The field line map approach to plasma turbulence simulations

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Motivation

Ultimate goal

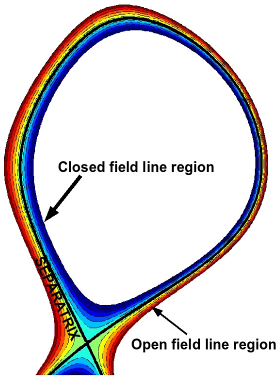
Prediction/Computation of anomalous transport/turbulence in edge and scrape-off layer

Why?

- Boundary region may have high influence on overall performance of reactor [Stangeby90,McCracken93]
- Many phenomena occurring in edge/SOL not yet fully understood
- Prediction of heat loads on divertor plates

Major challenges

1. Complex physical model
2. Complex geometry



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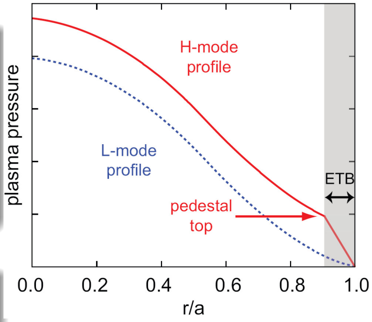


Major challenges

1. Complex physical model
2. Complex geometry

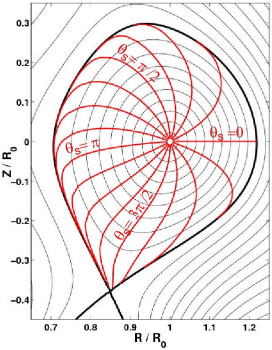
Coordinates

Field-aligned coordinates [D'haeseleer et al.90]

- Structures strongly elongated along field lines $k_{\|} \ll k_{\perp}$
- Scale separation via transformation to field-aligned coordinates/grids
- **BUT: ILL DEFINED ON SEPARATRIX**

Flux-aligned coordinates

- Ill defined on X/O-point [Mattor95], can be circumvented numerically
- However: X-point remains 'special', resolution imbalance



Goal

- Development and implementation of numerical concept, which avoids field/flux-aligned coordinates → applicable to separatrix
- Application to simplified plasma turbulence model

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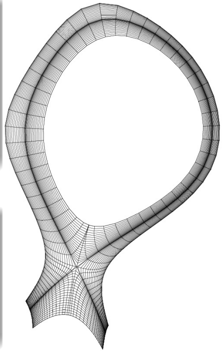

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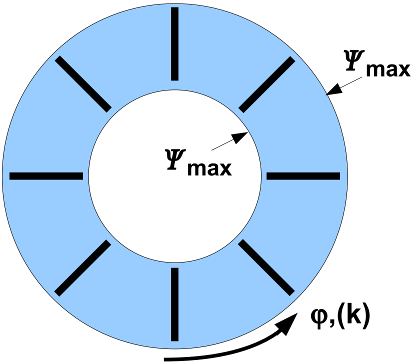
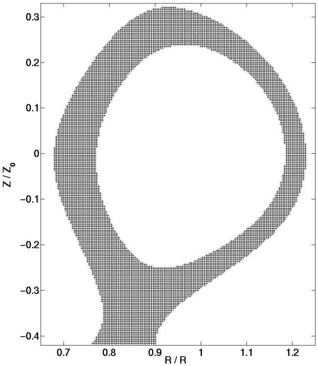
Overview

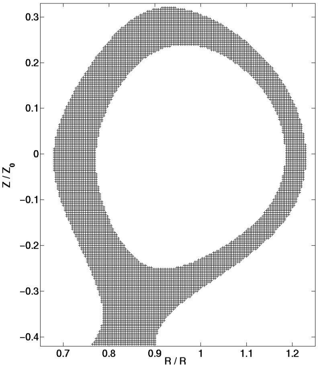
- See Flux Coordinate Independent approach (FCI) *[Ottaviani11,Hariri and Ottaviani13, Hariri et al.14]*, F. Hariri's talk on Tuesday
- Cylindrical grid $R_i, Z_j, \varphi_k \rightarrow$ no singularities[1] or special points
- Fieldline-following discretisation for parallel operators
- Grid sparsification in toroidal direction ($k_{\|} \ll k_{\perp}$)





[1]in relevant region

Perpendicular operators



Assumption $B_{tor} \gg B_{pol}$
$\rightarrow$ Stencil remains within poloidal plane
$\rightarrow$ Use of standard finite-difference methods

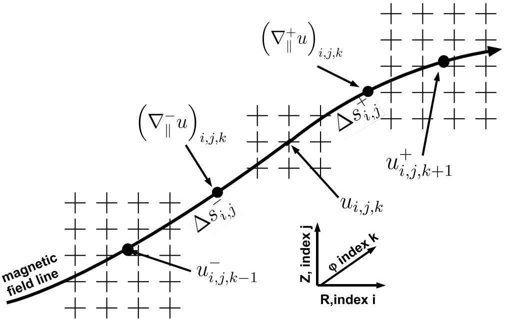
Parallel operators

- Stencil covers neighbouring poloidal planes
- Discretisation via finite difference along magnetic field lines
- Fieldline tracing and interpolation

$$R^{\pm} = \int_0^{\pm\Delta\varphi} \frac{B^R}{B^\varphi} d\varphi, \; Z^{\pm} = \int_0^{\pm\Delta\varphi} \frac{B^Z}{B^\varphi} d\varphi,$$

$$\left(\nabla_{\parallel}^{\pm} u\right)_{i,j,k} = \pm \frac{u_{i,j,k\pm1}^{\pm} - u_{i,j,k}}{\Delta s_{i,j}^{\pm}},$$

$u_{i,j,k}^{\pm}$ via 2D interpolation



- Express via matrices $\mathbf{Q}^{\pm}$, i.e.:

$$\mathbf{q}^{\pm} = \mathbf{Q}^{\pm}\mathbf{u}$$

$$\mathbf{q}^{\pm} := \left(\left(\nabla_{\parallel}^{\pm} u\right)_{1,1,1}, \left(\nabla_{\parallel}^{\pm} u\right)_{2,1,1}, \ldots\right), \quad \mathbf{u} := \left(u_{1,1,1}, u_{2,1,1}, \ldots\right)$$

Parallel diffusion

$$\mathcal{D}_{\parallel} u := \nabla \cdot \left[\mathbf{b} \left(\nabla_{\parallel} u \right) \right]$$

Naive scheme

- Assume: $\mathcal{D}_{\parallel} \approx \nabla_{\parallel}^2$
- Discretisation via further finite difference along magnetic field lines:

$$\left(\mathcal{D}_{\parallel}^{naive} u \right)_{i,j,k} = \frac{2}{\Delta s_{i,j}^{+} + \Delta s_{i,j}^{-}} \left[\nabla_{\parallel}^{+} u_{i,j,k} - \nabla_{\parallel}^{-} u_{i,j,k} \right]$$

- However: Better scheme possible

Parallel diffusion: Support operator method

- Motivated from *[Günter et al. (2005 and 2007)]*
- Construct scheme which mimics 'good' property on discrete level, i.e. self-adjointness ($u, v = 0$ at boundaries):

$$\left\langle u, \mathcal{D}_{\parallel} v \right\rangle = \int\limits_V u \nabla \cdot \left[\mathbf{b} \left(\nabla_{\parallel} v \right) \right] \, dV = - \int\limits_V \nabla_{\parallel} u \nabla_{\parallel} v \, dV \tag{1}$$

$$\rightarrow \nabla_{\parallel}^{\dagger} = -\nabla \cdot [\mathbf{b} \circ] , \quad \mathcal{D}_{\parallel}^{\dagger} = \mathcal{D}_{\parallel}$$

Support operator method *[Shaskov (1996)]*

Mimic integral equality 1 on discrete level

1. Define discrete space for scalars SG and fluxes (gradients) $FG^{\pm}$ with corresponding inner product
2. Define and discretise prime operator: $\nabla_{\parallel} \rightarrow \mathbf{Q}^{\pm} : SG \rightarrow FG^{\pm}$
3. Use integral equality 1 to construct derived operator

Parallel diffusion: Support operator method

Discrete spaces:

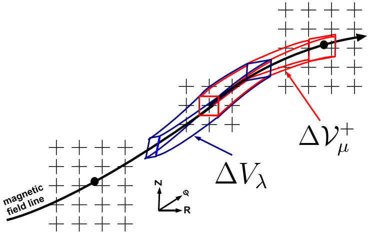
- Scalars SG : cylindrical grid
- Fluxes $FG^{\pm}$: staggered along field lines
- Inner products:

$$\langle u, v \rangle_{SG} := \sum_{\lambda} u_\lambda v_\lambda \Delta V_\lambda$$

$$\left\langle q^{\pm}, p^{\pm} \right\rangle_{FG^{\pm}} := \sum_{\mu} q^{\pm}_\mu p^{\pm}_\mu \Delta \mathcal{V}_\mu$$

Greek indices denote summation over all grid points

- Two possibilities $'\pm'$ (will be combined later)



Parallel diffusion: Support operator method

Discrete parallel gradient, discrete inner products, integral equality

Discrete parallel diffusion operator

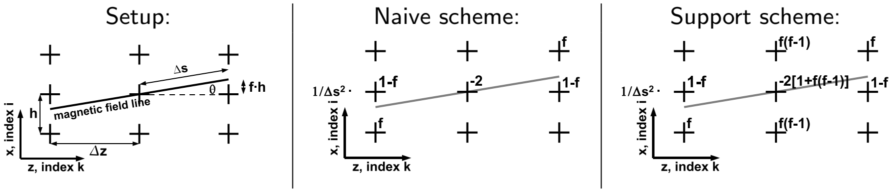
$$\boxed{\mathbf{D}^{\pm,supp}_{\parallel,\sigma,\lambda} = -\sum_{\mu} \mathbf{Q}^{\pm}_{\mu,\lambda} \mathbf{Q}^{\pm}_{\mu,\sigma} \frac{\Delta \mathcal{V}^{\pm}_{\mu}}{\Delta V_{\lambda}}}$$

Notes

- if volumes equal: $\mathbf{D}^{\pm,supp}_{\parallel} = -\left(\mathbf{Q}^{\pm}\right)^{T} \mathbf{Q}^{\pm}$
- Fusion of $'\pm'$ choice: $\mathbf{D}^{supp}_{\parallel} = \frac{1}{2}\left(\mathbf{D}^{+,supp}_{\parallel} + \mathbf{D}^{-,supp}_{\parallel}\right)$
- Conserves L1-norm (energy)
- Decreases L2-norm $\rightarrow$ numerically stable regardless of interpolation method

Simple 2D model problem

- $x \sim$ coordinate within poloidal plane, $z \sim$ toroidal coordinate
- Uniform magnetic field inclined by $\tan\theta = \frac{f\,h}{\Delta z}$ with respect to grid
- Linear interpolation along x (1d)



- Stencil for support scheme larger
- For $f = 0, 1$, i.e. no displacement, both schemes yield standard second order finite-difference expression

Numerical diffusion

Problem

- Interpolation introduces erroneous numerical coupling among distinct field lines
  $\rightarrow$ Leads to numerical perpendicular 'diffusion', which is dependent on resolution
- Might overwhelm real (slow) perpendicular dynamics $\chi_{\parallel}/\chi_{\perp} \sim 1 \cdot 10^{10}$
- Extremely high resolutions might be needed

Scaling of numerical diffusion

Action of discrete parallel diffusion operator on mode $u = \exp\left(ik_x x + ik_z z\right)$

$$\mathbf{D}_{\parallel}^{naive} u = \left[-k_{\parallel}^2 - \frac{f(1-f)(k_x h)^{2}}{\Delta s^{2}} + \mathcal{O}\left(\frac{(k_x h, k_z \Delta z)^4}{\Delta s^2}\right)\right] u$$

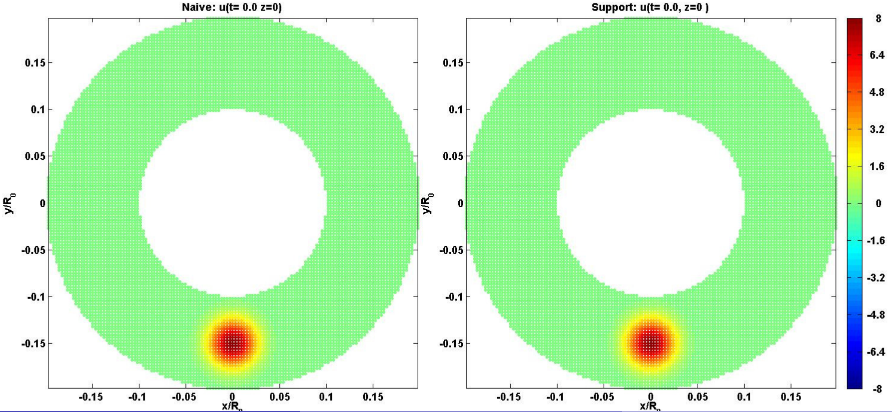
$$\mathbf{D}_{\parallel}^{supp} u = \left[-k_{\parallel}^2 + \mathcal{O}\left(\frac{(k_x h, k_z \Delta z)^{4}}{\Delta s^{2}}\right)\right] u$$

Support scheme exhibits better scaling $\rightarrow$ numerical diffusion drastically reduced

Numerical diffusion: Example

Example

- Parallel diffusion equation $\partial_t u = \chi_\parallel \mathcal{D}_\parallel u$
- Axial circular configuration with $q = 3$
- Initial state: $u(t=0,x,y,z) = \exp(-\frac{(x-x_0)^2+(y-y_0)^2}{\sigma^2}) \cdot \delta(z)$
- resolution: $N_z = 8$, $\frac{\sigma}{h} \approx 8.3$



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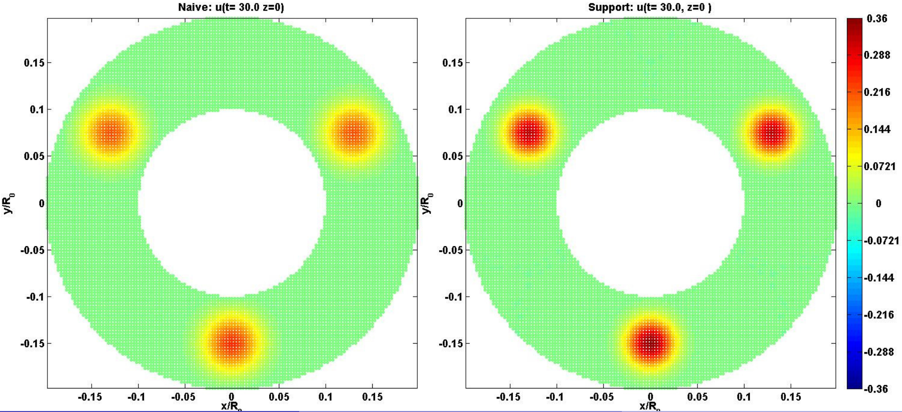

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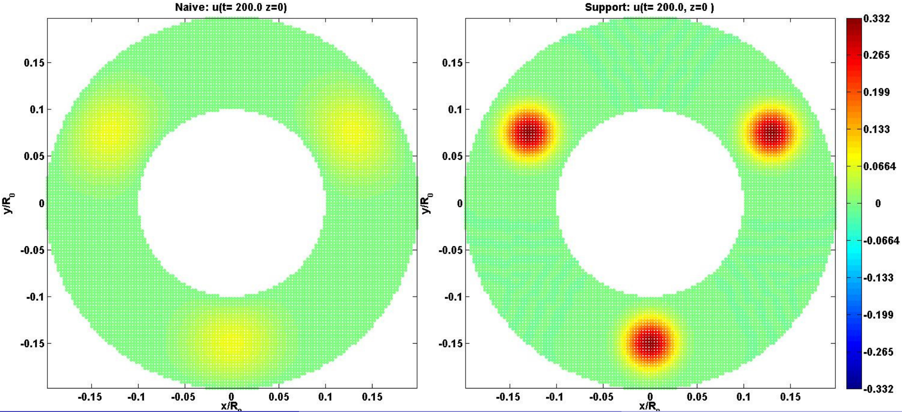
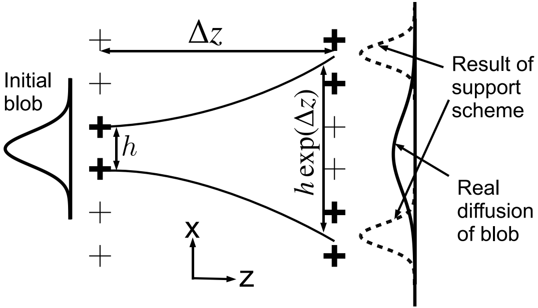


Map distortion

Magnetic field lines around X-point

- Lowest order expansion: $\mathbf{B} = B_0 \left[\mathbf{e_z} + \alpha \left(x\mathbf{e}_x - y\mathbf{e}_y\right)\right]$
- Distance between field lines diverges exponentially, i.e. $\delta(z) \propto \exp \alpha z$

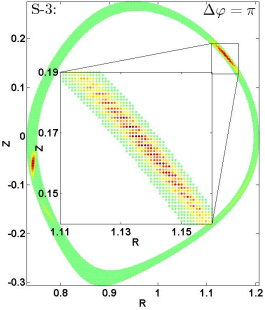


- With support scheme information is not only 'taken' but also 'sent' to neighbouring planes
- If points not properly connected erroneous wiggles may arise

Map distortion: Example

Result of diffusion of blob in flux surfaces close to separatrix:

Support scheme
Interpolation
$N_\varphi = 2$



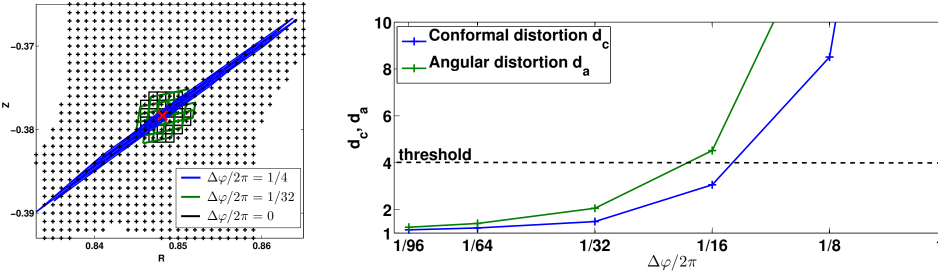
Map distortion: Remedy 1

- Quantify distortion via mapped quads:

$$d_c = \max_{i,j} \frac{\text{longest side of mapped quad } i,j}{\text{shortest side of mapped quad } i,j}, \qquad d_a = \max_{i,j} \frac{\text{largest angle of mapped quad } i,j}{\text{smallest angle of mapped quad } i,j}.$$

- Require enough toroidal resolution, such that map distortion remains below threshold

$$\boxed{d_c, d_a \leq 4}$$



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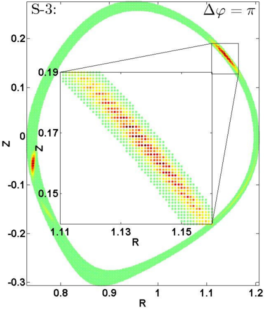
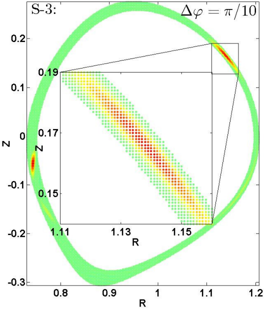


Support scheme
Interpolation
$N_\varphi = 20$



Note: Tiny oscillations on grid scale might still arise due to change of interpolation stamp *[Held15 et al., submitted]*, could be cured by small amount of high order perpendicular dissipation.

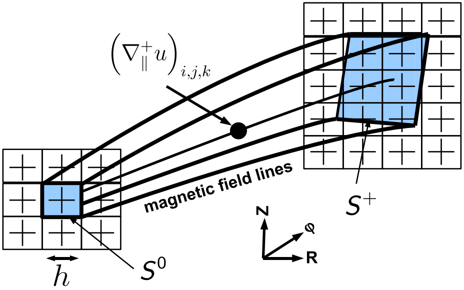
Map distortion: Remedy 2

Change parallel gradient to account for distorted field lines:

Coordinate free representation (Integration)

$$\nabla_{\parallel} u = \frac{1}{B}\nabla \cdot (u\mathbf{B}) = \frac{1}{B}\lim_{V\to 0}\frac{1}{V}\int_{\partial V} u\mathbf{B}\cdot d\mathbf{S}.$$

- Mimic surface integral on discrete level
- Integration over toroidal ends of flux box $\nabla_{\parallel}^{\pm} u = \pm\frac{1}{B_V \Delta\mathcal{V}}\left[\int_{S^{\pm}} uB_{tor}\,dS - \int_{S^0} uB_{tor}\,dS\right]$
- Combination with interpolation



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Result of diffusion of blob in flux surfaces close to separatrix:

Support scheme
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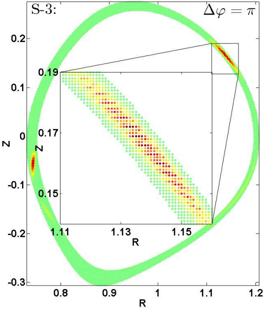
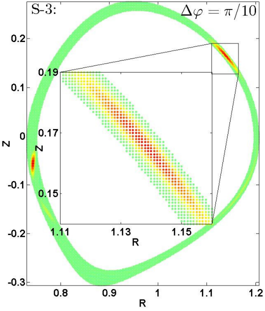
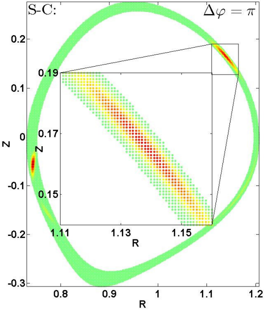


Support scheme
Interpolation
$N_\varphi = 20$



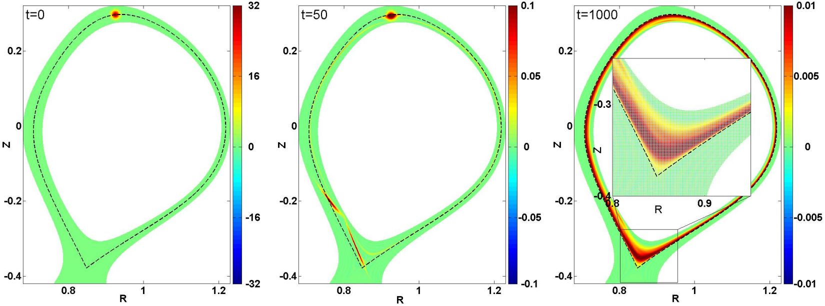
Support scheme
Integration
$N_\varphi = 2$



Application to separatrix

Example

- Initial state: Gaussian(R, Z)-delta(φ) blob located on separatrix
- resolution: $N_z = 16$, $\frac{\sigma}{h} = 10$
- Boundary conditions: $u = 0$ at divertor plates



- Improvement of parallel boundary conditions is ongoing (e.g. Neumann conditions)

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Normalised equations *[Hasegawa and Wakatani83]*:

Simple self-consistent 3D turbulence model (resistive drift-wave turbulence)

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_E \cdot \nabla\right) n = w_n \mathbf{v}_E \cdot \nabla \Psi\left(x_\perp\right) + \nu_n \nabla_\perp^6 n + \sigma \nabla \cdot \left[\mathbf{b} \nabla_\parallel \left(n - \phi\right)\right],$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_E \cdot \nabla\right) \nabla_\perp^2 \phi = + \nu_\phi \nabla_\perp^6 \left(\nabla_\perp^2 \phi\right) + \sigma \nabla \cdot \left[\mathbf{b} \nabla_\parallel \left(n - \phi\right)\right]$$

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- ν_n, ν_ϕ : viscosity coefficients
- σ : parallel conductivity, Ohm's law: $\sigma J_\parallel = \nabla_\parallel \left(n - \phi\right)$

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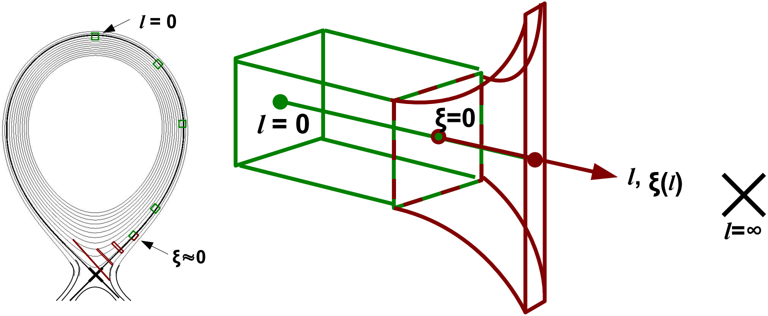
GRILLIX

- Model implemented for axisymmetric geometry with arbitrary poloidal cross section
- MPI + OpenMP parallelised

X-Point: Theoretical background

Flux box around reference magnetic field line approaching X-point



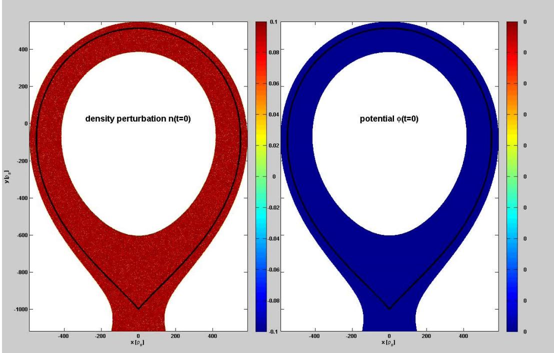
Basic picture *[Myra et al.]*

- Strong distortion of field-aligned structures towards X-point
- Drastic increase of $k_\perp$ towards X-point: $k_\perp(l) \xrightarrow[\xi \gg \alpha^{-1}]{} k_{\perp 0} \exp\left(\alpha \xi(l)\right)$

  $\rightarrow$ Operators with highest $k_\perp$ dependence dominant near X-point, i.e. dissipation
- X-point tends to disconnect structures $\rightarrow$ increase of $k_\parallel$

Axial diverted geometry[2]

Initial state

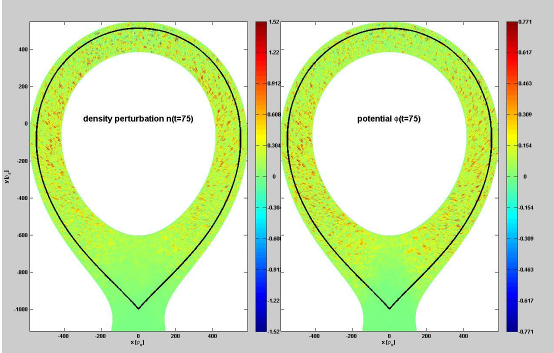


[2]Parameters reflect roughly:

T_e =80eV n_{e0} =4.5 · 10^{13}cm^{-3}, B =2.5T, R_0 =165cm, a =30cm, L_n =3.65cm, M_i =3670m_e, q_{95} ≈3/2

Axial diverted geometry[2]

Linear phase



Observations

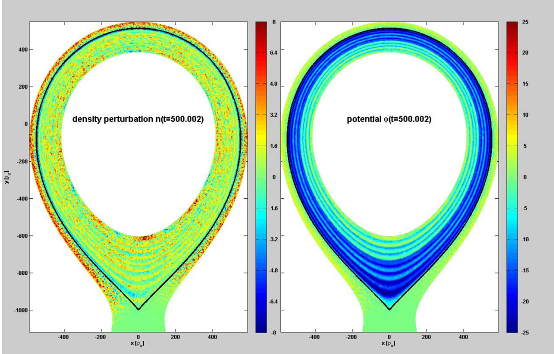
- Strongest effective drive at top
- Fluctuations towards sides driven by parallel currents
- No Fluctuations near X-point

[2]Parameters reflect roughly:

T_e =80eV n_{e0} =$4.5 \cdot 10^{13}\text{cm}^{-3}$, B =2.5T, R_0 =165cm, a =30cm, L_n =3.65cm, M_i =3670m_e, q_{95} ≈3/2

Axial diverted geometry[2]

Turbulent phase



Observations

- Automatic development of flux aligned structures
- Clear and sharp separation between open and closed flux surfaces visible

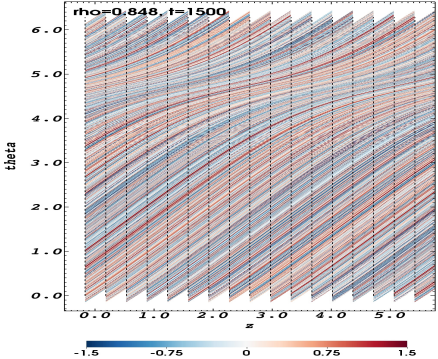
[2]Parameters reflect roughly:

T_e =80eV n_{e0} =$4.5 \cdot 10^{13}$cm^{-3}, B =2.5T, R_0 =165cm, a =30cm, L_n =3.65cm, M_i =3670m_e, q_{95} ≈3/2

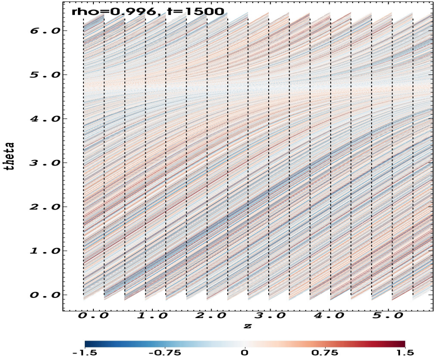
View along magnetic field lines:

Nonadiabaticity $n - \phi$ on flux surface...

...well inside:



...near separatrix



Observations

- structures are numerically smooth along field lines
- Fluctuations damped near X-Point $\rightarrow$ X-point disconnects structures $\rightarrow$ increase of $k_{\parallel}$
- Similar to resistive X-point mode *[Myra et al.00]*

Table of Contents

1. Introduction
2. Field line map
3. Application to simple turbulence model: Hasegawa-Wakatani
4. Outlook and summary

Recent developments and Outlook

- Extension to full-f:
  geometric multigrid solver for nonlinear polarisation ✓

$$\nabla \cdot (n \nabla_\perp \phi) = rhs$$

- Additional moments (parallel transport model ✓, thermal fluctuations) towards electromagnetic drift reduced Braginskii model
- Realistic boundary conditions (ongoing)
- Experimental equilibria (eqdsk) ✓
- Extension to 3D geometries, i.e. stellarators (maybe)
- Study of blob propagation in realistic geometry (ongoing → *M.Siccinio*)
- Cross verification against similar codes (GBS, FENICIA, TOKAM3D, FELTOR, BOUT++)
- Investigate effect of geometry on turbulent transport and heat exhaust, relevant for ITER and DEMO

Summary

Field line map

- Cylindrical/Cartesian grid, sparsified in toroidal/axial direction
- FCI: Not based on field/flux aligned coordinates → applicable to separatrix, X/O-points
- Discretisation of perp. operators straight forward (2nd order finite differences)
- Parallel operators via field line tracing and interpolation/integration
- Reduction of numerical diffusion via self-adjoint discretisation with support operator method
- Effects of map distortion identified and resolved (recommendation: use integration-interpolation)

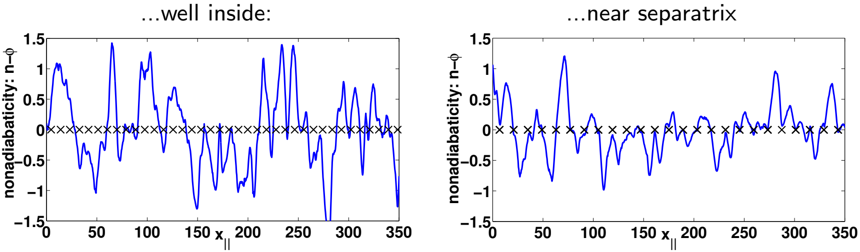
Application to simple turbulence model

- Hasegawa-Wakatani model implemented in parallel code GRILLIX
- Automatic development of field aligned and zonal structures (with Cartesian grid!!)
- Application to X-point geometry:
  - Strong shear enhances dissipation and leads to disconnection of structures
  - Increase of $k_{||}$
  - Confirmed with GRILLIX

Backup slides

View along magnetic field lines:

...along sample magnetic field line running in flux surfaces...



crosses (x) denote positions where field line passes bottom, i.e. where field line has its closest approaches to X-point

Observations

- Fluctuations strongly damped near X-point
- X-point disconnects structures → increase of $k_{||}$

→ Similar to resistive X-point mode *[Myra et al.00]*, though different physical model → Generic property of X-point

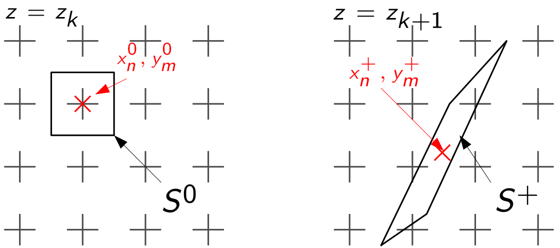
Integration-Interpolation method (detailed)

$$\nabla_{\parallel} u = \frac{1}{B} \lim_{V\to 0} \frac{1}{V} \int_{\partial V} u\mathbf{B}\cdot d\mathbf{S} \quad \Longrightarrow \quad \mathbf{Q}^{+} u = \frac{1}{B\Delta\mathcal{V}^{+}} \underbrace{\left[\int_{S^+} uB_{tor}\, dS_{tor} - \int_{S^0} uB_{tor}\, dS_{tor}\right]}_{\text{mimic}}$$

$$\int_{S^0} uB_{tor}\, dS_{tor} = \sum_{n,m=1}^{2^X} u(x_n^0, y_m^0, z=z_k) B_{tor}(x_n^0, y_m^0) \frac{h^2}{2^{2X}}, \qquad \int_{S^+} uB_{tor}\, dS_{tor} = \sum_{n,m=1}^{2^X} u(x_n^+, y_m^+, z=z_{k+1}) B_{tor}(x_n^+, y_m^+) \Delta S^+,$$

$u(x_n^0, y_m^0, z_k)$, $u(x_n^+, y_m^+, z_{k+1})$ via interpolation, B_{tor} analytically available, $\Delta S^+ = \frac{h^2}{2^{2X}} \frac{B_{tor}(x_n^0, y_m^0)}{B_{tor}(x_n^+, y_m^+)}$

X=0:



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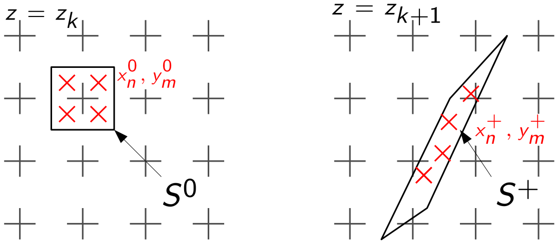
X=1:



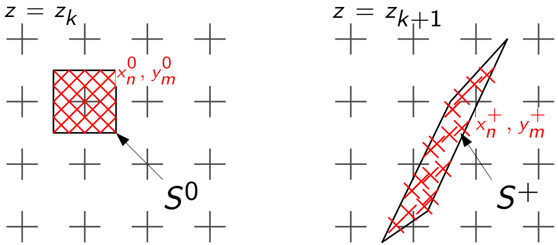
Integration-Interpolation method (detailed)

$$\nabla_{\parallel} u = \frac{1}{B} \lim_{V \to 0} \frac{1}{V} \int_{\partial V} u\mathbf{B} \cdot d\mathbf{S} \quad \Longrightarrow \quad \mathbf{Q}^{+} u = \frac{1}{B \Delta \mathcal{V}^{+}} \underbrace{\left[\int_{S^{+}} u B_{tor} dS_{tor} - \int_{S^{0}} u B_{tor} dS_{tor} \right]}_{\text{mimic}}$$

$$\int_{S^0} u B_{tor} dS_{tor} = \sum_{n,m=1}^{2^X} u(x_n^0, y_m^0, z = z_k) B_{tor}(x_n^0, y_m^0) \frac{h^2}{2^{2X}}, \qquad \int_{S^+} u B_{tor} dS_{tor} = \sum_{n,m=1}^{2^X} u(x_n^+, y_m^+, z = z_{k+1}) B_{tor}(x_n^+, y_m^+) \Delta S^+,$$

$u(x_n^0, y_m^0, z_k)$, $u(x_n^+, y_m^+, z_{k+1})$ via interpolation, B_{tor} analytically available, $\Delta S^+ = \frac{h^2}{2^{2X}} \frac{B_{tor}(x_n^0, y_m^0)}{B_{tor}(x_n^+, y_m^+)}$

X=2:

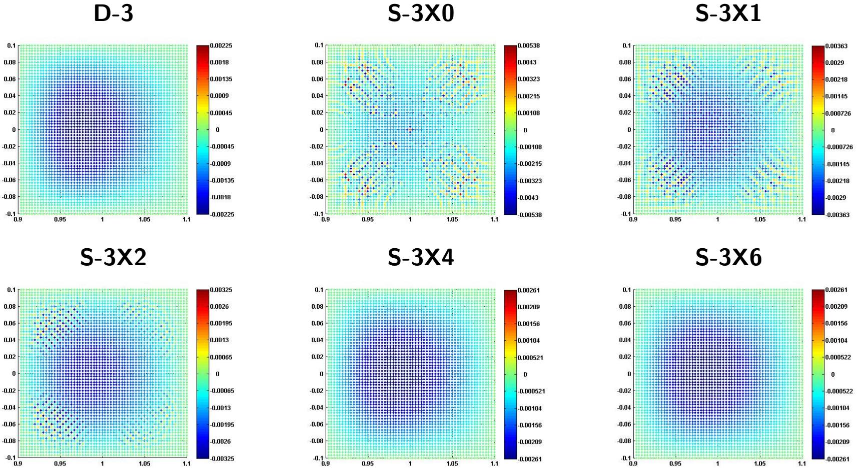


Consistency of parallel diffusion operator in general geometry

Considered case *[Held15]*:

$$\Psi(R,Z) = \cos\left(\frac{\pi}{2}(R - R_0)\right)\cos\left(\frac{\pi}{2}Z\right), \quad u(R,Z,\varphi) = -\Psi(R,Z)\cos(\varphi)$$

Difference to analytic result:



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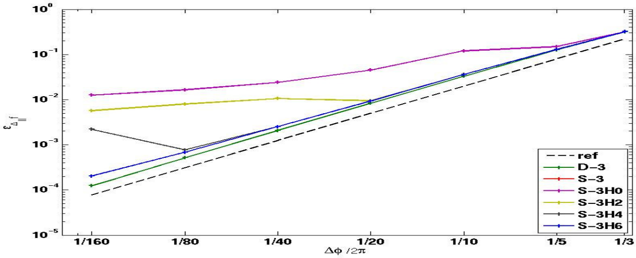
Quantify numerical error $\epsilon_{\Delta_\| u} := \frac{\left|(\mathcal{D}_\| u)_{numeric} - (\mathcal{D}_\| u)_{analytic}\right|_2}{\left|(\mathcal{D}_\| u)_{analytic}\right|_2}$



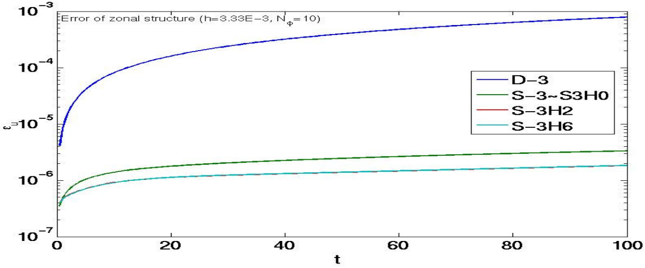
- Second order accuracy in toroidal direction can be achieved
- Prerequisite: sufficiently high perp. resolution, sufficiently high X to account for map distortion

Numerical diffusion in general geometry

Considered case *[Held15]*:

$$\Psi(R,Z) = \cos\left(\frac{\pi}{2}(R-R_0)\right)\cos\left(\frac{\pi}{2}Z\right), \quad u(R,Z,\varphi,t=0) = 0.1\Psi(R,Z)^2$$

Measure numerical diffusion: $\epsilon_u(t) = \frac{|u(t)-u(t=0)|_2}{|u(t=0)|_2}$



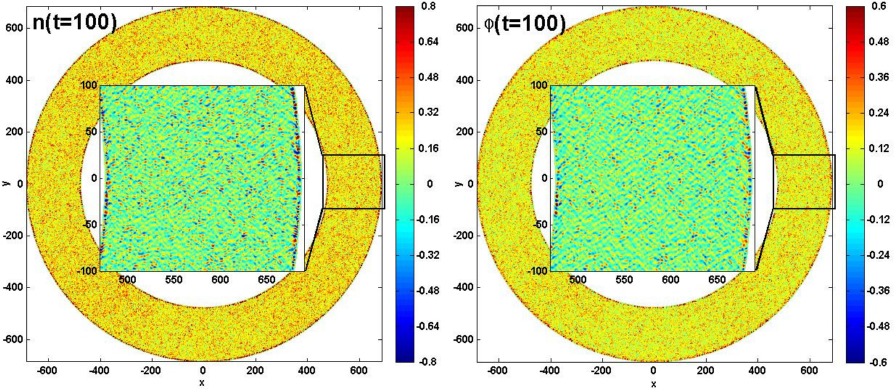
- Lower numerical diffusion with support scheme compared to naive scheme also in general geometries

Axial circular geometry

Demontstration simulation

T_e =80eV, n_{e0} =$4.5 \cdot 10^{13}$cm^{-3}, B =2.5T, R_0 =165cm,

a =30cm, $L_n = |n_{e0}/(\nabla n_{e0})| = 3.65$cm, M_i =3670m_e, q_0 =$3/2, \hat{s} = 0.7$



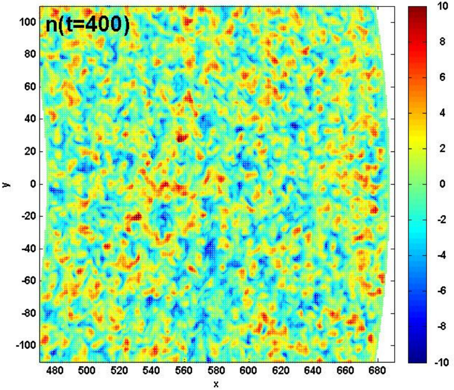
Linear phase: poloidally propagating drift waves

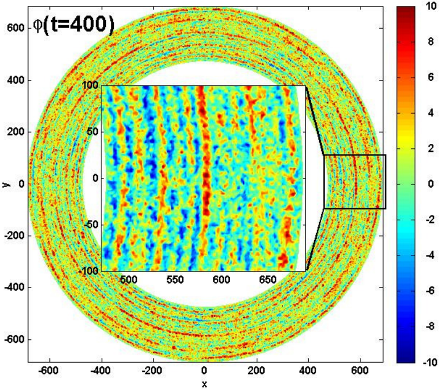
Axial circular geometry

Demontstration simulation

$T_e = 80\text{eV}, \quad n_{e0} = 4.5 \cdot 10^{13}\text{cm}^{-3}, \quad B = 2.5\text{T}, \quad R_0 = 165\text{cm},$

$a = 30\text{cm}, \quad L_n = |n_{e0}/(\nabla n_{e0})| = 3.65\text{cm}, \quad M_i = 3670 m_e, \quad q_0 = 3/2, \hat{s} = 0.7$





Onset of turbulent phase: Eddy mitosis

Axial circular geometry

Demontstration simulation

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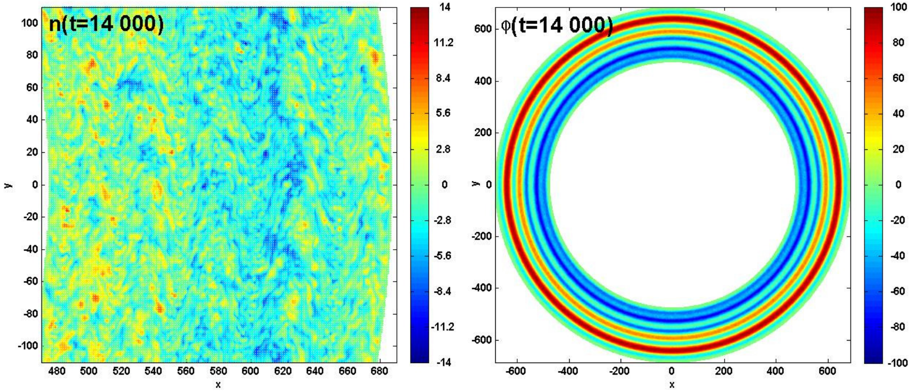
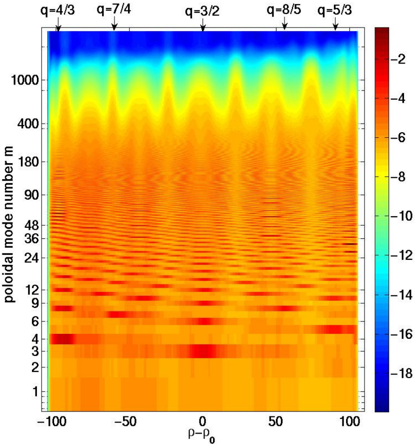


Saturated phase: Zonal flow

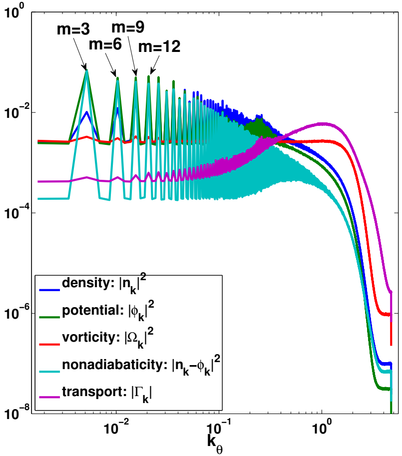
Axial circular geometry

Poloidal spectra:

$\log|\phi_{k\theta}|^2$



spectra at $\rho = \rho_0,\ q = 3/2$



$k_{\|} \approx 0$ structures on rational surfaces in accordance with geometry

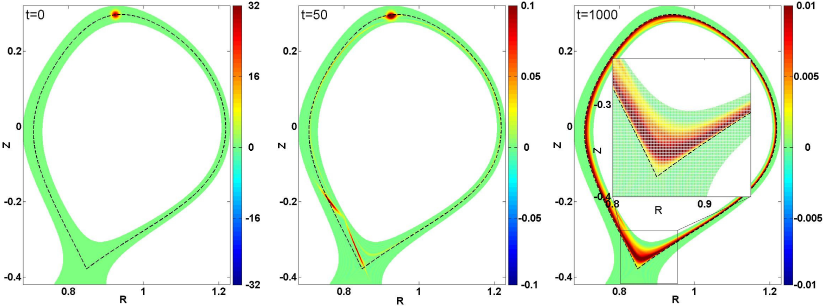
Toroidal Geometry

GRILLIX (A.Stegmeir, see talk on Thursday)

- FCI applied to toroidal geometries
- Discretisation of parallel diffusion
- Based on integral representation for parallel gradient to cope with map distortion

$$\nabla_{\parallel} u = \frac{1}{B} \nabla \cdot (u\mathbf{B}) = \frac{1}{B} \lim_{V \to 0} \frac{1}{V} \int_{\partial V} u\mathbf{B} \cdot d\mathbf{S}.$$

Simulation of temperature blob in realistic toroidal geometry (parallel diffusion):



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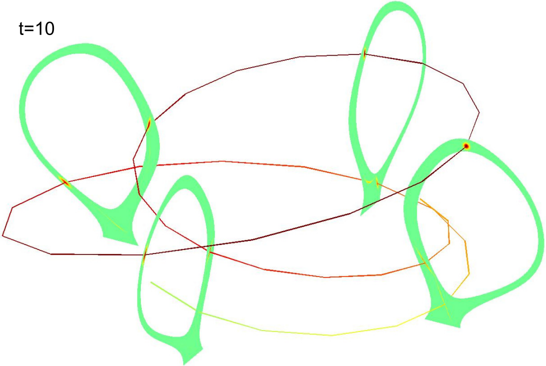
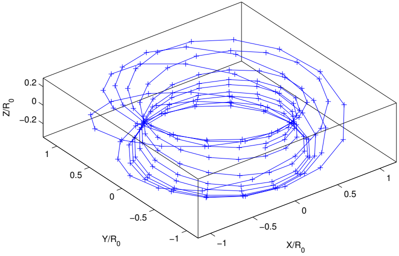
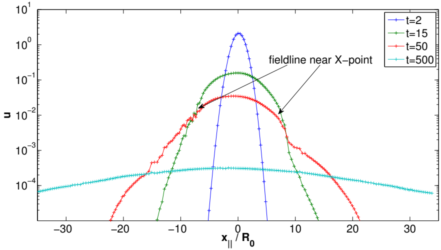
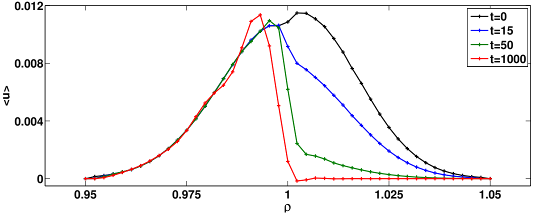


Structure along sample magnetic field line





Co



of Flux surface average: