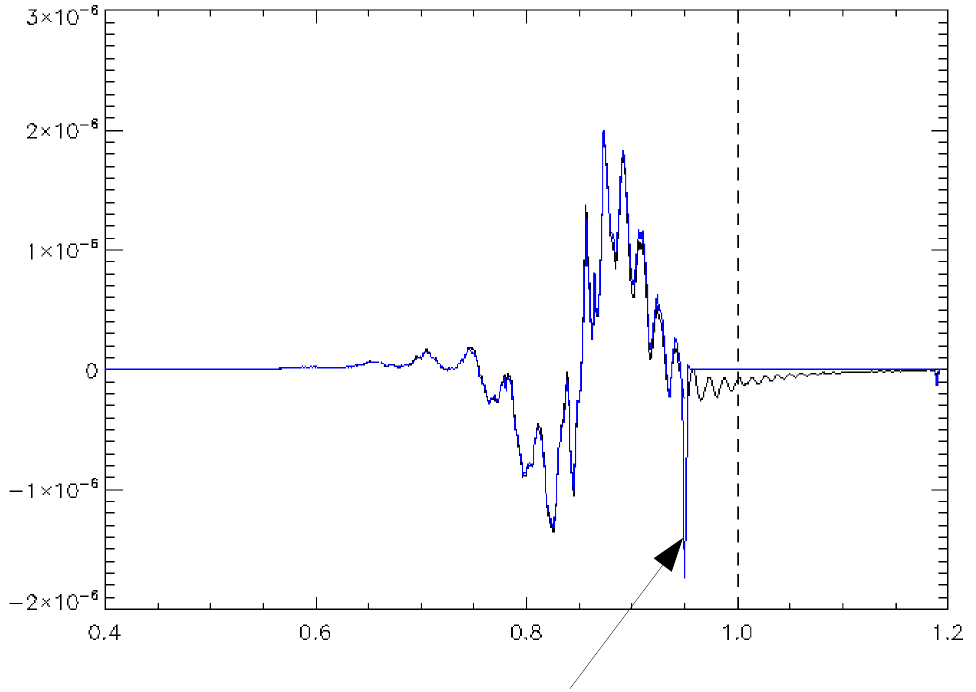
$$\frac{\partial A_{||}}{\partial t} = -\Theta\nabla_{||}\phi + (1-\Theta)\left(A_{||}^{target} - A_{||}\right)/\tau_{jvac} \qquad \Theta = \begin{cases} 1 & \text{plasma} \\ 0 & \text{vacuum} \end{cases}$$

At each timestep, the "target" state is calculated from the current A using:

$$A_{||}^{target} = \nabla_\perp^{-2}\left(\Theta\nabla_\perp^2 A_{||}\right)$$

Provided time-constant is small enough, field in vacuum relaxes to a self-consistent state with no vacuum currents.

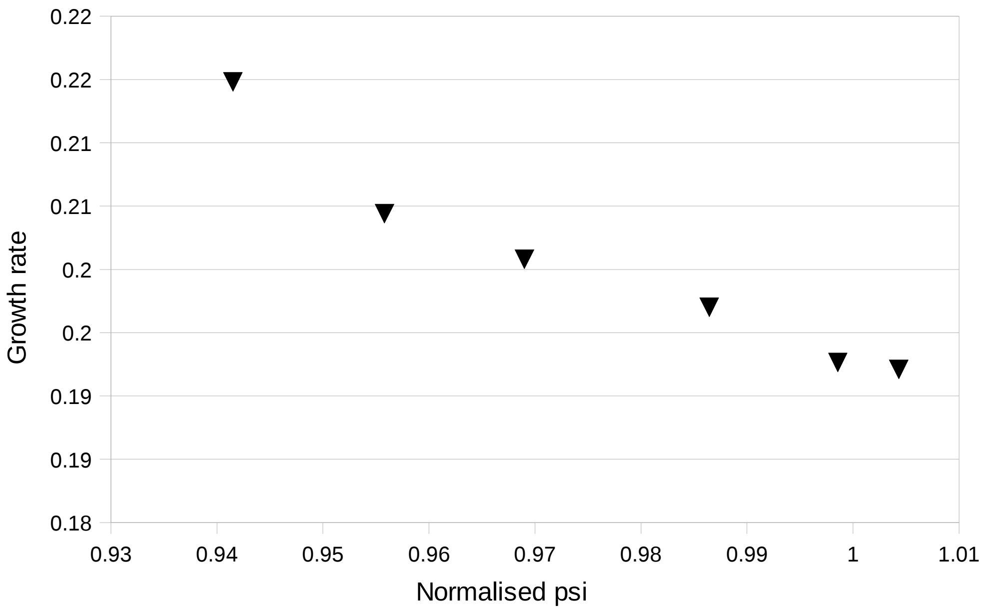
Moving plasma-vacuum interface changes Θ during nonlinear evolution

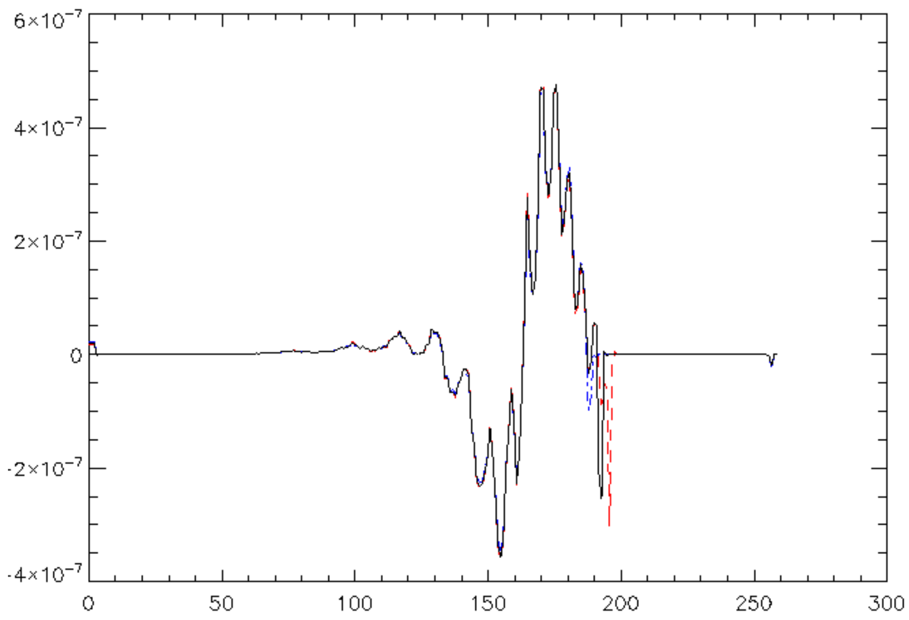


Surface current is formed

Sensitivity to boundary location

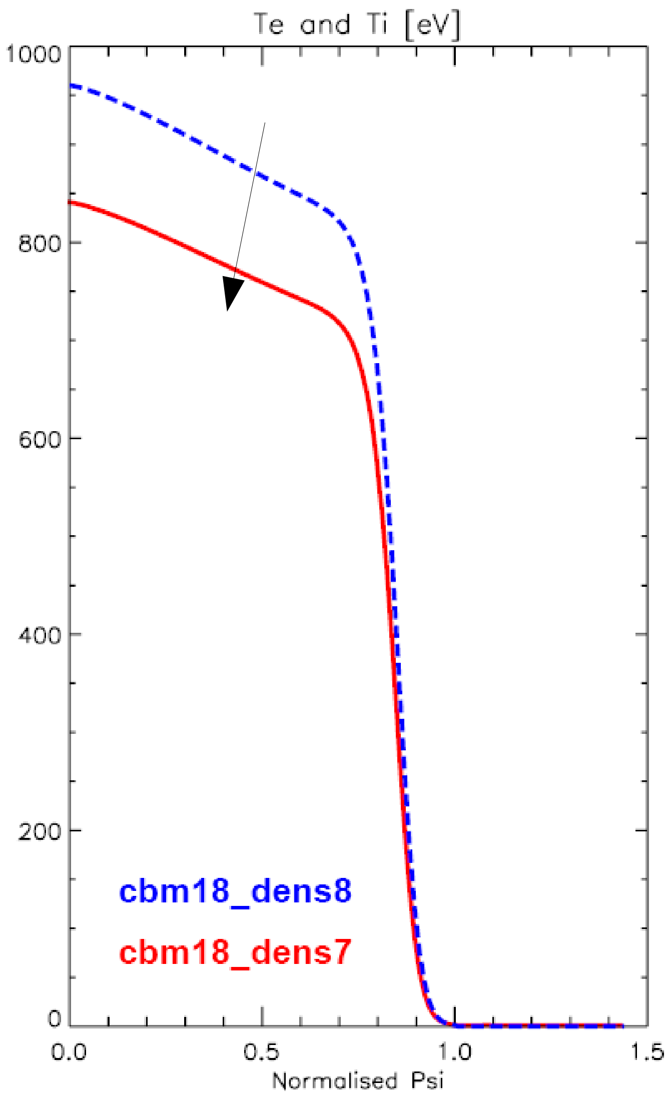
Plasma-vacuum boundary determined by a threshold in pressure
Allows motion of boundary during nonlinear stage



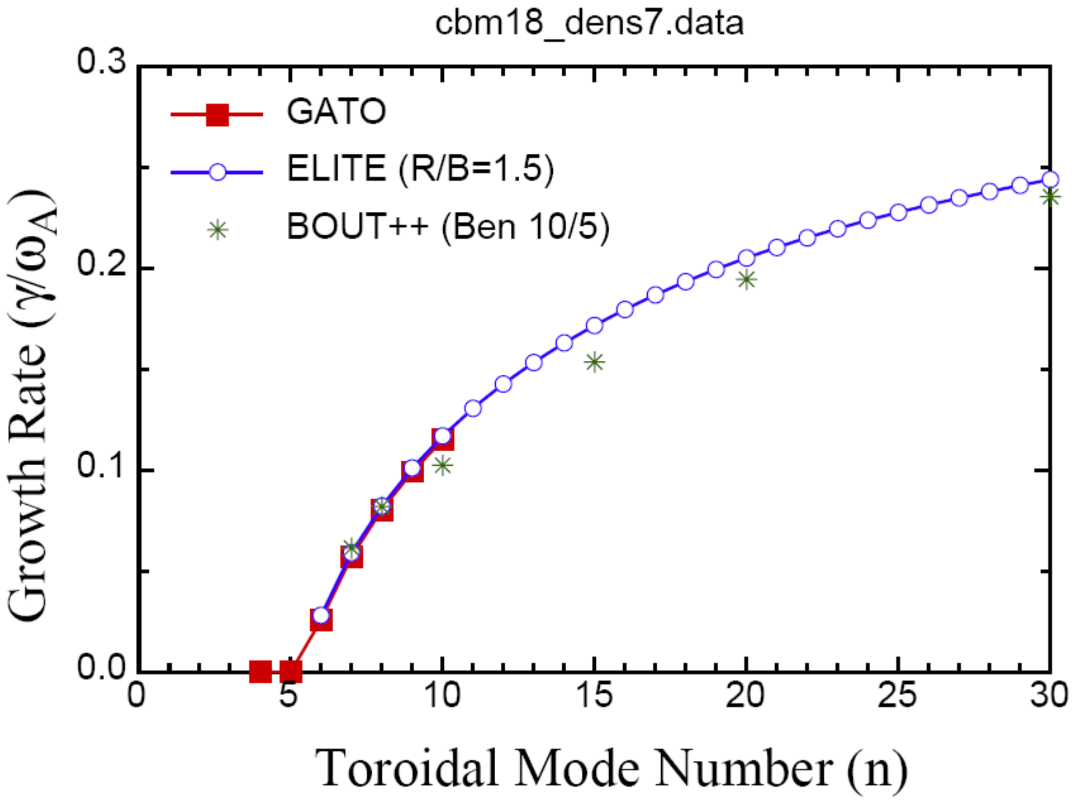


Since this case is strongly ballooning, it has only a small dependence on plasma-vacuum location.

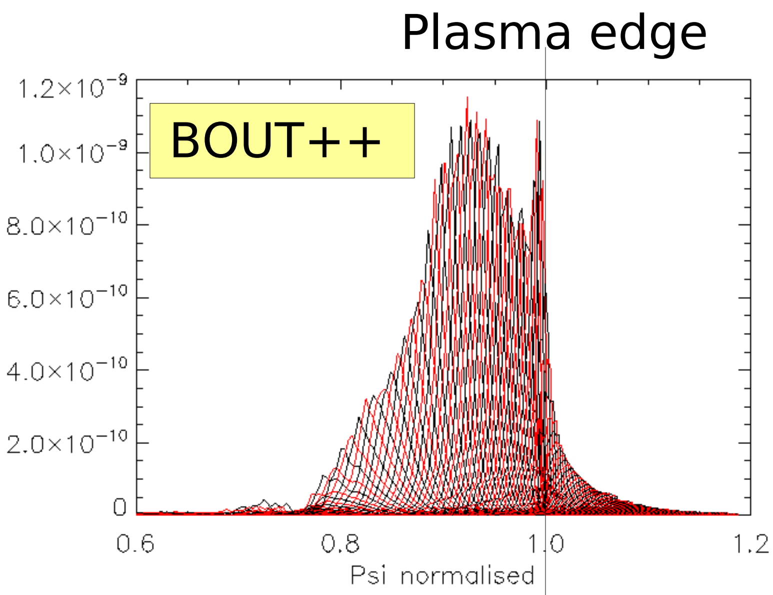
Lower growth-rate case



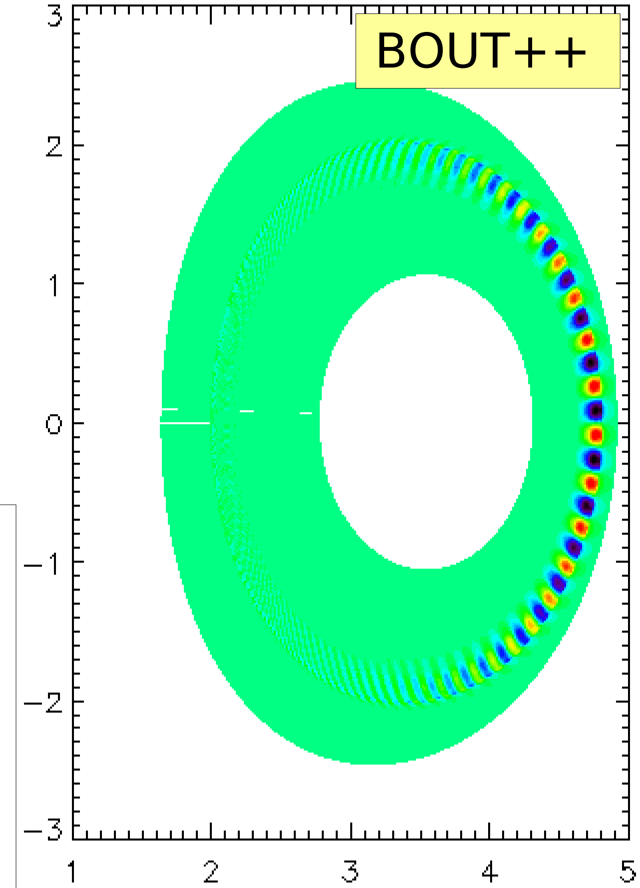
- Reducing the pressure gradient to lower growth-rates
- Still get good agreement between ELITE and BOUT++

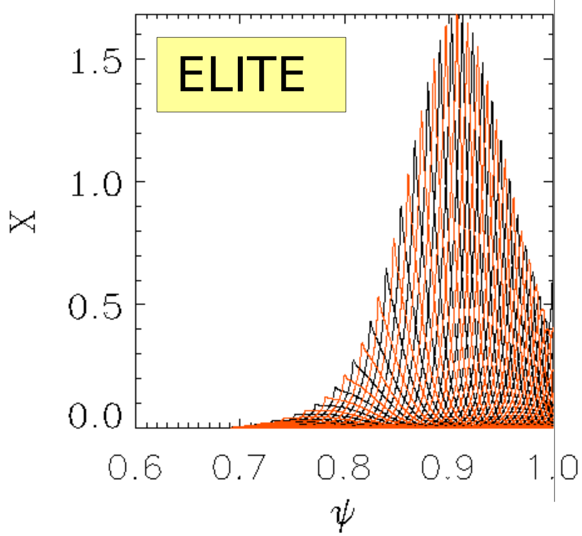


Shaped equilibria



Shaped plasma closer to marginal stability





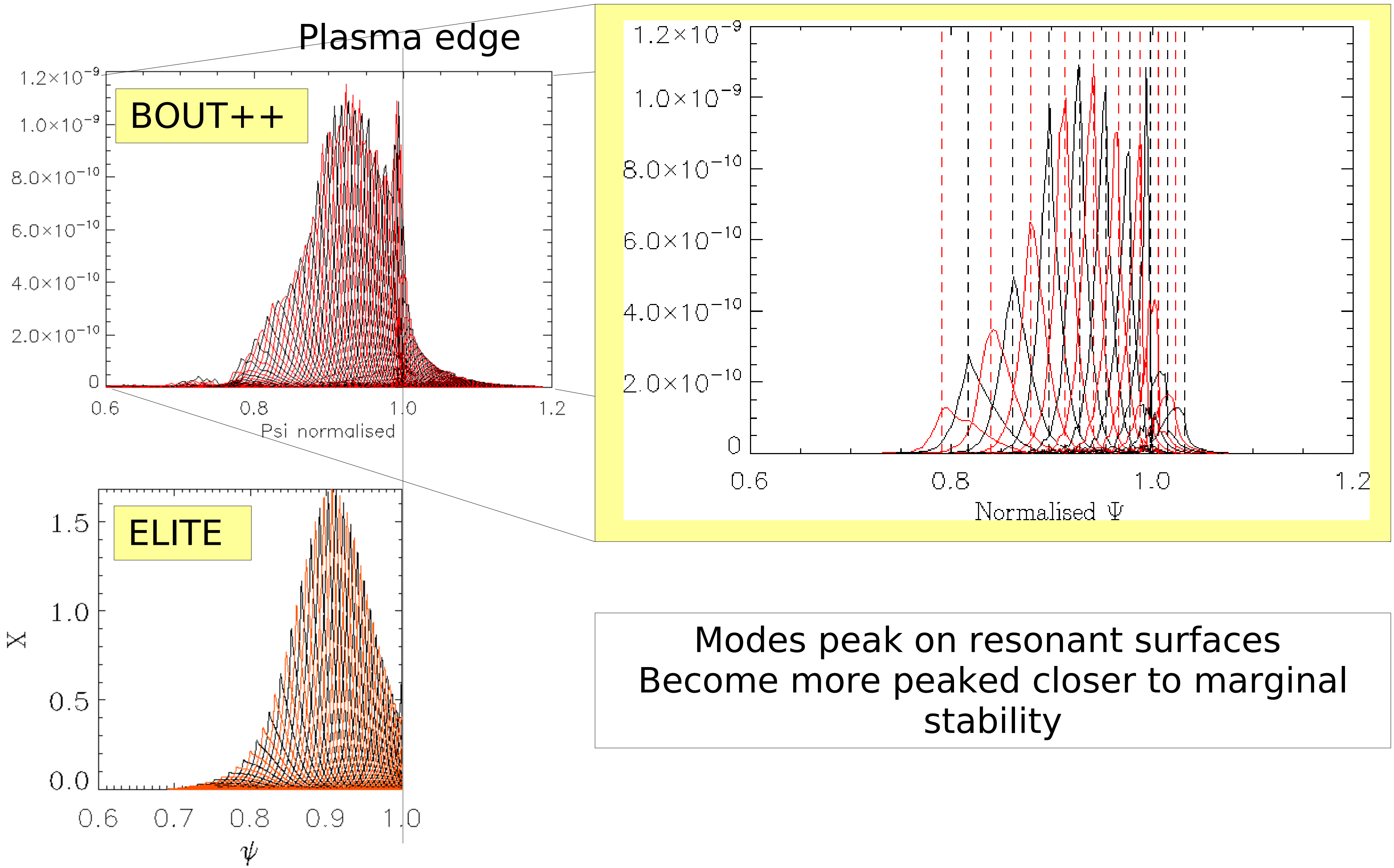
<u>Growth rate</u>

ELITE 0.012 w_A

BOUT++ 0.027 w_A

Larger relative error
fine balance between large
competing effects
Absolute error is still small.

Shaped equilibria



Modes peak on resonant surfaces
Become more peaked closer to marginal stability

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  - Modification of linear growth-rates
  - Nonlinear results
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Diamagnetic effects

Linear ideal MHD simulations agree well with ELITE linear code. Extending the code gradually by adding diamagnetic drift effects.

After gyroviscous cancellation, the diamagnetic modifies the vorticity (and additional nonlinear terms).

$$\rho_0 \frac{d\omega}{dt} = B_0^2 \mathbf{b} \cdot \nabla \left(\frac{J_{||}}{B_0} \right) + 2\mathbf{b}_0 \times \kappa_0 \cdot \nabla p \qquad \omega = \frac{1}{B} \nabla_\perp^2 \phi + \frac{1}{B} \nabla_\perp^2 \left(\frac{P_i}{en} \right)$$

Ohms law unmodified here (no Grad Te)

Diamagnetic stabilisation

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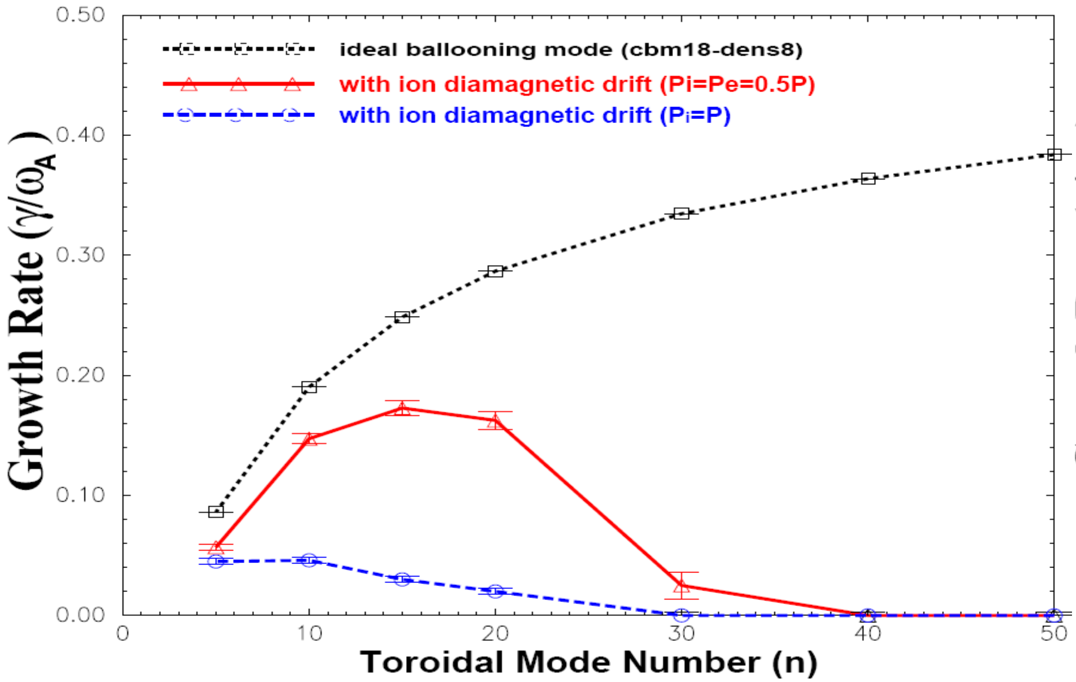

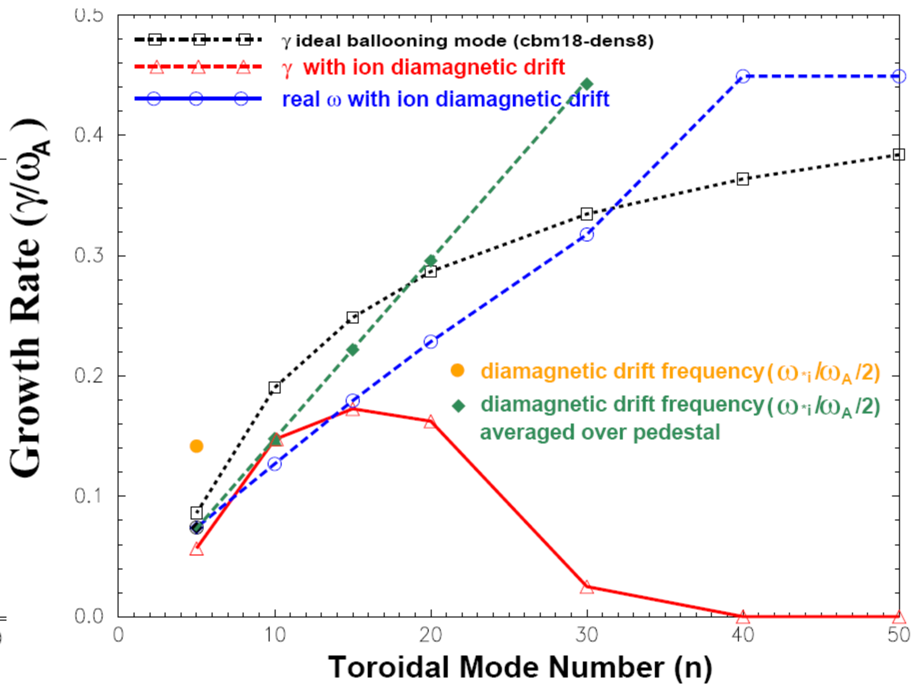

Equilibrium ExB flow

- Equilibrium is stationary, so there should be an E x B flow to balance the diamagnetic drift:

$$E_r = \frac{1}{Z_i e n}\frac{\partial P}{\partial r} \qquad \mathbf{V}_E = \frac{1}{B^2}\mathbf{B}\times\nabla\left(\phi + \phi_0\right)$$

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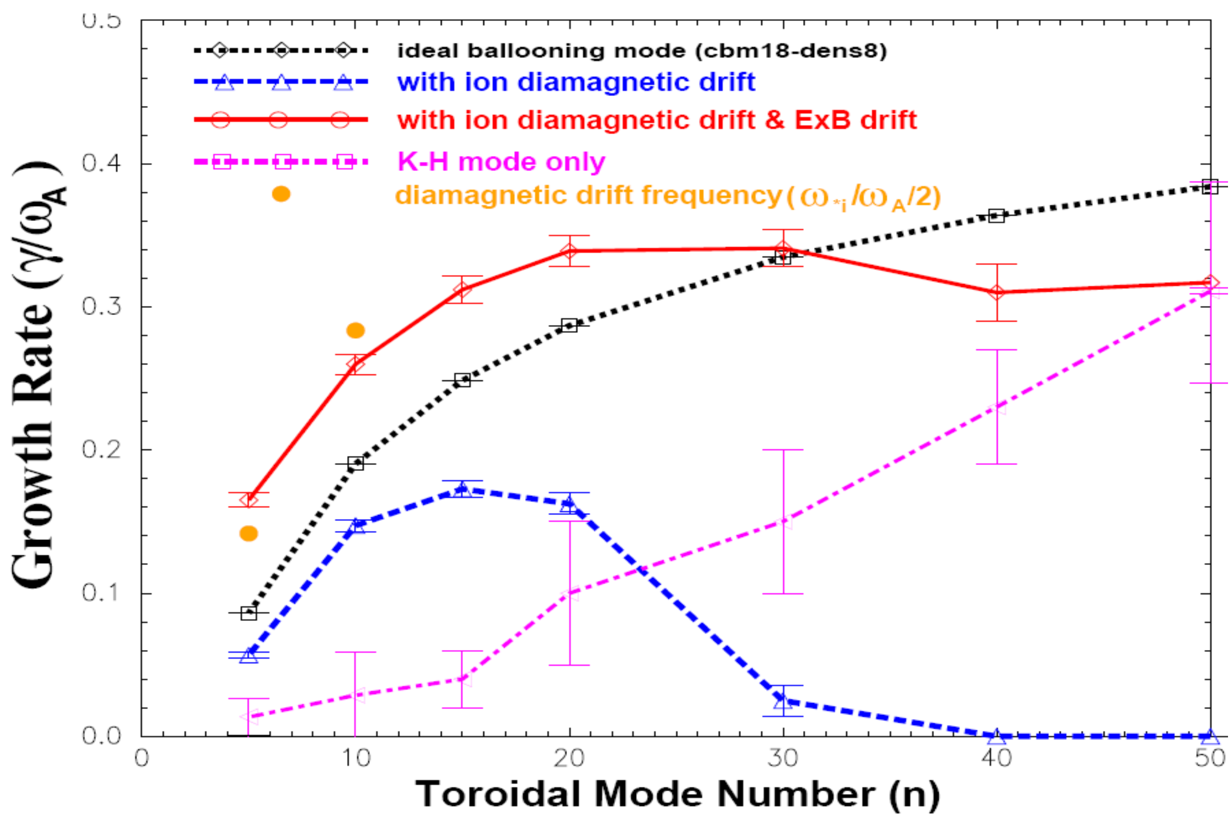
This flow shear drives another type of instability (possibly K-H)

Raises the growth-rate above ideal for low-n

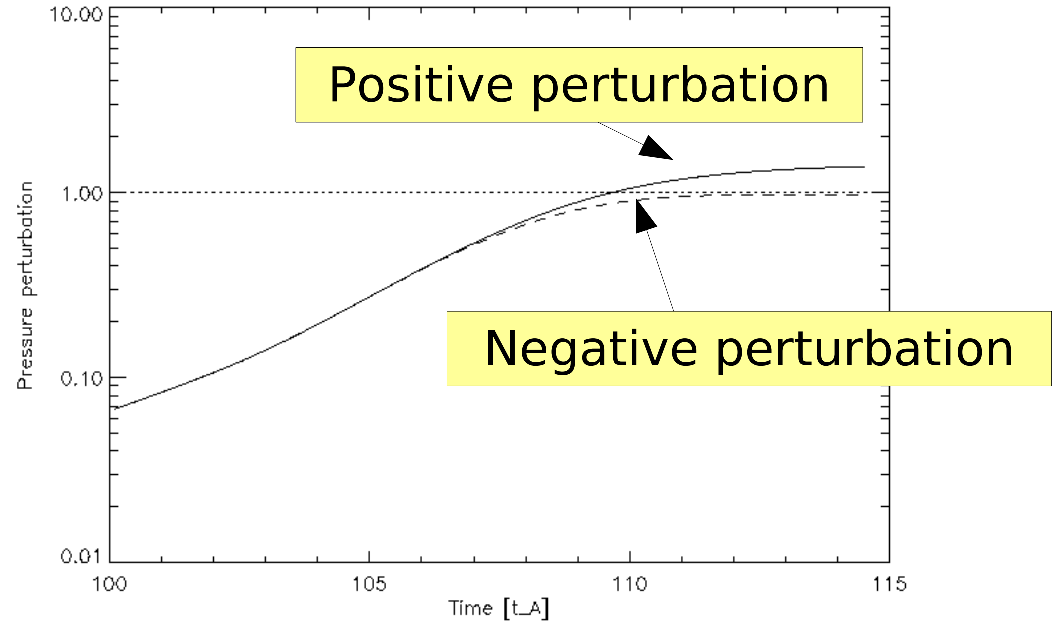
Test case still far above marginal, so Strong K-H drive



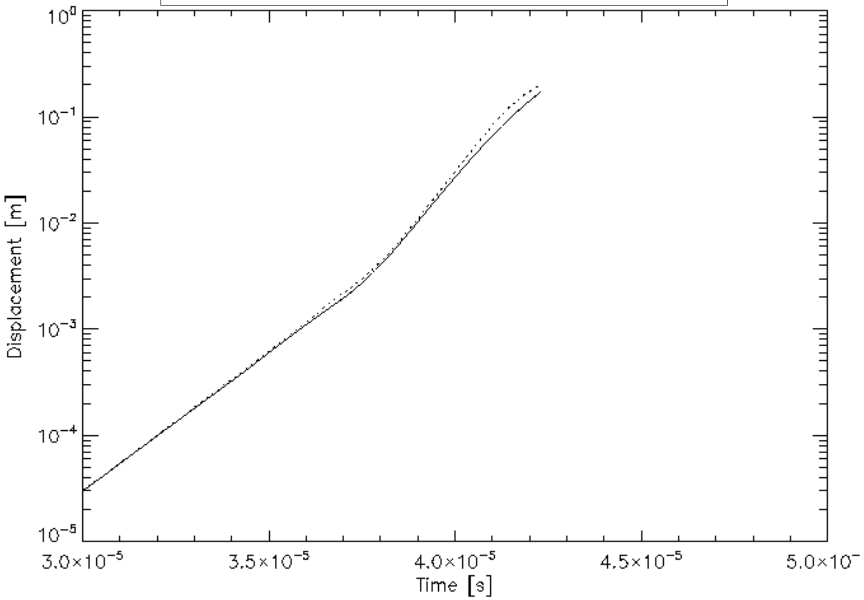
Non-linear growth

MHD case (no diamagnetic drift)

Pressure perturbation at fixed location saturates (as it must to avoid negative values)



Radial displacement



Instead, plot radial displacement of a given flux-surface

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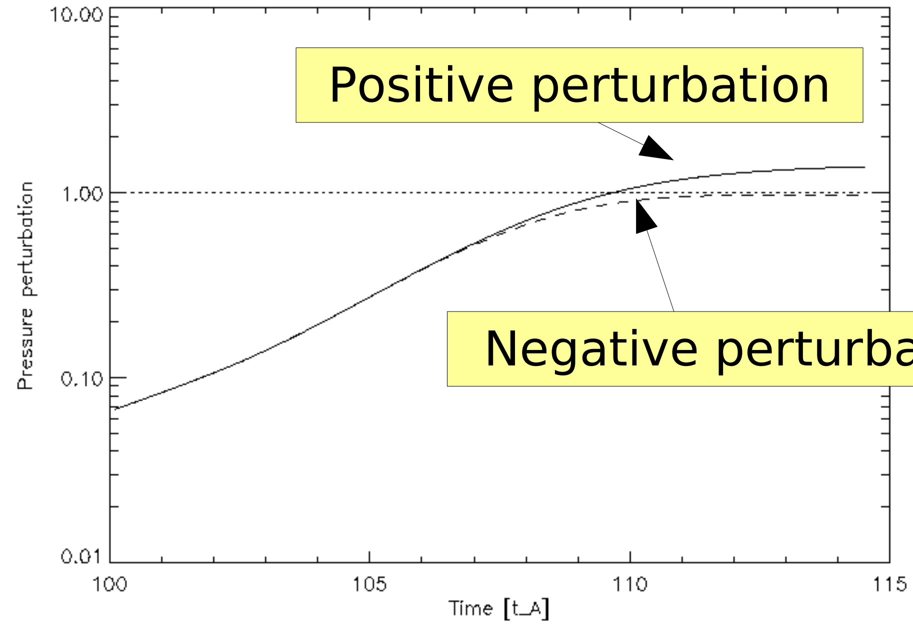
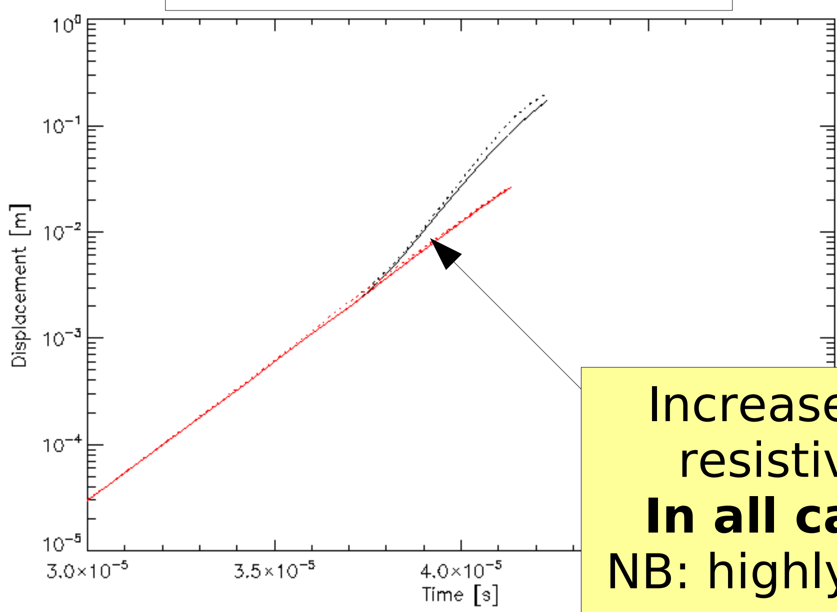


Instead, plot radial displacement of a given flux-surface

NB: Logarithmic scale

Radial displacement



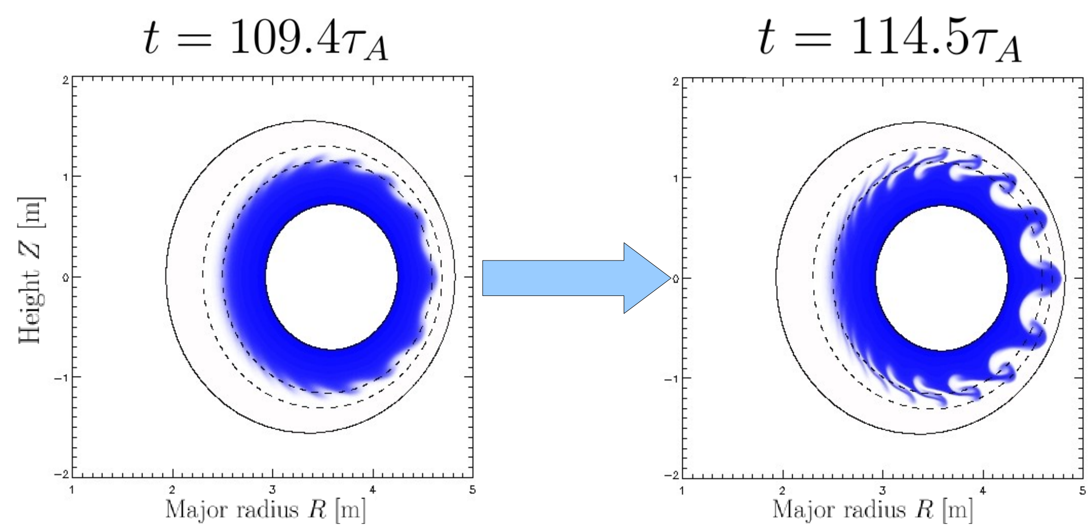
Increase in growth-rate is due to introduction of resistivity. Compare with ideal MHD run (red)

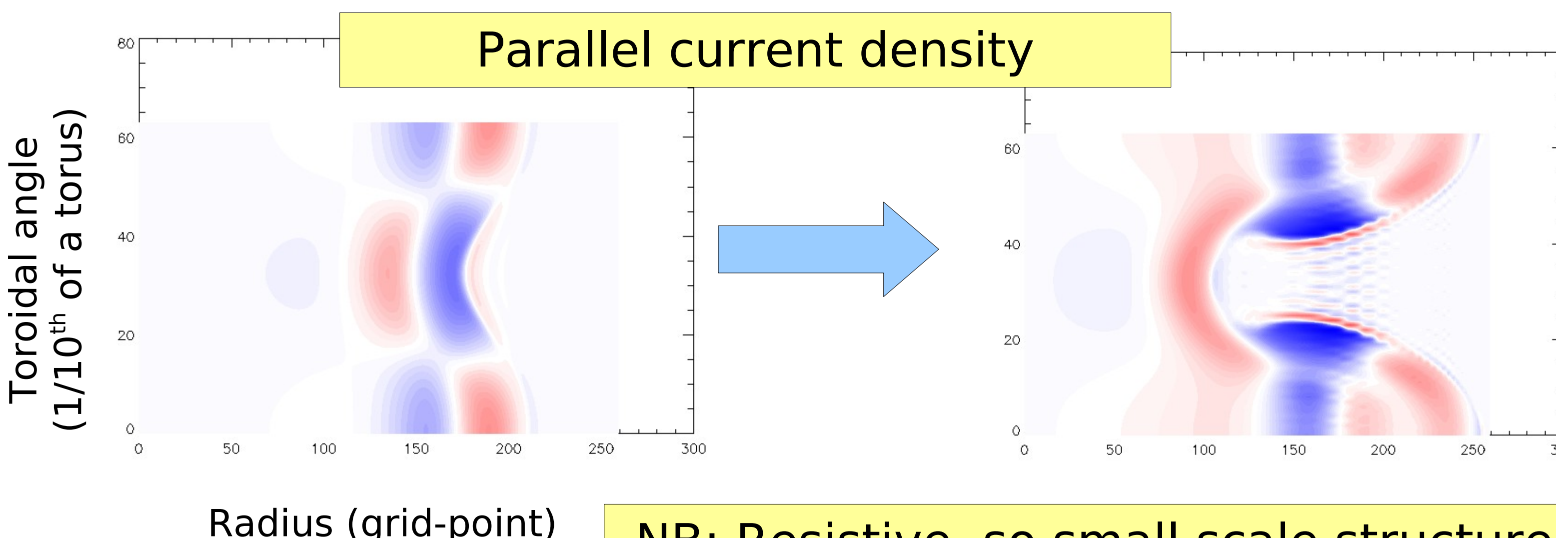
In all cases, filament accelerates outwards

NB: highly unstable, so non-linear stage dominated by linear drive

Nonlinear evolution

- Resistive MHD shows eruption of filaments which accelerate outwards.
- Plasma-vacuum interface maintained despite motion of the plasma.

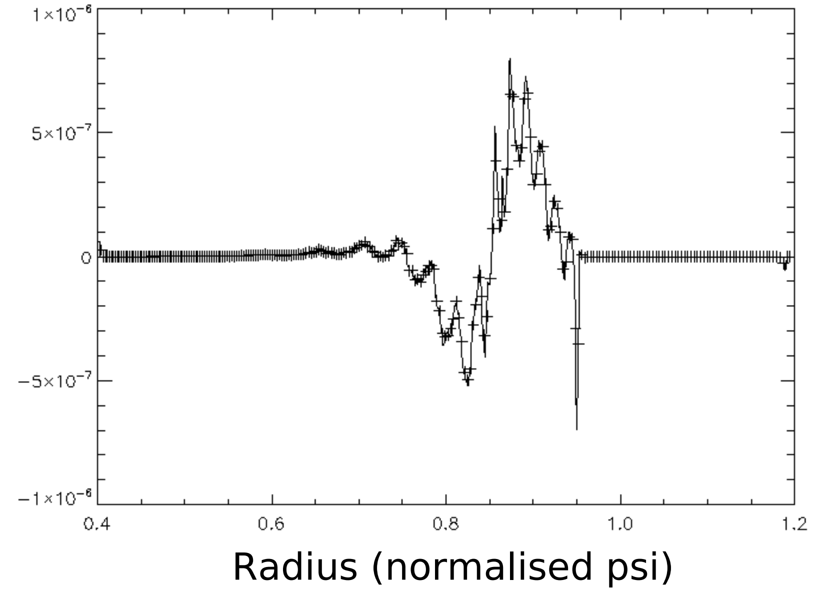


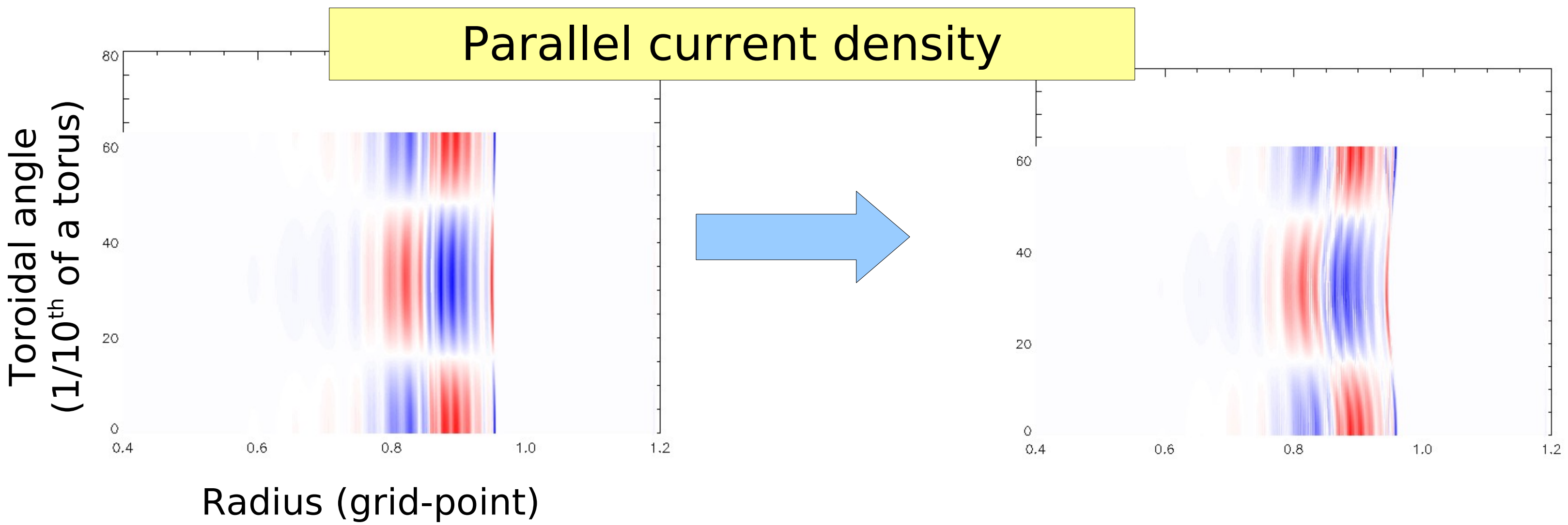


NB: Resistive, so small scale structure removed

Nonlinear evolution

- Ideal MHD
- Small-scale radial structure (current sheets) at rational surfaces
- Nonlinear motion of current sheets leads to numerical problems. Timestep -> 0.





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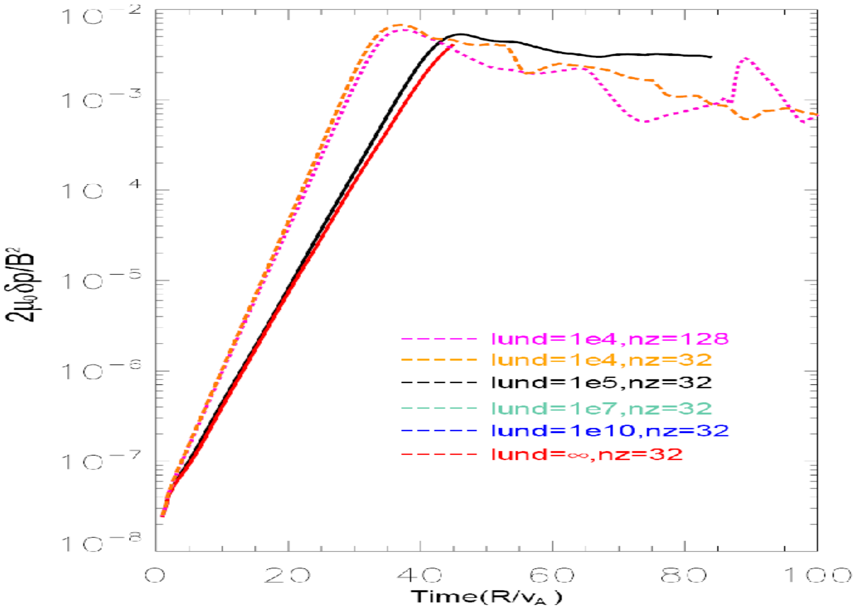
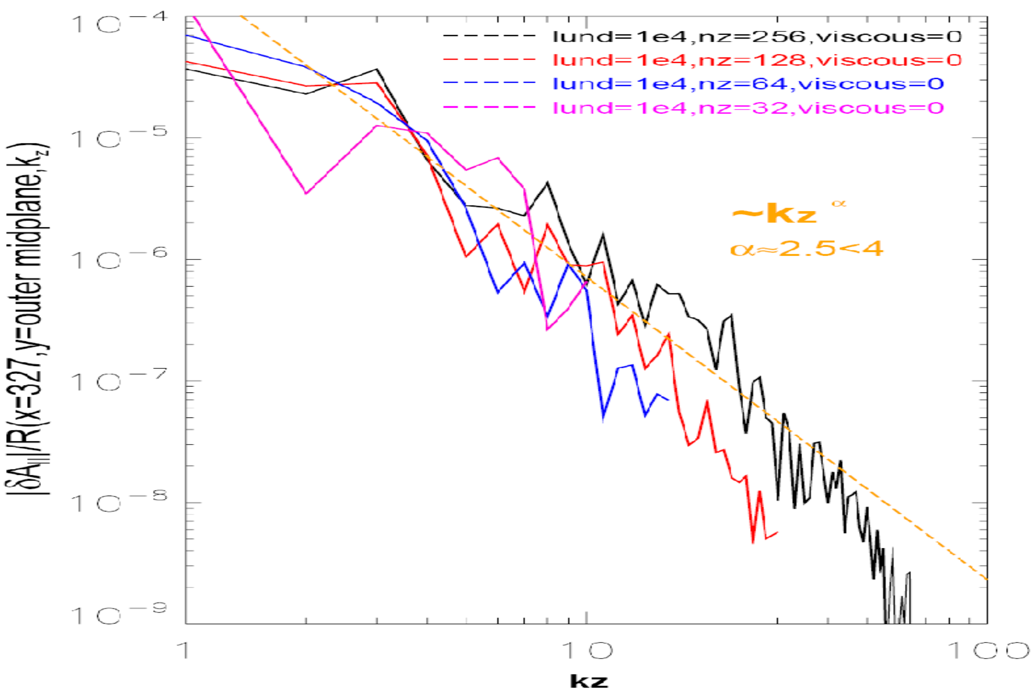
Nonlinear evolution

- Diamagnetic effects (and resistivity)
- Shearing breaks up emerging filament
- Results in dynamics similar to turbulence, with a power spectrum





ELM simulations summary

- BOUT++ can simulate linear ballooning modes, agreeing well with ELITE
  - Converging on a standard set of test cases: BOUT++, NIMROD, JOREK and M3D-c1 all find good agreement with ELITE for this ballooning case.
  - Each of these codes use quite different numerical methods
- Preliminary results incorporating diamagnetic effects show:
  - Suppression of high-n modes as expected
  - That associated E_r drives another type of instability
- Nonlinear results show eruption of plasma filaments
  - Very different results when incorporating diamagnetic effects
  - Currently require enhanced resistivity for numerical stability

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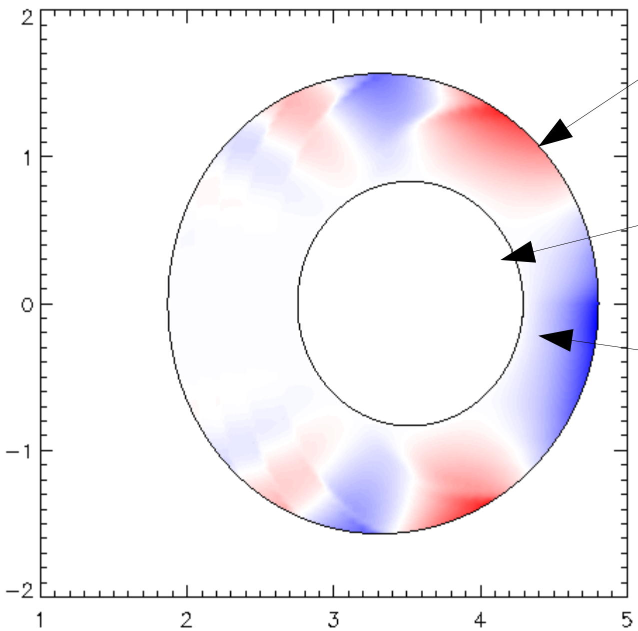
BOUT++ RMP simulations

Initial runs using simple model for external field coils
Similar test case (cbm18 dens 6). Ideally stable to low n modes

Parallel magnetic potential



Apply an m,n perturbation at the domain outer boundary

Perturbation set to zero on inner boundary

Solve $\nabla_\perp^2 A_{||} = 0$ inside domain

Linearly ramp up the external field (~10^{-4} T) on a timescale of 10^{-4} s (282 t_A)

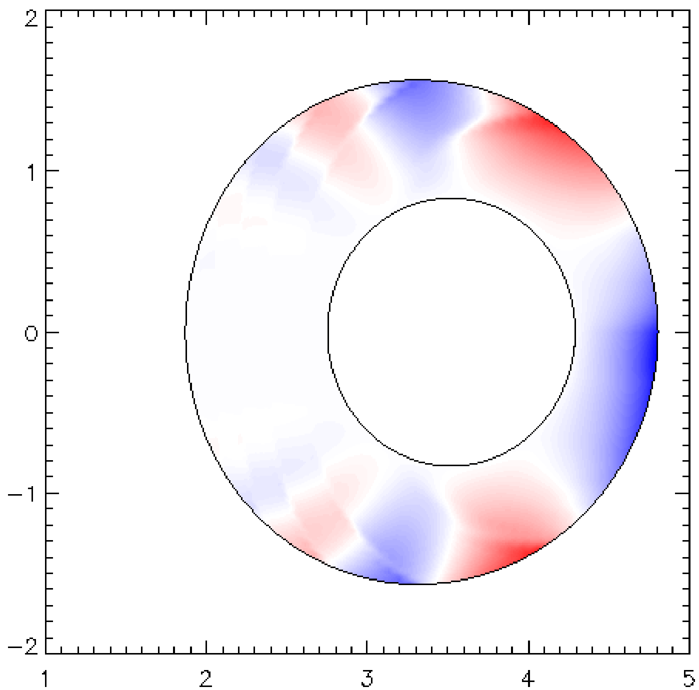
Include non-linear effects, but only retain n = 3 mode

RMP simulations

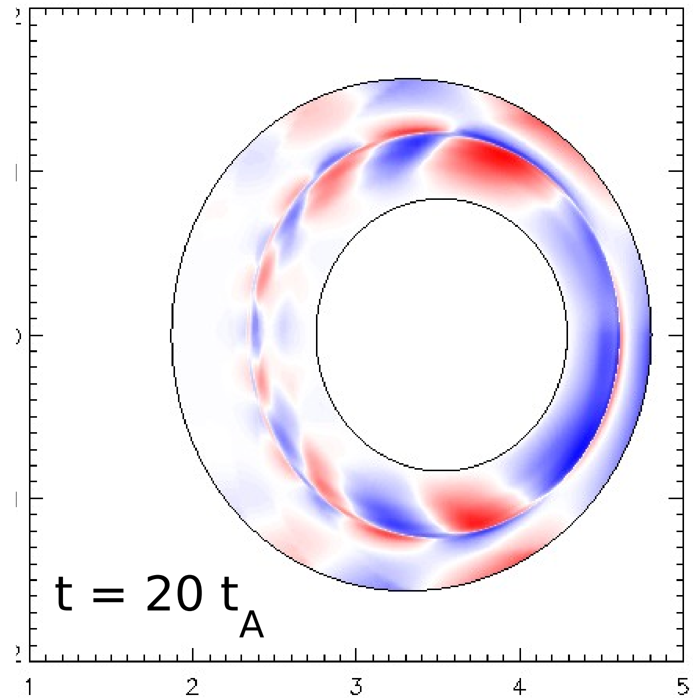
Simulating an ideal plasma. What does the plasma response look like?

NOTE: Not intended to be a faithful representation of the real thing, but to give some insight into the plasma physics.

Vacuum field



During ramp phase



Observe field amplification

RMP simulations

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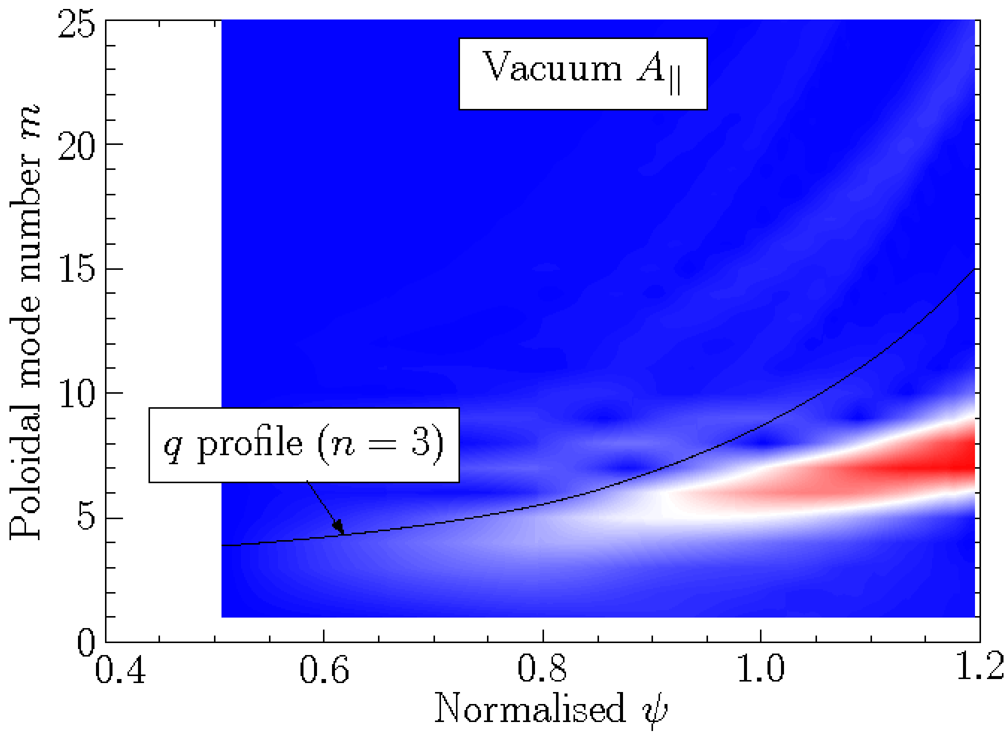
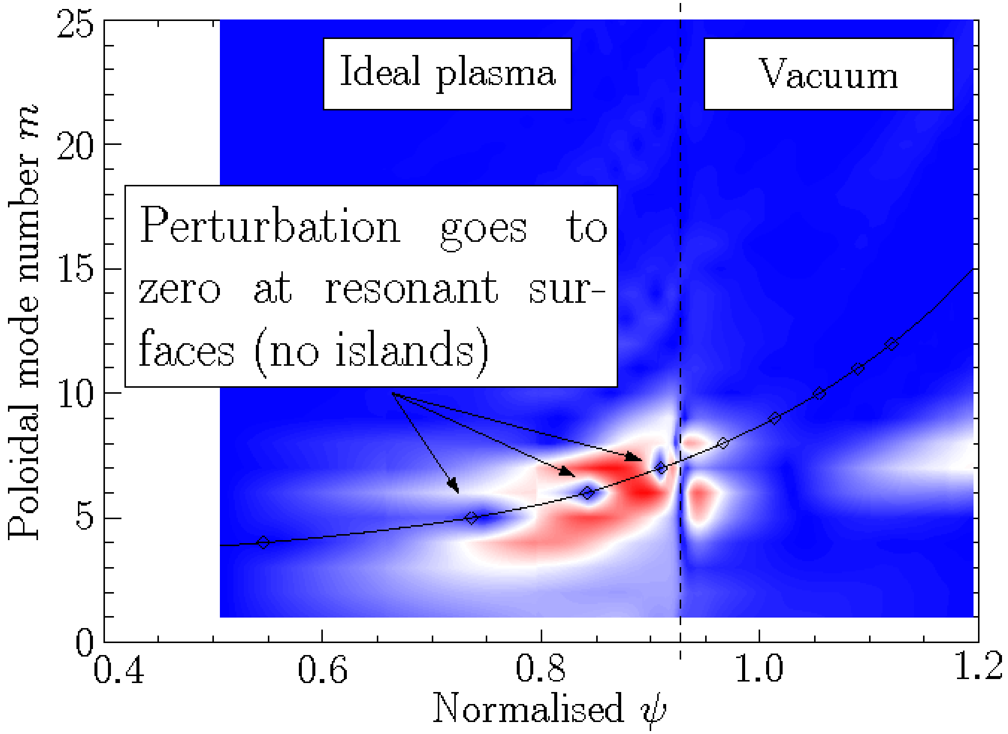
Vacuum field



During ramp phase



→ Field structure can look quite different in the presence of a plasma

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RMP simulations

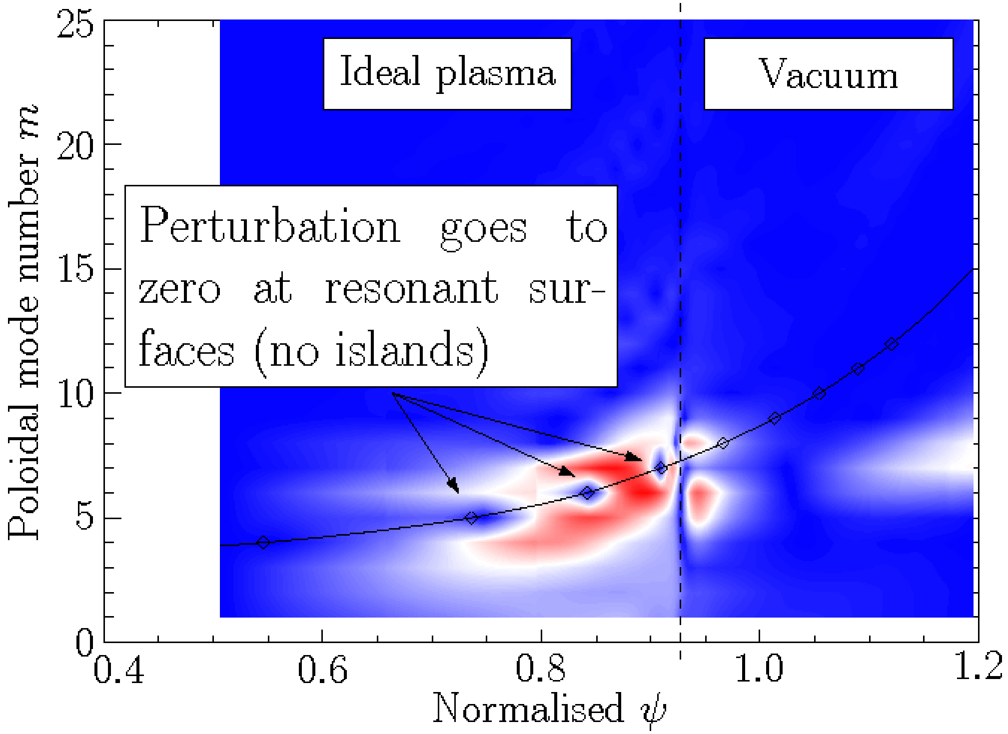
- Ideal MHD
- As externally applied field changes, drives surface current
- JxB force distorts plasma surface (here seen as parallel current driving vorticity)
- Distortion transmitted inside plasma (since ~incompressible)

Simulations suffer same problem as ELMs: Large perturbation of the flux surfaces leads to numerical problems

Can't filter out high-n modes since they're needed to maintain positive pressure.

Edge plasma effect, since delta-P is larger than P_0.

During ramp phase



Outline of talk

- The BOUT++ code
  - Equations solved, equilibria used, ...
- Ideal MHD simulation of ELMs
  - Linear results and comparison with ELITE
- Diamagnetic effects
  - Modification of linear growth-rates
  - Nonlinear results
- Simulation of RMPs
- Handling large delta-B / B in a field-aligned code
- Conclusions / Future work

Limits to current simulations

- Nonlinear simulations require high resistivity to avoid numerical problems
    - This is a common problem with ELM simulations
- Large field perturbations cause high mode-numbers, and grid misalignment.

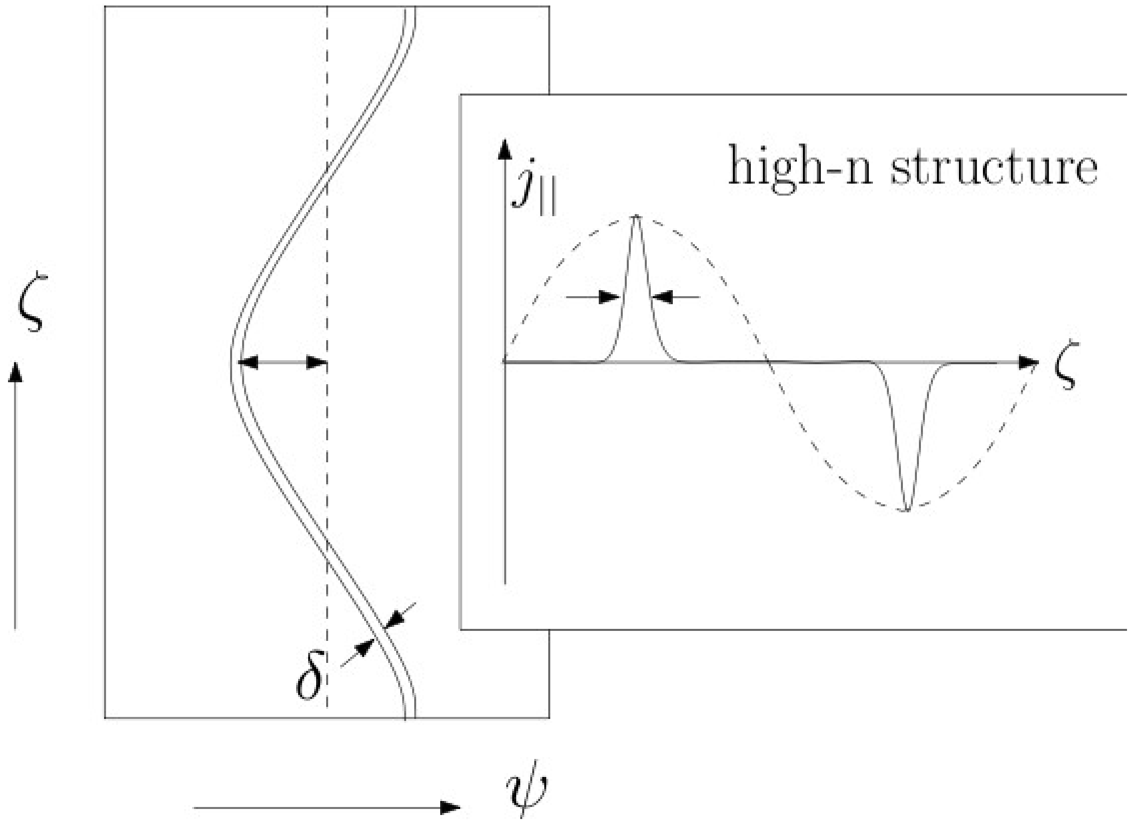
Limits to current simulations

- Nonlinear simulations require high resistivity to avoid numerical problems
  - This is a common problem with ELM simulations
- Large field perturbations cause high mode-numbers, and grid misalignment.
- <u>High toroidal mode-numbers</u>

Narrow structures in radial direction (~1cm)

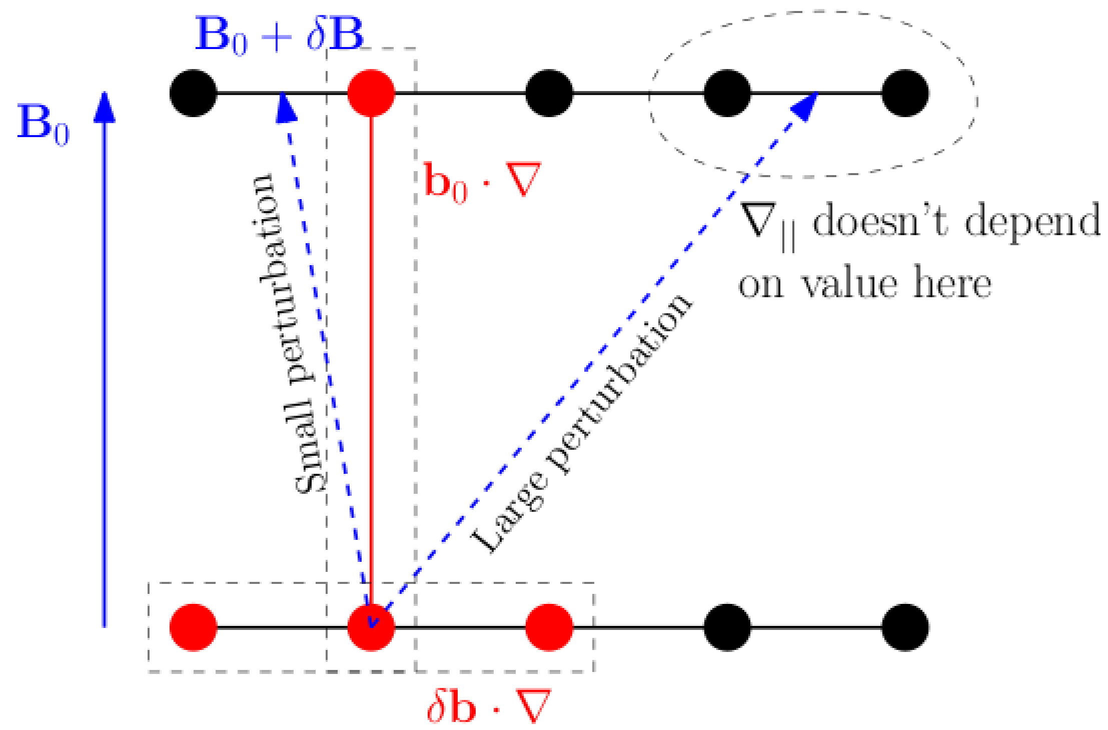
Distortion of flux surface rotates into toroidal direction

Corresponds to very high mode-numbers (~3000)



Parallel derivatives

Perturbed parallel derivatives
calculated using red points:
Equilibrium + perpendicular



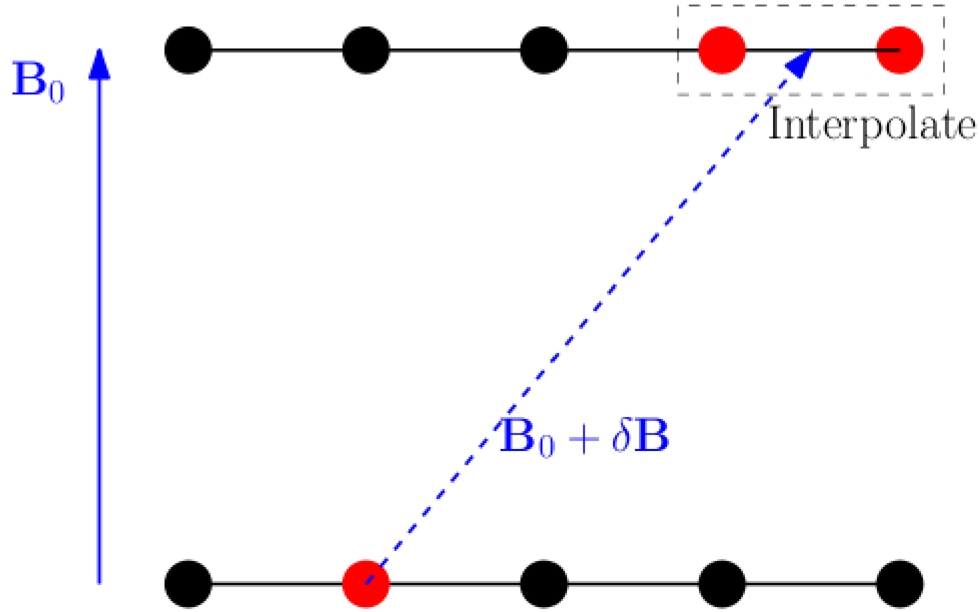
For small delta-B, field-line stays close to stencil points

For large perturbations, calculated parallel derivative doesn't depend on grid-points along the magnetic field

One way around both these problems is to use a very high resolution in parallel and toroidal directions -> Lose advantages of field-alignment!

Moving stencil method

- One possibility would be to move the grid-points to maintain alignment. Has problems with non-ideal plasma, time-evolving metric tensor, and grid tying itself into knots
- Rather than move the grid-points, move the stencils by interpolation, and differentiate along the perturbed field-line.

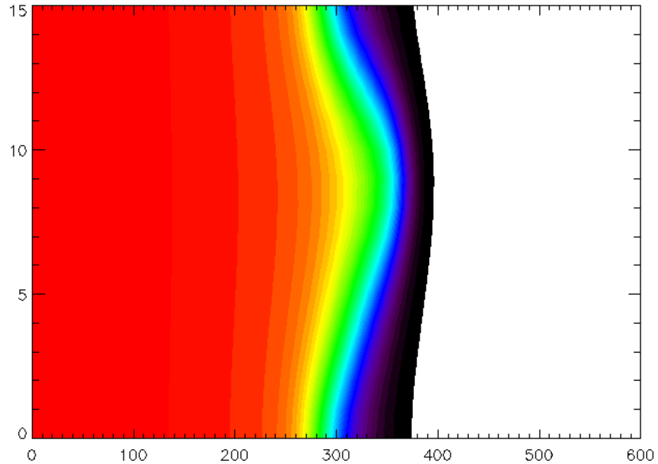


Method implemented in BOUT++, and currently being tested...

Moving stencil method: Initial results

Difficult part is projecting field-lines whilst maintaining numerical stability. Currently using quasi-staggered 1st-order method.

Appears to allow much larger perturbations with lower toroidal resolution than previously.



Aim to allow significant magnetic field perturbations, whilst maintaining efficiency of field-aligned code.

<u>Allow efficient simulations of turbulence + large-scale MHD</u>

Future work

- Two approaches being followed to suppress small-scale structures:
  - Add additional physics e.g. Diamagnetic drift. Could also include Hall term, turbulence-induced anomalous resistivity.
    Has advantage of adding extra physics, but moves away from testable solutions.
  - Novel moving stencil method for adaptive parallel derivatives.
- Plasma model doesn't include parallel dynamics yet
  - Plan to add model for loss mechanisms
- Model application of magnetic fields from more realistic coil sets on more realistic equilibria
  - Need to apply coils to stable equilibria

Summary

- BOUT++ is a framework which allows new methods to be tried relatively quickly, and additional terms and equations easily added.
- Linear ideal ballooning mode shows good agreement with ELITE
  - Nonlinear results show eruption of filaments accelerating outwards
- Diamagnetic effects suppress ballooning mode, but associated electric field drives another type of instability
  - Nonlinear collapse appears different to resistive MHD, and more like broadband turbulence.
- RMP simulations of ideal plasmas show penetration of fields through distortion of plasma surface. Structure inside plasma quite different to applied field.

- BOUT++ Employs a novel technique to handle the plasma-vacuum interface
- Being used to develop a moving stencil method to combine efficient simulation of turbulence with large-scale MHD modes

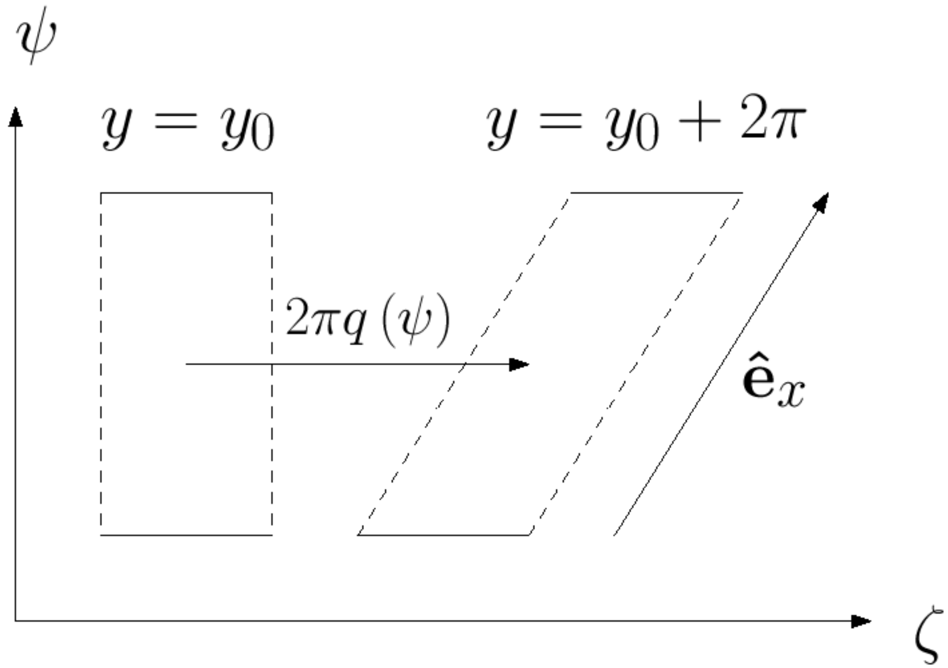
Thankyou!

Extra slides...?

Shifted radial derivatives

Field-aligned coordinates have a problem:
differencing stencils are discontinuous

Caused by magnetic shear. Following a bundle of field-lines poloidally around the tokamak, it is sheared in the toroidal direction.



Where the field-line bundle is connected back onto itself, numerical stencils jump

Covariant basis vectors

$$\mathbf{e}_x = \frac{1}{RB_\theta}\hat{\mathbf{e}}_\psi + IR\hat{\mathbf{e}}_\zeta$$

$$\mathbf{e}_y = \frac{h_\theta}{B_\theta}\mathbf{B} = h_\theta\hat{\mathbf{e}}_\theta + \nu R\hat{\mathbf{e}}_\zeta$$

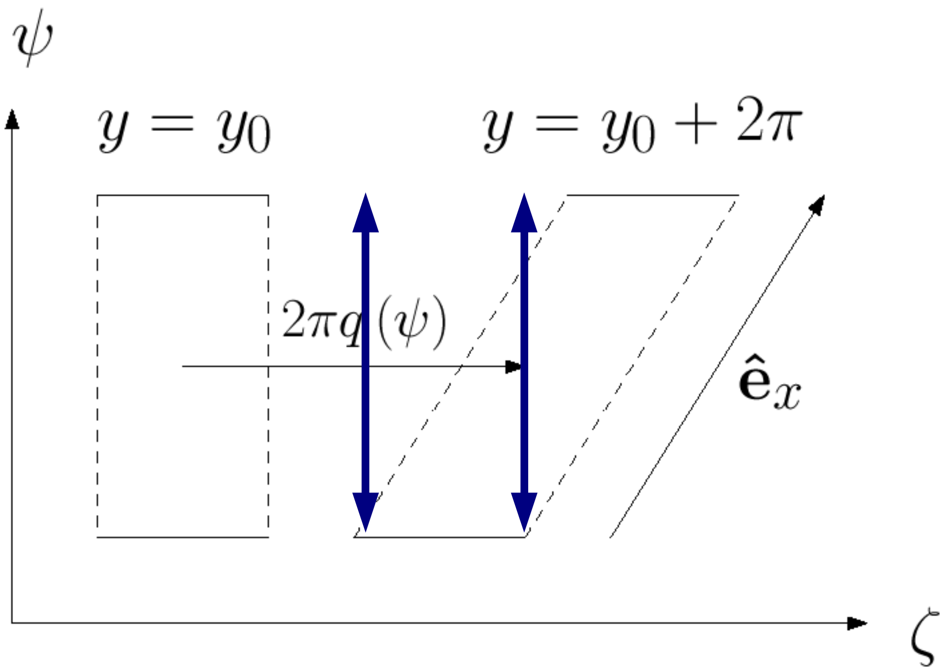
$$\mathbf{e}_z = R\hat{\mathbf{e}}_\zeta$$

$$I = \int_{\theta_0}^{\theta} \frac{\partial \nu(\psi,\theta)}{\partial\psi} d\theta$$

Integrated shear

Shifted radial derivatives

Solution: always take derivatives directly in ψ, rather than x.
Called "quasi-ballooning" coordinates



Differencing stencils are now always continuous in space

Radial derivatives now require interpolation in toroidal angle. This is done using FFTs.

Covariant basis vectors

$$\mathbf{e}_x = \frac{1}{RB_\theta}\hat{\mathbf{e}}_\psi + \cancel{IR\hat{\mathbf{e}}_\zeta}$$

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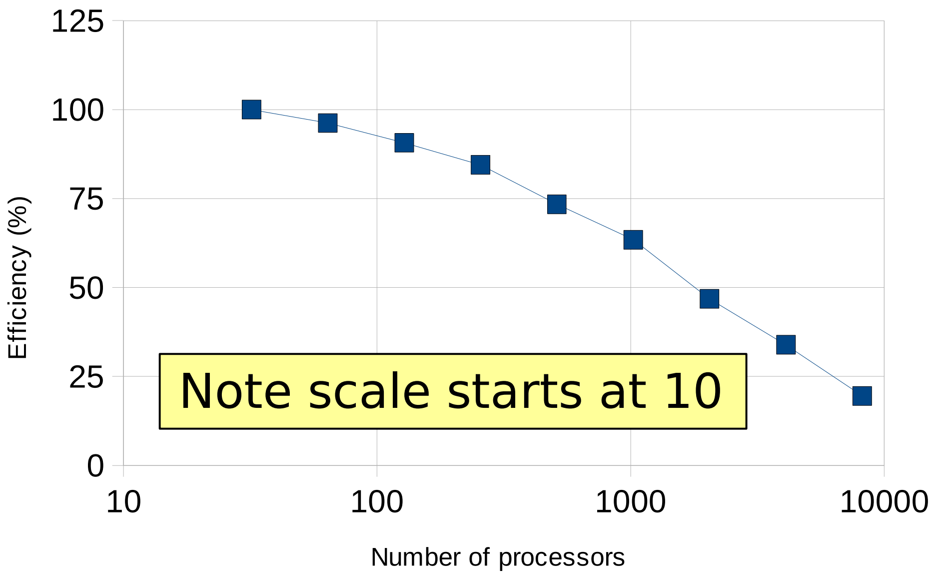
Integrated shear

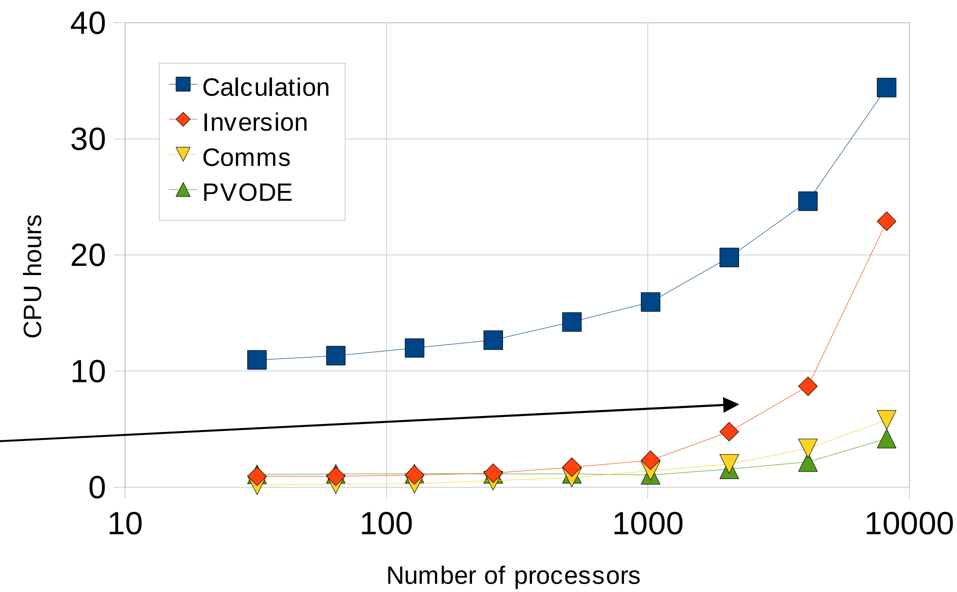
A.M. Dimits, Phys. Rev. E **48** (1993), p. 4070

Parallel scaling: ELM problem

- Large (ish) grid, in range for non-linear ELM problems on Cray XT4 (Franklin at NERSC, and HECToR)
  - Grid size 256 x 256 x 128 (25,165,824 evolving values)



This problem runs efficiently (>50%) on up to 2048 processors

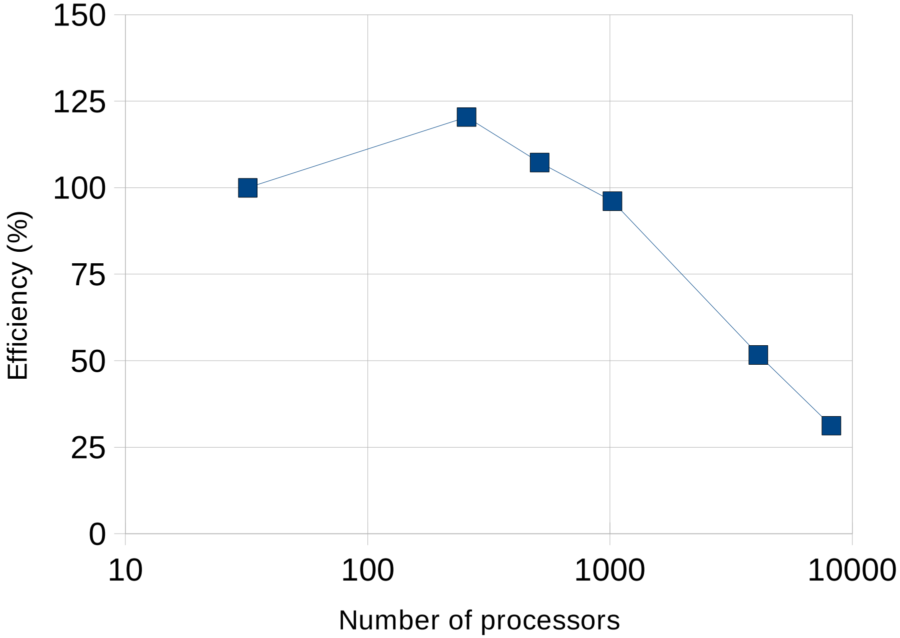


Laplacian Inversion algorithm: Only basic parallelisation of serial code. Efficiency suffers for NP > NY (256)

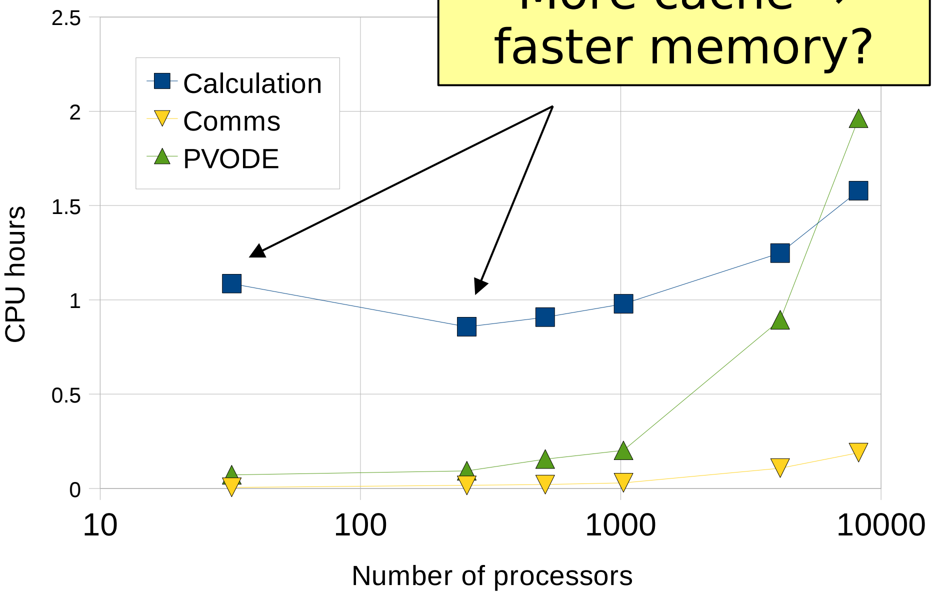
Parallel scaling: 2D Ideal MHD

- Non-linear full ideal MHD: No inversion
  - 2D Grid 512 x 512 (2,097,152 evolving variables)

In this case efficient on 4096 processors



PVODE seems to limit the parallelism in this case → Not so easy to improve



More cache → faster memory?