

stella Update: Full-Flux Annulus

G. O. Acton^{1,2,3}, M. Barnes¹, S. Newton²,
F. I. Parra⁵, W. Dorland⁶, H. Thienpondt⁴

¹Rudolf Peierls Centre For Theoretical Physics, University of Oxford, Oxford, OX1 3PU, UK

²Culham Centre for Fusion Energy, United Kingdom Atomic Energy Authority,
Abingdon, OX14 3EB, UK

³Max-Planck-Institut für Plasmaphysik, Teilinstitut Greifswald, Germany

⁴Laboratorio Nacional de Fusion, CIEMAT, 28040 Madrid, Spain

⁵Princeton Plasma Physics Laboratory, Princeton, NJ 08540, USA

⁶Department of Physics, University of Maryland, College Park, MD 20742, United States of America

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1. Introduction to **stella**
2. Motivation for Full-Flux Annulus
3. Flux Annulus Formalism
4. Results

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- Each term in the gyrokinetic (GK) equation is solved independently

$$\frac{\partial g_\nu}{\partial t} + \underbrace{\mathcal{S}_\nu[g_\nu, \varphi_\nu] + \mathcal{M}_\nu[g_\nu]}_{\text{Implicit}} + \underbrace{\mathcal{D}_\nu[g_\nu, \varphi_\nu] + \mathcal{G}_\nu[\varphi_\nu] + \mathcal{N}_\nu[g_\nu, \varphi_\nu]}_{\text{Explicit}} = \mathcal{C}_\nu[\{g_{\nu'}\}, \{\varphi_{\nu'}\}],$$

streaming
mirror
drifts
non-linear
collisions

$$\partial_t g_\nu = \sum_{i=1}^3 (\partial_t g_\nu)_i \quad \left| \quad \begin{aligned} (\partial_t g_\nu)_1 + \mathcal{D}_\nu[g_\nu, \varphi_\nu] + \mathcal{G}_\nu[\varphi_\nu] + \mathcal{N}_\nu[g_\nu, \varphi_\nu] &= \mathcal{C}_\nu \\ (\partial_t g_\nu)_2 + \mathcal{M}_\nu[g_\nu] &= 0 \\ (\partial_t g_\nu)_3 + \mathcal{S}_\nu[g_\nu, \varphi_\nu] &= 0 \end{aligned} \right.$$



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$$\mathcal{S}_\nu \doteq v_{\text{th}} v_{\parallel} \hat{\mathbf{b}} \cdot \nabla_z \left(\frac{\partial g_\nu}{\partial z} + \frac{Z_\nu}{T_\nu} \frac{\partial \varphi_\nu}{\partial z} F_{0,\nu} \right)$$



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$$\frac{g_\nu^{n+1} - g_\nu^n}{\Delta t} = -v_{\text{th}} v_{\parallel} \hat{\mathbf{b}} \cdot \nabla z \left(\frac{\partial g_\nu^n}{\partial z} + \frac{Z_\nu e}{T_\nu} \frac{\partial \varphi_\nu^n}{\partial z} F_{0,\nu} \right) \quad (1)$$



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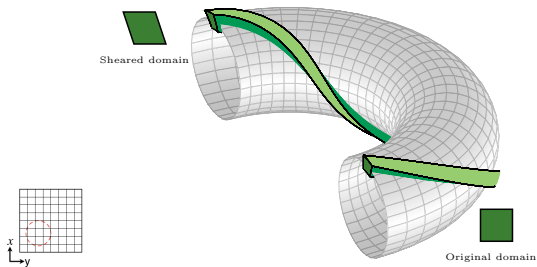
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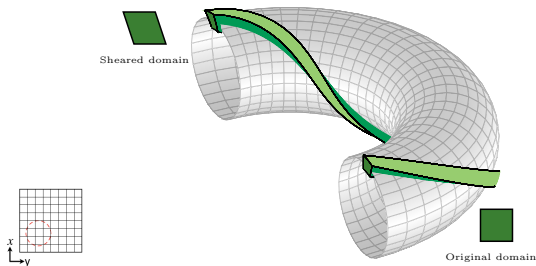
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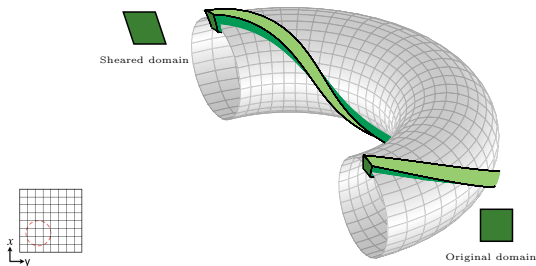
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- Uses $\{v_{\parallel}, \mu\}$ for the velocity space coordinates \rightarrow good for stellarators



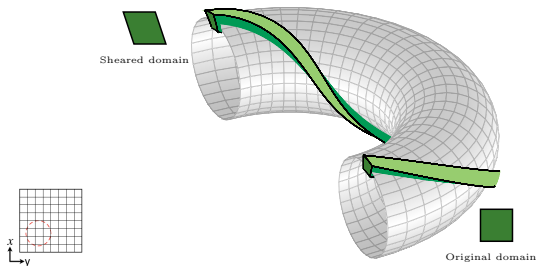
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- Simulation coordinates: $(x, y, z) \rightarrow (\psi, \alpha, \zeta)$
- Initialise some δf and ϕ at $t = 0$ on simulation domain
- Evolve gyrokinetic equation pseudo-spectrally
 - Decay in v_{\parallel} ; $g(t, \mathbf{x}, v_{\parallel} \rightarrow \pm\infty, \mu) \rightarrow 0$
 - Turbulence is taken as periodic in perpendicular directions, $k_x, k_y \gg 1/L$
 - Use twist-and-shift boundary conditions in z to capture extended modes

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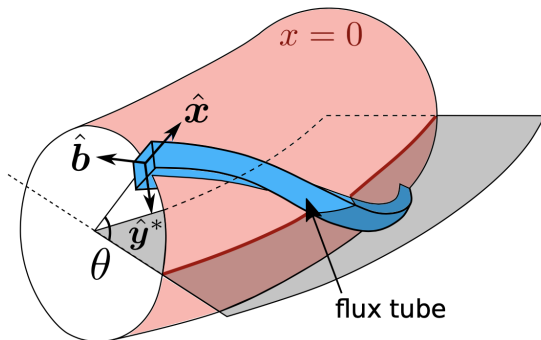


Image: Nicolas Christen, Bistable turbulent transport in fusion plasmas with rotational shear (2021)

- Flux-tube simulations are sufficient for tokamaks because we can stitch our flux tubes together

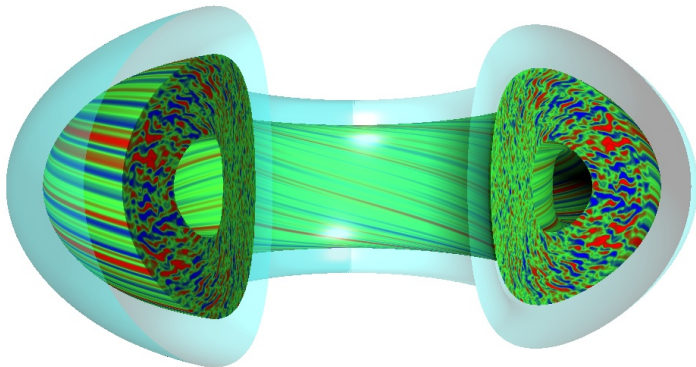


Image: J.Candy, Waltz, GYRO simulation of DIII-D

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Flux tube formalism: pros and cons

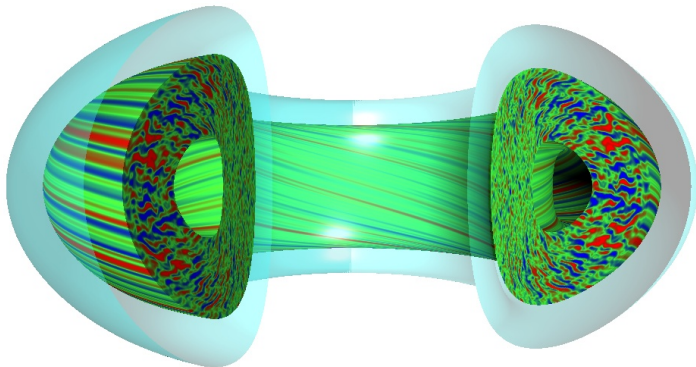


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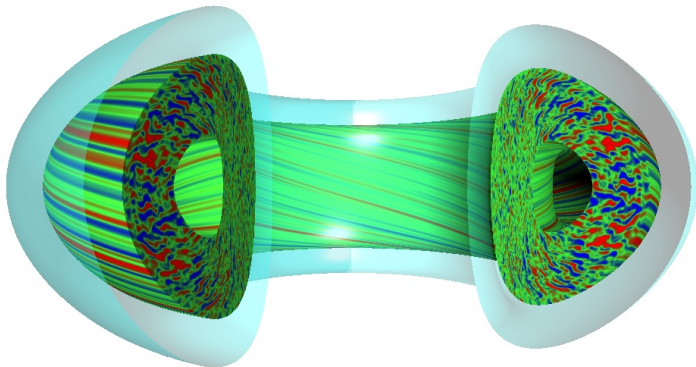


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- Easy to interpret: normal modes are well defined

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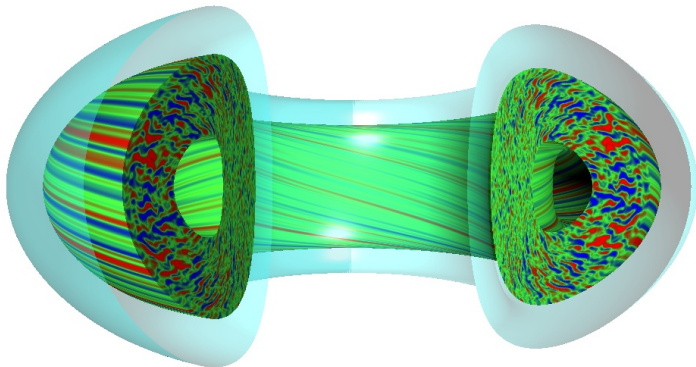
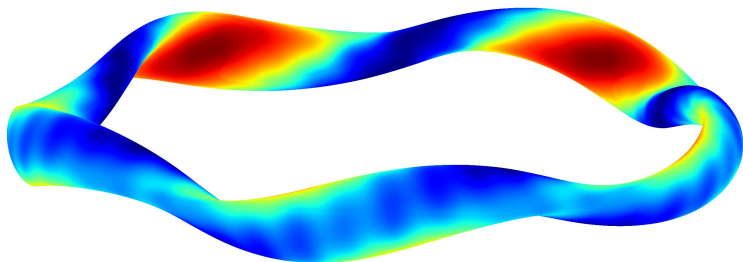


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- Easy to interpret: normal modes are well defined
- Retains spectral accuracy in spacial derivatives

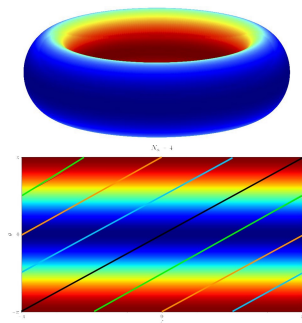
Flux tube formalism: pros and cons



- Fast codes: perform many simulations in quick succession
- Easy to interpret: normal modes are well defined
- Retains spectral accuracy in spacial derivatives
- Does not capture global effects like coupling between different field lines

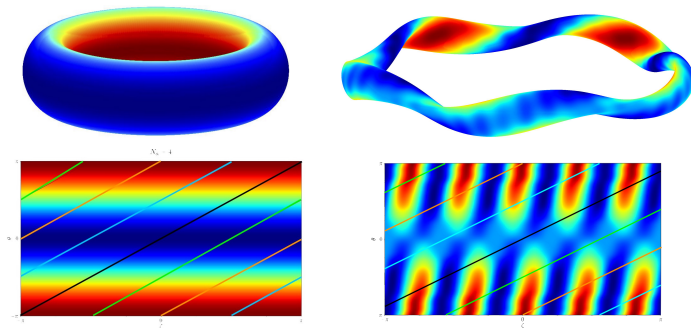
Motivation

- Axisymmetry means all field lines are equivalent



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- Stellarator magnetic geometry varies with field line: single field line is **not** sufficient!
- Modes on different field lines interact \rightarrow complicates algorithms due to α -inhomogeneity
- Particularly relevant for zonal flows

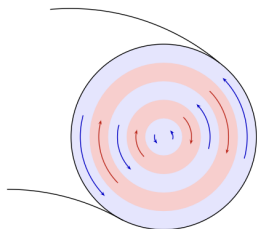


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Flux annulus formalism: motivation



- Stellarator geometry varies with field line
- Method of stitching together flux tubes no longer holds

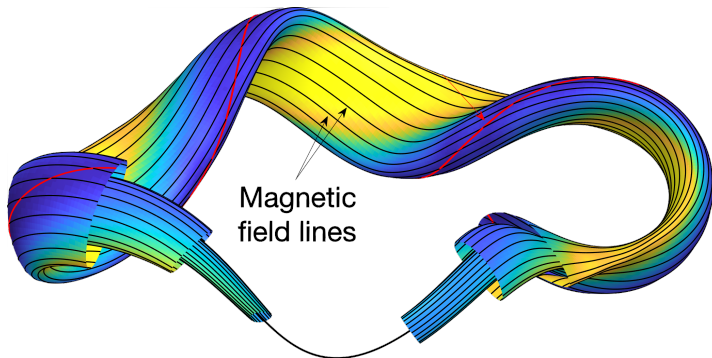
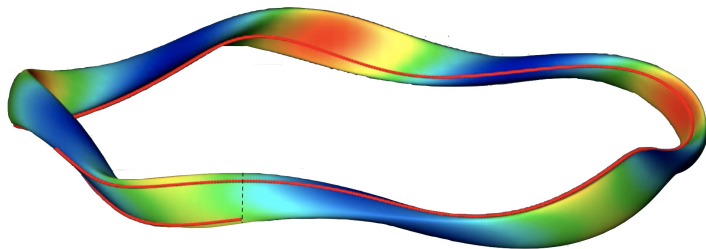


Image: UMD stellarator group

Flux annulus framework



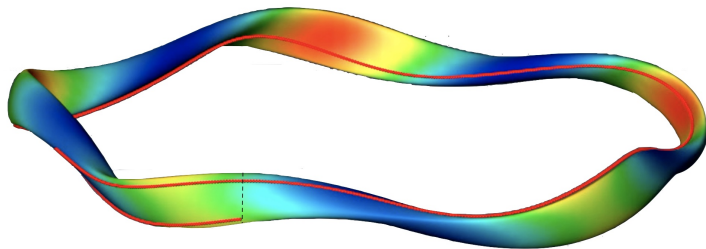
- Domain is now 2π in ζ , not 2π in θ



Flux annulus framework



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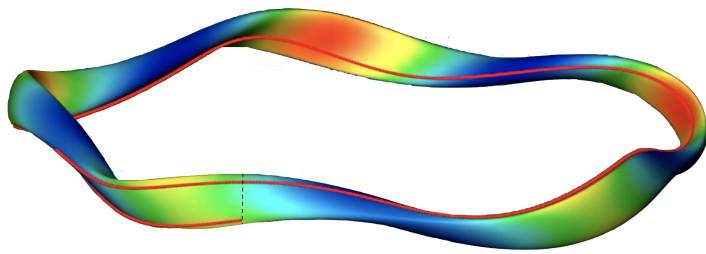


- Evolve pseudo-spectrally to retain spectral accuracy in derivatives

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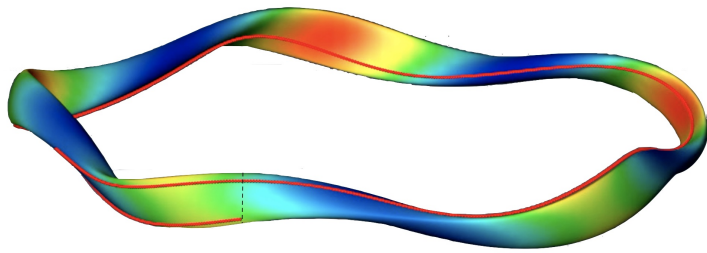


- Evolve pseudo-spectrally to retain spectral accuracy in derivatives
- N_y field lines that cover different geometry and are now coupled together

Flux annulus framework



- Domain is now 2π in ζ , not 2π in θ



- Evolve pseudo-spectrally to retain spectral accuracy in derivatives
- N_y field lines that cover different geometry and are now coupled together
- Apply twist-and-shift to entire poloidal domain

How 3D geometry modifies equations

- Geometry is no longer trivial
- But how does geometry enter our code?



How 3D geometry modifies equations



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Simplified notation GK:

$$\frac{\partial g}{\partial t} = (\text{geometric factors}) \cdot (\nabla g + \nabla \langle \phi \rangle_{\mathbf{R}})$$

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- Geometric factors are α -dependent
- Bessel functions $J_0(a_{\mathbf{k}})$ with $a_{\mathbf{k}} = \frac{k_{\perp} v_{\perp}}{\Omega_s}$

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- α -inhomogeneity leads to convolutions

How 3D geometry modifies equations

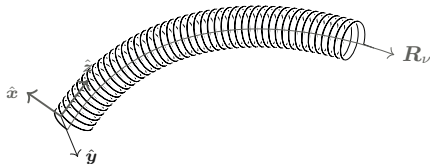


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- Gyro-averaging introduces coupling between different k_y -modes \rightarrow no longer a local operation



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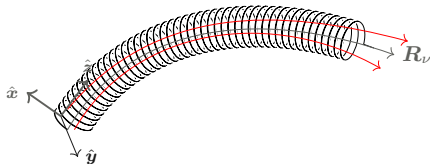


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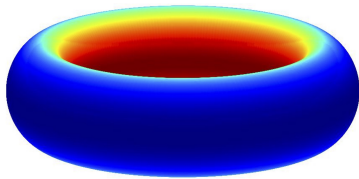
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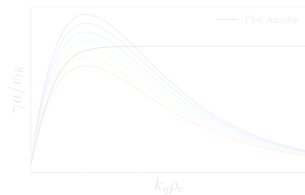
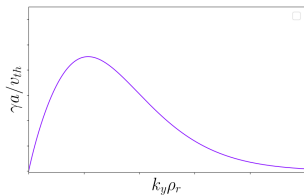
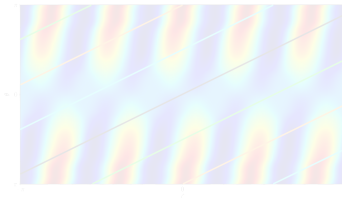
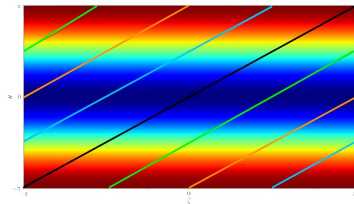
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- Geometric factors are α -dependent
- Bessel functions $J_0(a_k)$ with $a_k = \frac{k_{\perp} v_{\perp}}{\Omega_s} \leftarrow k_{\perp}$ and B in argument
- Gyro-averaging introduces coupling between different k_y -modes \rightarrow no longer a local operation
- Develop iterative-implicit method \rightarrow accurate treatment without stringent CFL restriction

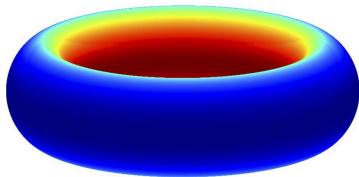
How 3D geometry modifies expectations



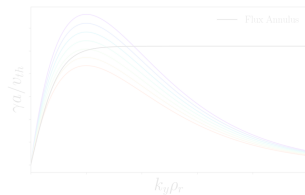
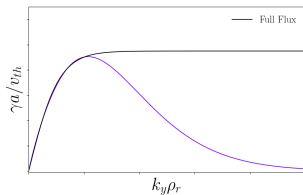
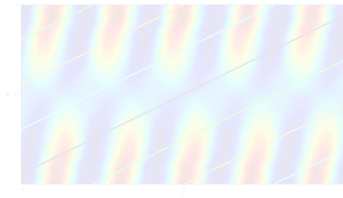
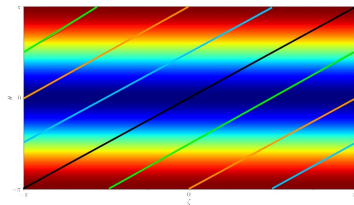
$N_p = 4$



How 3D geometry modifies expectations



$N_x = 4$



How 3D geometry modifies expectations

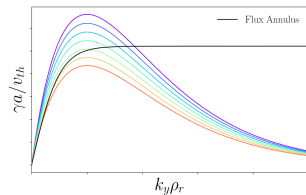
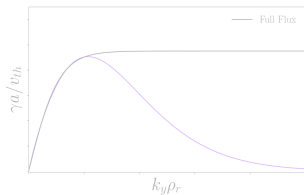
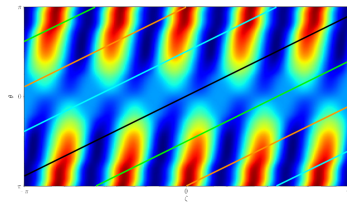
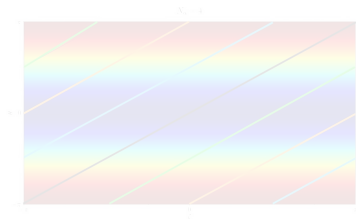
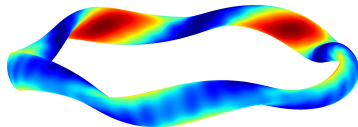
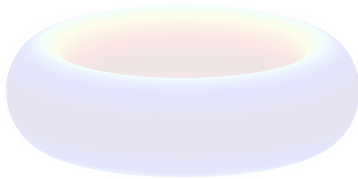


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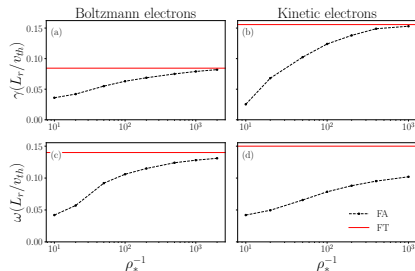
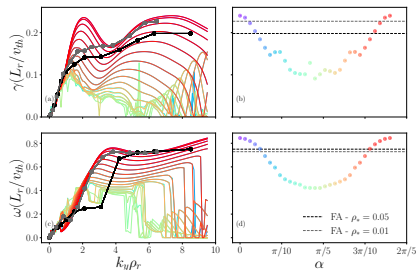
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Benchmarked



- Simulates gyrokinetic turbulence on a full-flux annulus in general 3D geometry
- Capable of simulating adiabatic and kinetic electrons

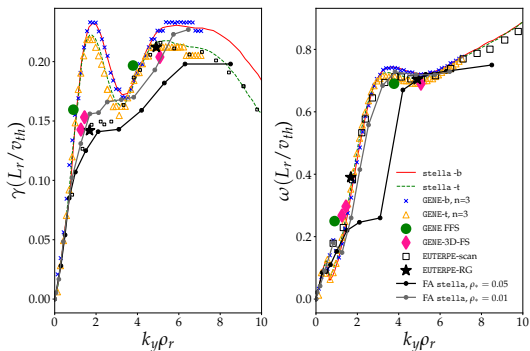
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- Has been benchmarked against stella flux tube code in appropriate limits



Benchmarked



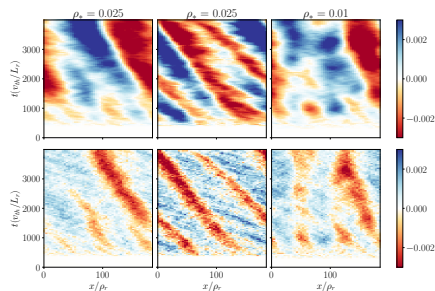
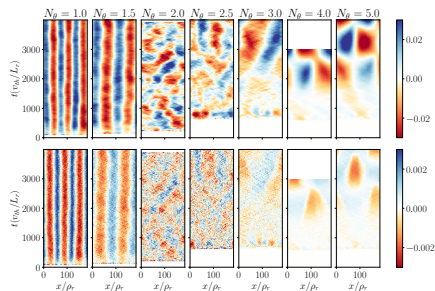
- Simulates gyrokinetic turbulence on a full-flux annulus in general 3D geometry
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- Shows good agreement with other full-surface codes



E. Sánchez, J. M. García-Regaña, A. B. Navarro, J. H. E. Proll, C. M. Moreno, A. González-Jerez, I. Calvo, R. Kleiber, J. Riemann, J. Smoniewski, et al.

Gyrokinetic simulations in stellarators using different computational domains.
Nuclear Fusion, 61(11):116074, 2021.

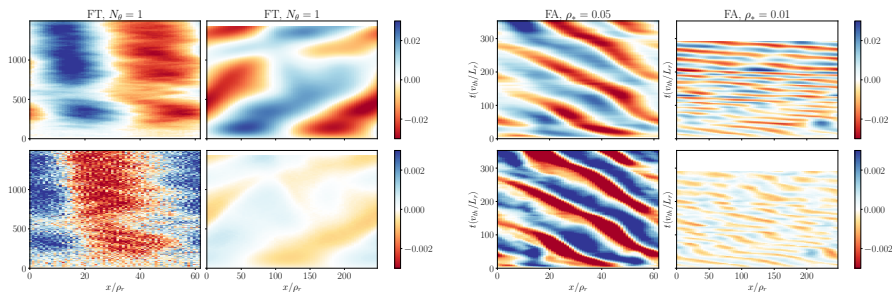
- Simulates gyrokinetic turbulence on a full-flux annulus in general 3D geometry
- Capable of simulating adiabatic and kinetic electrons
- Has been benchmarked against stella flux tube code in appropriate limits
- Shows good agreement with other full-surface codes
- Preliminary results shows differences between flux-tube and full-flux approaches with Boltzmann electrons



Benchmarked

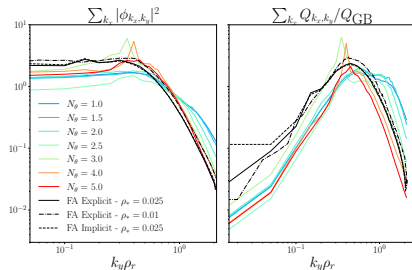
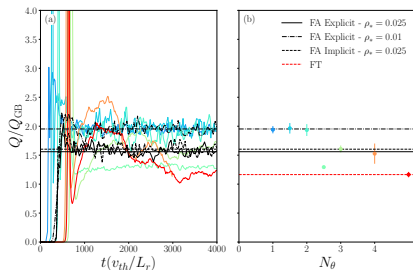


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- Boltzmann electrons:

Simulation Case	Time Step (dt)	CPU Hours
FT, $N_\theta = 1$	0.049666	26,880
FT, $N_\theta = 5$	0.030470	80,640
FA (explicit), $\rho_* = 0.025$	0.1	43,550
FA (implicit), $\rho_* = 0.025$	0.1	51,690
FA (explicit) ¹ , $\rho_* = 0.01$	0.1	35,420



¹ Reduced resolution



- Kinetic electrons:

<u>Parameter</u>	<u>FT 1</u>	<u>FT 2</u>	<u>FA 1</u>	<u>FA 2</u>
Δt	1.6577×10^{-2}	2.1195×10^{-2}	7.7464×10^{-3}	5.6368×10^{-3}
t_{final}	1500	1470	355	270
CPU hours	46,080	76,800	107,520	128,640

- $\Delta t = 1\text{E-}006$ for explicit kinetic electron simulations \rightarrow numerically unstable
- Implicit treatment allows $\Delta t \sim 5\text{E-}003$



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Simulation results: code efficiency



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Improvements

- NB: this was before **stella** improvements \rightarrow need to re-run with updated version
- Already identified inefficiencies
- Anticipate this can be reduced to $\sim \times 5$ speed of flux-tube
- Removing strong coupling (e.g. for CBC) improves code by ~ 10 times for KE

Summary and future work



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- Developed an iterative-implicit algorithm to deal with full-flux annulus effects, with kinetic electrons, in arbitrary geometry
- FFA **stella** has been benchmarked in appropriate limits and against existing codes

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- Developed an iterative-implicit algorithm to deal with full-flux annulus effects, with kinetic electrons, in arbitrary geometry
- FFA **stella** has been benchmarked in appropriate limits and against existing codes

Future Work

- Investigate how zonal flows are supported in stellarators
- Combine full-flux with electromagnetic **stella**
- Optimise for computational speed-up

Backup slides: Derivation of twist-and-shift boundary conditions

*

$$A(t, x, y, z) = \sum_k \hat{A}_{k_x, k_y}(t, z) e^{ik_y(y-y_0)+ik_x(x-x_0)} \quad (1)$$

Set $y_0 = 0$, $x_0 = 0$ $A(t, x, y(x, \theta, z), z) = A(t, x, y'(\theta, z + 2p\pi), z + 2p\pi)$

But $y = y(\theta, z)$

$$\sum_k \hat{A}_{k_x, k_y}(t, z) e^{ik_y y + ik_x x} = \sum_k \hat{A}_{k_x, k_y}(t, z') e^{ik_y(y'(\theta, z')) + ik_x x} \quad (2)$$

So $y'(\theta, z') = y + \frac{\partial y}{\partial z} 2\pi p = y + 2\pi p \frac{\partial y}{\partial \alpha} \frac{\partial \alpha}{\partial z} = y - 2\pi p \iota(\psi) \frac{\partial y}{\partial \alpha}$ Remembering

$\iota(\psi) = \iota(\psi_0) + \iota' \frac{\partial \psi}{\partial x}$ so $y' = y - 2\pi p \iota(\psi_0) \frac{\partial y}{\partial \alpha} - 2(x - x_0) \pi p \iota' \frac{\partial y}{\partial \alpha} \frac{\partial \psi}{\partial x}$

$$\sum_k \hat{A}_{k_x, k_y}(t, z) e^{ik_y y + ik_x x} = \sum_k \hat{A}_{k_x, k_y}(t, z + 2\pi p) e^{ik_y y + i(k_x - 2\pi p \iota' \frac{\partial y}{\partial \alpha} \frac{\partial \psi}{\partial x} k_y) x' - i 2\pi p k_y \iota p \frac{\partial y}{\partial \alpha}} \quad (3)$$

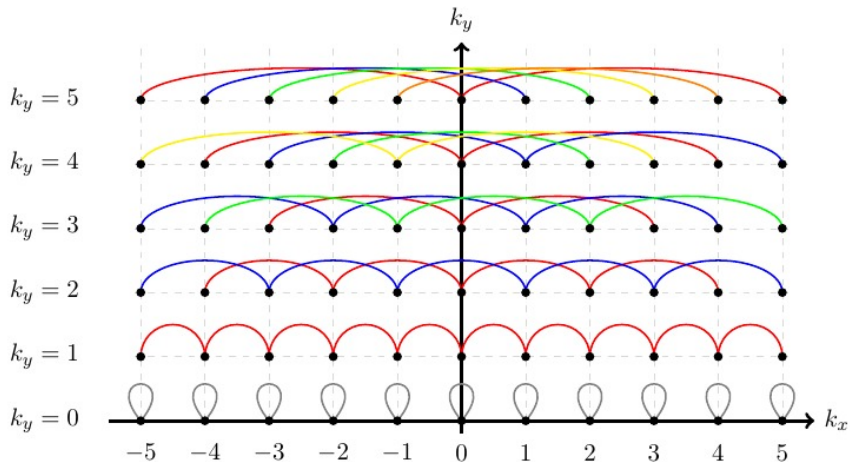
Let $\delta k_x = 2\pi p \iota' \frac{\partial y}{\partial \alpha} \frac{\partial \psi}{\partial x} k_y$ and $\Delta = -2\pi p k_y \iota \frac{\partial y}{\partial \alpha}$

$$\sum_k \hat{A}_{k_x, k_y}(t, z) e^{ik_y y + ik_x x} = \sum_k \hat{A}_{k_x, k_y}(t, z + 2\pi p) e^{ik_y y + i(k_x - \delta k_x) x'} e^{i\Delta} \quad (4)$$

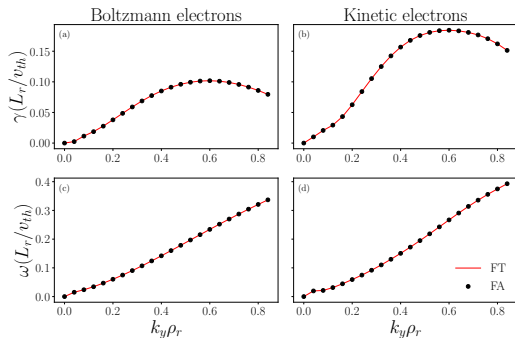
So relate $k_x = k'_x - 2\pi p \iota' \frac{\partial y}{\partial \alpha} \frac{\partial \psi}{\partial x} k_y$

Backup slides: Eigenmode chains

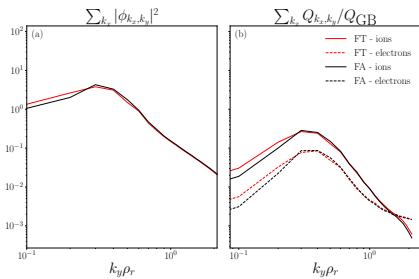
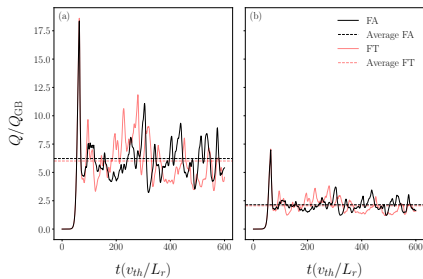
*



Backup slides: Miller geometry linear comparison



Backup slides: Miller geometry nonlinear comparison



Backup slides: Adiabatic, W7X comparison between GX and stella

