The Flux-Coordinate Independent Approach

Farah Hariri

Contributors:

M. Ottaviani, Y. Sarazin, P. Hill, G. Latu, M. Mehrenberger, E. Sonnendrücker, L. Villard

1 EPFL, Swiss Plasma Center, 1015 Lausanne, Switzerland
2 CEA Cadarache, Saint Paul Lez Durance, France
3 University of York, UK
4 University of Strasbourg, France
5 Max-Planck-Institute, IPP Garching, Germany
• Motivation: plasma anisotropy
  Inability to simulate X-point geometry

• The flux coordinate independent (FCI) method to deal with plasma anisotropy and X-point geometry

• Relation to various field-alignment methods

• Applications:
  with the FENICIA finite difference code
  with the GYSELA semi-Lagrangian code
  with BOUT++/GRILLIX/FELTOR

• 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

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

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

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

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

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

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

Solutions of turbulence models have

\[ L_\parallel \sim qR, \ L_\perp \sim \rho_i, \]

\[ \nabla_\parallel \ll \nabla_\perp \]

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

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

⇒ Substantial waste of computer resources when using a uniform grid spacing
Motivations (1): Anisotropy allows for a reduction of the number of grid points

Key considerations:

a) Point reduction can be carried out in almost any direction

b) Information about a function at *missing* grid points can be reconstructed

c) Derivatives can be carried out using the interpolated values at missing grid pts
Motivations (2): Tackling the X-point geometry

X-points in Magnetic Islands & in Tokamak Configurations are singular

$q$ diverges at the X-point

⇒ It is numerically challenging to implement $\nabla_{\|}$ in the X-point neighborhood
An extreme case: $\nabla_{\parallel} = 0$ on a rational surface

Single helicity solution

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

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 $\varphi$), but not that on $\varphi$, or
- the dependence on $\varphi$ (at any given value of $\theta$), but not that on $\theta$, or
- the dependence on any line on the ($\theta, \varphi$) 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

Motivation
Anisotropy: grid reduction
Review field-aligned coordinates
FCI
Applications
FENCIA: ITG instability & turbulence
SW, X-point
Interaction of turbulence with an island
GRILLIX
FELTOR
GYSELA
Summary

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

Reduction in $\varphi$
Ballooning (S. Cowley et al., 1991)

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

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

- Reduction of points is in \(\theta\)
- The small scale dependence is in \(\varphi\)
- Like in the linear ballooning representation
- Most common method in codes
- Can not deal with X-points
2D field-aligning transformations

with shifts (Scott, 2001)

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

- Reduction of points is in \( \theta \)
- The small scale dependence is in \( \varphi \)
- Like in the linear ballooning representation
- Most common method in codes
- Can not deal with X-points
2D field-aligning transformations

Ottaviani, 2009

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

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

- Reduction of points is in \(\phi\)
- The small scale dependence is in \(\theta\)
- Not efficient for flexible coding
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

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

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**
  
  \[
  \frac{d}{ds} f(x(s), y(s), z(s)) = -[\psi, f] + \frac{\partial f}{\partial z} = \nabla_{||} f
  \]

- **2nd order FD expression**
  
  \[
  \nabla^{\text{FD}}_{||} f = \frac{f(s + \Delta s) - f(s - \Delta s)}{2\Delta s}
  \]

The values of \( f \) at \( s \pm \Delta s \) are obtained by combining **field line tracing & interpolation at end points**. \( \nabla_{||} \) can be computed for any magnetic field **including stochastic ones**.

F. Hariri *et al.*, PoP 21, 082509 (2014)
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.
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 points:**
- Flux coordinates not needed, only a field line mapper is needed.
- 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.
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.

**Advantages:**
- Reduce the number of points along $z$
- Can use any coordinate system in the poloidal plane
- Can tackle any magnetic configuration: **X-points**
Likewise, in the toroidal case

- Field line equations:
  
  \[
  \frac{dR}{ds} = R \frac{B_R}{B_\varphi}
  \]
  
  \[
  \frac{dZ}{ds} = R \frac{B_Z}{B_\varphi}
  \]
  
  \[
  \frac{d\varphi}{ds} = 1
  \]

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

- Straightforward implementation of FCI by choosing the toroidal angle as a parameter to track the position along a field line

F. Hariri et al., PoP 21, 082509 (2014)
FCI for kinetic semi-Lagrangian codes

Example: simple electrostatic problem, large scale limit

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

Equations of motion:

1. Splitting \((r, \theta)\) and \(\varphi\) motions
   \[\implies \text{coupling } \perp \text{ and } \parallel \text{ dynamics:} \]
   \[
   \begin{cases}
   \frac{dr}{dt} = \mathbf{v}_E \cdot \nabla r \\
   \frac{d\theta}{dt} = \mathbf{v}_E \cdot \nabla \theta + \mathbf{v}_\parallel/q \, R \\
   \frac{d\varphi}{dt} = \mathbf{v}_\parallel/R
   \end{cases}
   \]

2. Splitting \(\mathbf{v}_E\) and \(\mathbf{v}_\parallel\) motions using the FCI spirit
   \[\implies \text{decoupling } \perp \text{ and } \parallel \text{ dynamics:} \]
   \[
   \begin{cases}
   \frac{dr}{dt} = \mathbf{v}_E \cdot \nabla r \\
   \frac{d\theta}{dt} = \mathbf{v}_E \cdot \nabla \theta \\
   \frac{d\varphi}{dt} = \mathbf{v}_\parallel/R \\
   \end{cases}
   \]
   and
   \[
   \begin{cases}
   \frac{d\theta}{dt} = \mathbf{v}_\parallel/q \, R \\
   \frac{d\varphi}{dt} = \mathbf{v}_\parallel/R
   \end{cases}
   \]
• Finding the foot of the trajectories using semi-Lagrangian (backward) method

\[ \theta^* = \theta(t) = \theta_i(t + \Delta t) - (v_{||}/q R) \Delta t \]
\[ \varphi^* = \varphi(t) = \varphi_j(t + \Delta t) - (v_{||}/R) \Delta t \]

• Interpolating to find the distribution function at \((\theta^*, \varphi^*)\)
Codes adopting the FCI approach

Part of 3 ER Projects (2015-2017). It is now implemented in:

1. **FENICIA** 3D fluid code  
   [F. Hariri and M. Ottaviani, CPC, 2013]

2. **BOUT++** 3D fluid code (York)  
   [B. Shanahan, B. Dudson, J. Phys conf. series, 2015]

3. **GRILLIX** 3D fluid (Garching)  
   → A. Stegmeir, talk on Thursday

4. **FELTOR** 3D gyrofluid code (Innsbruck)  
   → M. Held, Poster today

5. **GYSELA** 5D full-f gyrokinetic code (CEA)  
   [G. Latu and M. Mehrenberger]
FENICIA: ITG turbulence simulations

Solves a gyrofluid model in cylindrical geometry:

\[
\begin{align*}
\partial_t \tilde{n} + [\phi, \log(n0)] - [\phi, \rho_\star^2 \nabla^2 \phi] + C_\parallel \nabla_\parallel u_\parallel &= D_n \nabla^2_\perp \tilde{n} \\
\partial_t u_\parallel + [\phi, u] + C_\parallel (\frac{1}{\tau} \nabla_\parallel \tilde{n} + \nabla_\parallel \phi + \nabla_\parallel T_\parallel) &= D_u \nabla^2_\perp u_\parallel \\
\partial_t T_\parallel + [\phi, T_\parallel] + \frac{2}{\tau} C_\parallel \nabla_\parallel u_\parallel - \chi_\parallel \nabla^2_\parallel T_\parallel &= D_{T_\parallel} \nabla^2_\parallel T_\parallel \\
\partial_t T_\perp + [\phi, T_\perp] - \chi_\parallel \nabla^2_\parallel T_\perp &= D_{T_\perp} \nabla^2_\perp T_\perp \\
\phi &= \tilde{n}
\end{align*}
\]

\[\gamma \approx 11.4\]

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

---

log(E) as a function of time where \(E = \int (\phi^2 \, dV)\)

0 0.1 0.2 0.3 0.4
0 2 4 6

Potential fluctuations level
Convergence at \(N_z = 15\)
movie: 3D evolution of density fluctuations
Consider an equilibrium with a magnetic island:

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

in a slab domain periodic in $y$ and $z$

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

$$\nabla_\parallel \equiv b \cdot \nabla = -[\psi, .] + \partial_z$$

**Sound wave model**

$$\begin{cases}
\partial_t \phi + C_\parallel \nabla_\parallel u = 0 \\
\partial_t u + \frac{1+\tau}{\tau} C_\parallel \nabla_\parallel \phi = 0
\end{cases}$$
Convergence achieved 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 \((m, n) = (24, 1)\)
movie: evolution of a perturbation across the separatrix
Convergence achieved across the separatrix

Convergence with respect to NZ

Moving difference (norm of volume average)

Number of grid points $N_z$
FENICIA main application: Interaction of 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.

**Figure:** island width $\omega = 4\rho_i$

**Figure:** island width $\omega = 8\rho_i$

**Main finding from the island width scan:**

Turbulence can cross the separatrix and penetrate $\sim 4\rho_i$ into the island (roughly the turbulence correlation length)

GRILLIX: application of FCI in toroidal X-point geometry

GRILLIX (A. Stegmeir, see talk on Thursday)

- FCI applied to toroidal X-point geometry
- Discretisation of parallel diffusion
- Based on integral representation for parallel gradient to cope with map distortion
- Hasegawa-Wakatani simulations

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

![Temperature blob simulation](image_url)
We present a thermal full-F gyrofluid model in a 2D slab geometry. The model consists of the zeroth (\( T_0 \)), first (\( T_1 \)), and second (\( T_2 \)) moments of the Boltzmann equation. The field-aligned component of the electron drift velocity is given by\(^4\):

\[
\mathbf{v}_d = \frac{e}{m_e} \left( \mathbf{E} + \mathbf{v}_s \times \mathbf{B} \right)
\]

\( \mathbf{v}_s \) is the fluid bulk velocity, \( \mathbf{E} \) is the electric field, and \( \mathbf{B} \) is the magnetic field. The parallel component of the drift velocity is given by\(^4\):

\[
\mathbf{v}_{d,\parallel} = \frac{e}{m_e} \left( \mathbf{E}_\parallel + \mathbf{v}_s \times \mathbf{B}_\perp \right)
\]

\( \mathbf{E}_\parallel \) is the parallel electric field, and \( \mathbf{B}_\perp \) is the perpendicular component of the magnetic field. The thermal and field-aligned components are connected through the magnetic field line map, which formulates the numerical approximation to the parallel diffusion operator and the parallel gradient along the magnetic field line. To this end the detailed curve of the magnetic field is traced out to the next point along the magnetic field line. To this end the detailed curve of the magnetic field is traced out to the next point along the magnetic field line.

### Outline
- Full-F Gyrofluid Models In 2D
- Field-aligned coordinates
- Applications
  - FENCIA: ITG instability & turbulence
  - SW, X-point
  - Interaction of turbulence with an island
- GRILLIX
- FELTOR
- GYSELA

### Summary

**FELTOR (M. Held, see Poster today)**

- FCI in toroidal X-point geometry run on GPUs
- with discontinuous Galerkin methods
- 3D full-f Gyrofluid model with FLR effects

---

**Drift-Wave Turbulence In Global X-Point Geometry**

On the left the electron density during an ideal ballooning mode blowout is shown. The developed drift-wave turbulent state is given in the center, while on the right the footprint of zonal flows appears for the flux surface averaged vorticity. In the 3D fields of the electron parallel velocity (left) and the electron density (right) the characteristic flute mode structure appears. The spatial resolution is \( P_{\theta Z} = 3, P_r = 1, N_r = 120, N_Z = 160, N_r = 20 \).
GYSELA: application of FCI within a semi-Lagrangian code

GYSELA code:
Test of ITG growth rate in a 4D ($\mu = 0$) gyrokinetic model. Comparison: Uniform grid vs FCI semi-Lagrangian method

Figure: Potential energy as a function of time

G. Latu et al., https://hal.inria.fr/hal-01098373
Robustness of FCI in semi-Lagrangian schemes

<table>
<thead>
<tr>
<th>Reference case</th>
<th>Standard approach: $N_\varphi=128$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Radial coordinate R</strong></td>
<td><strong>Vertical coordinate Z</strong></td>
</tr>
<tr>
<td>0</td>
<td>50</td>
</tr>
<tr>
<td>Poloidal mesh $[0-2\pi]$</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>50</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Standard approach: $N_\varphi=32$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Radial coordinate R</strong></td>
</tr>
<tr>
<td>0</td>
</tr>
<tr>
<td>Poloidal mesh $[0-2\pi]$</td>
</tr>
<tr>
<td>0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Aligned approach: $N_\varphi=32$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Radial coordinate R</strong></td>
</tr>
<tr>
<td>0</td>
</tr>
<tr>
<td>Poloidal mesh $[0-2\pi]$</td>
</tr>
<tr>
<td>0</td>
</tr>
</tbody>
</table>

G. Latu et al., 2015 (in preparation)
• 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
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.