The flux coordinate independent approach to plasma turbulence simulations

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Outline

• Motivation: plasma anisotropy and turbulence codes
• The flux coordinate independent (FCI) method to deal with plasma anisotropy
• Relation to various field-alignment methods
• Applications and tests:
  with the FENICIA finite difference code
  with the GYSELA semi-Lagrangian code
• Conclusions
The computational problem

Global, uniform grid, machine like ITER $a = 2m, R = 6m$

- Resolve the ion Larmor radius with four grid points, 1mm grid spacing
- Poloidal plane: $N_R \times N_Z = 4000 \times 4000$ points
- Toroidal direction 36000 points

$$N_{\text{points}} \sim \rho_*^{-3} \sim 6 \times 10^{11}, \text{unaffordable}$$

If one could work with a fixed ($\rho_*$-independent) number of toroidal points:

- $N_R = N_Z = 4000$, as before
- Perhaps $N_\phi = 64$

$$N_{\text{points}} \sim \rho_*^{-2} \sim 10^9, \text{feasible}$$

Achievable with a flux coordinate independent (FCI) method
Turbulence is anisotropic

Solutions of turbulence models have

\[ L_{\parallel} \sim qR, \quad L_{\perp} \sim \rho_i, \quad \nabla_{\perp} \gg \nabla_{\parallel} \]

Fluctuations in the \((\varphi, \theta)\) plane

Spectrum in the \((n,m)\) plane

Substantial waste of computer resources when using a uniform grid spacing
Anisotropy allows for a reduction of the number of grid points

Key considerations

a) Point reduction can be carried out in almost any direction (not perpendicular to the field lines).

b) Information about a function at missing grid points (due to point reduction) can be reconstructed with interpolation to the desired precision.

c) Mathematical operations, such as derivatives, can be carried out using the interpolated values at the missing grid points when needed.
An extreme case: $\nabla_{\parallel} = 0$ on a rational surface

Single helicity solution

$$f(r, \theta, \phi) = f(r, m\theta - n\phi)$$

In order to reconstruct the **full** dependence of $f$ on the three coordinates one needs the dependence on $r$ and

- the dependence on $\theta$ (at any given value of $\phi$), **but not** that on $\phi$, or
- the dependence on $\phi$ (at any given value of $\theta$), **but not** that on $\theta$, or
- the dependence on any line on the ($\theta, \phi$) plane **not parallel** to the magnetic field
The usual case: $\nabla_{\parallel} \approx 0$

Multiple helicity solutions, weak parallel gradient, on a discretised domain

$$f = f(r, \theta, \varphi), \quad \nabla_{\parallel} \sim 1/L_{\text{system}}$$

In order to reconstruct approximately but adequately the full dependence of $f$ on the three coordinates one needs the dependence on $r$ and

- the dependence on $\theta$, to a high accuracy and that on $\varphi$, to a lesser accuracy or
- the dependence on $\varphi$, to a high accuracy, and that on $\theta$, to a lesser accuracy or
- the dependence on any line on the $(\theta, \varphi)$ plane not parallel to the magnetic field, to a high accuracy, and the dependence on any line on the $(\theta, \varphi)$ plane not perpendicular to the magnetic field, to a lesser accuracy
Examples of grids with point reduction

Reduction in $\theta$
Most turbulence codes
Linear ballooning theory

Reduction in $\varphi$
Flux coordinate independent (FCI): point reduction directly in 3D

An FCI grid in Cartesian coordinates, with point reduction in z
Flux coordinate independent (FCI): point reduction directly in 3D

An FCI grid in Cartesian coordinates, with point reduction in z

with superimposed circular flux surfaces
FCI: the grid is independent of the flux surfaces

The same grid can be used for:
FCI: the grid is independent of the flux surfaces

The same grid can be used for:

Circular magnetic surfaces
FCI: the grid is independent of the flux surfaces

The same grid can be used for:

Circular magnetic surfaces and X-point configurations
Evaluation of differential operators with FCI: finite difference (FD) approach

Parallel derivative:

- Field line equations (straight geometry case)
  \[ \frac{dx}{ds} = b_x = \frac{\partial \psi}{\partial y} \]
  \[ \frac{dy}{ds} = b_y = -\frac{\partial \psi}{\partial x} \]
  \[ \frac{dz}{ds} = 1 \]

- Derivative along the line
  \[ \frac{d}{ds} f(x(s), y(s), z(s)) = -[\psi, f] + \partial f / \partial z = \nabla_\parallel f \]

- 2nd order FD expression
  \[ \nabla_{\text{FD}}^\parallel f = \frac{f(s+\Delta s) - f(s-\Delta s)}{2\Delta s} \]

The values of \( f \) at \( s \pm \Delta s \) are obtained by combining field line tracing with interpolation at end points.

F. Hariri, P. Hill, M. Ottaviani and Y. Sarazin, PoP 21, 082509 (2014)
F. Hariri, P. Hill, M. Ottaviani and Y. Sarazin, PPCF (2015), ArXiv 1409.2393v1
Parallel derivative with FD and interpolation

The computation of a parallel derivative at a grid point (red point) requires finding the end of a field line arc (blue point).

The value of a function at the blue point is obtained by interpolation in the poloidal plane.
Parallel derivative with FD and interpolation

The computation of a parallel derivative at a grid point (red point) requires finding the end of a field line arc (blue point).

The value of a function at the blue point is obtained by interpolation in the poloidal plane.

Key considerations

- The interpolation in the poloidal plane is easily good since resolution is high to resolve the Larmor radius.
- The X-point region is not special; no singularity of the field lines, no degeneracy of the coordinate system.
- Stochastic field lines do not pose a problem.
- Perpendicular (poloidal plane) operations are straightforward.
Likewise, in the toroidal case

- Field line equations
  
  \[ \frac{dR}{ds} = \frac{RB_R}{B_\varphi} \]
  
  \[ \frac{dZ}{ds} = \frac{RB_Z}{B_\varphi} \]
  
  \[ \frac{d\varphi}{ds} = 1 \]

- Derivative along the line
  
  \[ \frac{d}{ds} f(R(s), Z(s), \varphi(s)) = \frac{RB}{B_\varphi} \nabla_\parallel f \]

Straightforward implementation in machine coordinates (FCI) by choosing the toroidal angle as a parameter to track the position along a field line.

F. Hariri, P. Hill, M. Ottaviani and Y. Sarazin, PoP 21, 082509 (2014)

F. Hariri, P. Hill, M. Ottaviani and Y. Sarazin, PPCF (2015), ArXiv 1409.2393v1
FCI for kinetic semi-Lagrangian codes

Example: simple electrostatic problem, large scale limit

\[
\frac{\partial f_{GC}}{\partial t} + \mathbf{v}_E \cdot \nabla \perp f_{GC} + \mathbf{v}_\parallel \nabla \parallel f_{GC} + \frac{q}{m} \mathbf{E}_\parallel \frac{\partial f_{GC}}{\partial \mathbf{v}_\parallel} = 0
\]

Splitting (not discussed here) leads to the sub-problem:

\[
\frac{\partial f_{GC}}{\partial t} + \mathbf{v}_\parallel \nabla \parallel f_{GC} = 0
\]

Exact solution with the method of characteristics

\[
f_{GC}(s, t + \Delta t) = f_{GC}(s - \Delta s, t)
\]

where \(s\) indicates a grid point, and \(s - \Delta s\) is generally a non-grid point obtained by following a field line by an amount \(\Delta s = \mathbf{v}_\parallel \Delta t\)

The value of the function at \(s - \Delta s\) is obtained by a **double interpolation**, first in the poloidal plane and then along the field line.
Relation to field-aligning transformations

Ballooning (PPPL, early ’90s) with shifts (Scott, 2001)

\[
\begin{cases}
\xi = \varphi - q(r)(\theta - \theta_k) \\
s = (\theta - \theta_k) \\
\rho = r
\end{cases}
\]

\[
\nabla_\parallel = \frac{1}{q(r)} \frac{\partial}{\partial s}
\]

- Most common method in codes
- \(\theta\) labels the position along a field line
- Reduction of points is in \(\theta\)
- The small scale dependence is in \(\varphi\)
- Like in the linear ballooning representation

Outline
Motivation
Anisotropy and grid point reduction
FCI
Relation to other methods
Tests and applications
DW, cylinder
SW, X-point
ITG instability and turbulence
Turbulence with an island
Summary
Relation to field-aligning transformations

Ottaviani, 2009

\[\begin{align*}
\xi &= \theta - \frac{1}{q(r)}(\varphi - \varphi_k) \\
\sigma &= (\varphi - \varphi_k) \\
\rho &= r
\end{align*}\]

\[\nabla_{||} = \frac{\partial}{\partial s}\]

FCI directly in 3D (this talk)

\[\begin{align*}
\xi^1 &= V^1(x) + C^1(x)(z - z_k) \\
\xi^2 &= V^2(x) + C^2(x)(z - z_k) \\
\sigma &= z - z_k
\end{align*}\]

- \(\xi\) chosen such that \(\nabla_{||} = \left(\frac{\partial}{\partial s}\right)_{\xi=\text{cst}}\)
- Point reduction is in \(z\) or \((\varphi)\)
Tests and applications

- Drift wave propagation in cylindrical geometry
- Sound wave propagation in X-point geometry
- ITG turbulence in cylindrical geometry
- Semi-Lagrangian code implementation: first tests
- ITG turbulence in a magnetic island: the question of profile flattening and the critical island width in NTM theory
Testing FCI: drift-wave propagation in cylindrical geometry

Consider a 3D Drift-Wave model:

\[
\begin{cases}
\frac{\partial \phi}{\partial t} + [\phi, N_0(r)] + C_\parallel \nabla_\parallel u = 0 \\
\frac{\partial u}{\partial t} + \frac{2}{\tau} C_\parallel \nabla_\parallel \phi = 0
\end{cases}
\]

- With initial condition:
  \( \phi(t = 0) = f(r) \times \cos(m\theta - n\phi) \)

- The relative error writes:
  \( E^2 = \frac{\langle (\phi_{\text{exact}} - \phi_{\text{num}})^2 \rangle}{\langle (\phi_{\text{exact}})^2 \rangle} \)

Parameters:
\[ C_\parallel = \frac{a}{(\rho_* R)} \]
\[ N_x = N_y = 400, N_z = 20 \]
\[ m = 30 \text{ and } n = 15 \]
EXCEEDS the Nyquist cutoff
Testing FCI: drift-wave propagation in cylindrical geometry

Consider a 3D Drift-Wave model:

\[
\begin{align*}
\frac{\partial}{\partial t} \phi + \left[ \phi, N_0(r) \right] + C_\parallel \nabla_\parallel u &= 0 \\
\frac{\partial}{\partial t} u + \frac{2}{\tau} C_\parallel \nabla_\parallel \phi &= 0
\end{align*}
\]

\( \text{With initial condition:} \)

\( \phi(t = 0) = f(r) \times \cos(m\theta - n\phi) \)

\( \text{The relative error writes:} \)

\[ E^2 = \frac{\langle (\phi_{\text{exact}} - \phi_{\text{num}})^2 \rangle}{\langle (\phi_{\text{exact}})^2 \rangle} \]

\( \text{Parameters:} \)

\( C_\parallel = a/(\rho_\star R) \)

\( Nx = Ny = 400, Nz = 20 \)

\( m = 30 \) and \( n = 15 \)

\( \text{EXCEEDS the Nyquist cutoff} \)

\( \text{Result:} \)

- The contribution to the error from the parallel dynamics is negligible
- The code is able to simulate drift-wave propagation with \( n \) exceeding the Nyquist cutoff


18 March 2015
Sherwood meeting 2015, NYU
Testing FCI: sound-wave propagation in X-point geometry

Consider an equilibrium with a magnetic island:

\[ \psi = -\frac{(x - 1)^2}{2} + A \cos(y) \]

in a slab domain periodic in \( y \) and \( z \)

\[ \mathbf{b} \equiv \nabla \times (\psi \mathbf{e}_z) + \mathbf{e}_z \]

\[ \nabla_{\parallel} \equiv \mathbf{b} \cdot \nabla = -[\psi, \cdot] + \partial_z \]

Sound wave model

\[
\begin{align*}
\partial_t \phi + C_{\parallel} \nabla_{\parallel} u &= 0 \\
\partial_t u + \frac{(1+\tau)}{\tau} C_{\parallel} \nabla_{\parallel} \phi &= 0
\end{align*}
\]
Comparison with analytic solutions at the exterior of the island

Analytic solution of the sound wave model:

\[
\begin{pmatrix}
\phi(\rho, \eta, t) \\
u(\rho, \eta, t)
\end{pmatrix}
= \begin{pmatrix}
\phi_0(\rho) \\
u_0(\rho)
\end{pmatrix}
\cos [m \eta - n z - \omega(\rho) t]
\]

with \((\rho, \eta)\) island flux coordinates and \(\omega\) the mode frequency

**Initial condition**
For \((m, n) = (24, 1)\)

![Diagram showing the analytic solution]
Initial conditions across the separatrix

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Initial conditions

Energy conservation

Convergence

Energy conservation

Convergence

18 March 2015 Sherwood meeting 2015, NYU
Tests with ITG instability and turbulence

Gyrofluid model for \( \phi, u_\parallel, T_\parallel \) and \( T_\perp \)
in cylindrical geometry

\[
\log(E) \text{ as a function of time where } E = \langle \phi^2 \rangle
\]

\[
\gamma \approx 11.4
\]

\[
\gamma_{\text{theory}} \approx 11.7
\]

Potential fluctuations level

Convergence at \( N_z = 15 \)
Testing FCI within a semi-Lagrangian code

GYSELA code:

Test of ITG growth rate in a 4D ($\mu = 0$) gyrokinetic model.

Comparison between the uniform grid and the FCI semi-Lagrangian method.

G. Latu et al., https://hal.inria.fr/hal-01098373
Application: turbulence with a magnetic island

Goal: explore the temperature profile flattening mechanism caused by an island in a turbulent environment. Of interest for the NTM threshold problem

Main finding from the island width scan: the critical width for profile flattening is proportional to the turbulence correlation length

[P. Hill et al., PoP (2015), accepted]
A flux coordinate independent (FCI) method has been devised to exploit the anisotropic nature of plasma turbulent fluctuation and reduce computational needs.
Summary

• A flux coordinate independent (FCI) method has been devised to exploit the anisotropic nature of plasma turbulent fluctuation and reduce computational needs.

• Benefits of the method are:
  • grid independence of magnetic geometry
  • natural applicability to X-point configurations, 3D geometries and stochastic field lines
Summary

- A flux coordinate independent (FCI) method has been devised to exploit the anisotropic nature of plasma turbulent fluctuation and reduce computational needs.

- Benefits of the method are:
  - grid independence of magnetic geometry
  - natural applicability to X-point configurations, 3D geometries and stochastic field lines

- Tests and applications carried out to a variety of situations:
  - drift wave propagation and ITG turbulence in cylindrical geometry
  - sound wave propagation in X-point geometry and application to the problem of turbulence with a magnetic island
  - development and tests of the method for semi-Lagrangian kinetic codes.