Overview over the edge fluid turbulence code GRILLIX

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BOUT++ ↔ GRILLIX

GRILLIX … :

... is a 3D fluid code for plasma edge/SOL turbulence in complex (diverted) geometries
... addresses problems related with edge confinement and heat exhaust

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<tr>
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<th>BOUT++</th>
<th>GRILLIX</th>
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<tbody>
<tr>
<td><strong>Model</strong></td>
<td>reduced fluid models (generic)</td>
<td>full-f drift reduced Braginskii</td>
</tr>
<tr>
<td><strong>Discretisation</strong></td>
<td>finite differences</td>
<td>finite differences</td>
</tr>
<tr>
<td><strong>‘Coordinates’</strong></td>
<td>globally field aligned (curvilinear)</td>
<td>FCI (locally field aligned)</td>
</tr>
<tr>
<td><strong>Language</strong></td>
<td>C++ (MPI)</td>
<td>Fortran (MPI + OpenMP) → C++ for GPU</td>
</tr>
<tr>
<td><strong>Community</strong></td>
<td>global, code publicly available</td>
<td>~ 10 persons located mainly at IPP</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Garching, code available on request</td>
</tr>
</tbody>
</table>
Drift reduced Braginskii model

Basic assumptions:

\[ \lambda_{mfp,\parallel} \ll R_0 \]
\[ \omega \ll \Omega_i \]
\[ \beta \ll 1 \]
\[ k_{\parallel} \ll k_{\perp} \]

plasma density
\[ \frac{\partial}{\partial t} n + \nabla \cdot (n \mathbf{v}_e) = 0 + k_{iz} n N \]

quasineutrality / vorticity
\[ \nabla \cdot \mathbf{j} = \nabla \cdot (e n \mathbf{v}_i - e n \mathbf{v}_e) = 0 \]

Drift reduction:
\[ \mathbf{v}_{e\perp} = \mathbf{v}_E + \mathbf{v}_e^* \]
\[ \mathbf{v}_{i\perp} = \mathbf{v}_E + \mathbf{v}_i^* + \mathbf{u}_{pol} \]
\[ \mathbf{v}_{e\perp}^* = \mp (\mathbf{B} \times \nabla \mathbf{v}_{e,i}) / e n \mathbf{B}^2 \]
\[ \mathbf{u}_{pol} = \frac{m_i}{e \mathbf{B}^2} \mathbf{B} \times \left( \frac{\partial}{\partial t} + \mathbf{v}_E \cdot \nabla \right) (\mathbf{v}_E + \mathbf{v}_i^*) \]

electromagnetic parallel dynamics
\[ \mathbf{E} = -\nabla \varphi - \partial_t A_\parallel \mathbf{b}, \quad \mathbf{B} = \mathbf{B}_0 + \nabla \times A_\parallel \mathbf{b}, \quad \mathbf{B} \approx \mathbf{B}_0 \]

electron heat
\[ \left[ \frac{\partial}{\partial t} + \mathbf{v}_e \cdot \nabla \right] T_e + \frac{2}{3} T_e \mathbf{v}_e \cdot \mathbf{v}_e = -\frac{2}{3n} \nabla \cdot \mathbf{q}_e + \frac{2}{3n} Q_e + S_{Te} \]

ion heat
\[ \left[ \frac{\partial}{\partial t} + \mathbf{v}_i \cdot \nabla \right] T_i + \frac{2}{3} T_i \mathbf{v}_i \cdot \mathbf{v}_i = -\frac{2}{3n} \nabla \cdot \mathbf{q}_i - \frac{2}{3n} P_i : \mathbf{v}_i \]

diffusive neutrals
\[ \frac{\partial}{\partial t} N = \nabla \cdot \frac{1}{n k_{cx}} \nabla N T_i - k_{iz} n N, \quad N \text{ fixed at the divertor} \]
Field aligned turbulence

- **High anisotropy**: structures are spaghettis ($k_\perp \gg k_\parallel$), aligned to magnetic field
- **Complex geometry**: divertor, X-point, advanced diverter configurations, stellarators

[https://bout.llnl.gov/](https://bout.llnl.gov/)
Flux-Coordinate Independent approach (FCI)

Basic concept:
- Set of few Cartesian planes
- Perpendicular operators ($\nabla_{\perp}$) straightforward
- Parallel operators ($\nabla_{\parallel}$) via field line tracing to neighbouring planes and interpolation within planes

Advanced features in GRILLIX:
- Flux box volume integration
- Toroidally staggered → mimetic finite differences
- Immersed boundary method
Geometric flexibility

Advanced divertor concepts

Linear

Limiter

Single null


A. Ross, PoP 26, 2019

W. Zholobenko, CPP, 2019

W. Zholobenko, NF 61, 2021

W. Zholobenko, CPP, 2019

W. Zholobenko, NF 61, 2021

Validations: AUG

ASDEX Upgrade L-mode simulation in realistic geometry and at realistic parameters

- Neutral gas density at divertor tunable
- Good match with experimental profiles with
  \[ N_{\text{div}} = 5 \times 10^{17} \text{ m}^{-3} \]
- \[ P_{\text{exp}} = 750 \text{kW} \sim P_{\text{sim}} = 530 \text{kW} \]

W. Zholobenko, NF 61:116015, 2021
Validations: TCV-X21

- First validation of turbulence codes in diverted geometry
- Multicode validation (GBS, GRILLIX, TOKAM3X)
- Experimental and simulation data published (open access)
- Rigorous quantification of validation results

D.S. Oliveira and T. Body, NF 62:096001, 2022
Towards stellarators

- Locally Cartesian at $\varphi_k$
- Field aligned boxes $[\varphi_k - \Delta \varphi/2, \varphi_k + \Delta \varphi/2]$
- Non-conformal at $\varphi_k + \Delta \varphi/2$
- Actually non-straight smooth lines
Towards stellarators

\[ \partial_t u = \nabla \cdot \left[ b \nabla_{||} u \right] \]

T. S. Pederson, Nat. Commun. 7:13493, (2016)

- Blob traces out magnetic field lines
- Superiority of mimetic discretisation methods holds true in 3D geometries
- Full turbulence model in GRILLIX currently adapted

The field lines making up a magnetic surface are visualized in a dilute neutral gas, in this case primarily water vapour and nitrogen \((pn \approx 10^{-6} \text{ mbar})\).
Landau-Fluid closure

Heat flux most susceptible to kinetic effects

- Braginskii closure:
  \[ q^{BG} = \chi_e \nabla || T_e, \quad \chi_e = 3.2 \frac{n T_e \tau_{ei}}{m_e} \]

- Free streaming limiter:
  \[ q^{LIM} = \left( \frac{1}{q^{BG}} + \frac{1}{\alpha q^{FS}} \right)^{-1} \]
  - Free parameter \( \alpha \)

- Landau-fluid closure:
  - Self-consistent heat flux limiter
  - Non-local effects
  - Requires set of full 3D solves within FCI

J.G. Chen et al., CPC 236:128, 2019
Landau-Fluid closure

C. Pitzal et al., in preparation, 2023
Performance

Parallelisation concept
- MPI domain decomposition across planes
- OpenMP within planes

ITER Q=10 scenario
- Resolution: $3\rho_s @OMP$ separatrix, 16 plane
- Number of mesh points: 11 437 831 \times 16

<table>
<thead>
<tr>
<th>#OMP threads</th>
<th>Speedup</th>
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<tbody>
<tr>
<td>2</td>
<td>2.0</td>
</tr>
<tr>
<td>5</td>
<td>4.9</td>
</tr>
<tr>
<td>10</td>
<td>8.9</td>
</tr>
<tr>
<td>20</td>
<td>17.9</td>
</tr>
<tr>
<td>40</td>
<td>23.8</td>
</tr>
</tbody>
</table>
Elliptic solver

Elliptic Problem:

\[ \lambda \phi - \nabla \cdot (c \nabla_{\perp} \phi) = b \]

on an set of 2D poloidal planes independently (no MPI)

- for logically unstructured grid
- inhouse developed GMRES with geometric multigrid preconditioner
- Being ported to GPU (C++/Fortran interoperability)

<table>
<thead>
<tr>
<th>Algorithm:</th>
<th>time per solve [s]</th>
</tr>
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<tbody>
<tr>
<td>GMRES with geometric multigrid preconditioner</td>
<td>3.99</td>
</tr>
<tr>
<td>DIRECT (MKL)</td>
<td>72.80</td>
</tr>
<tr>
<td>PETSC -ksp_type gmres, -pc_type hypre</td>
<td>57.26</td>
</tr>
</tbody>
</table>
Code framework

Numerical and algorithmic tools for Flux-Coordinate Independent approach (Equilibra, meshes, solvers, operators)

Fluid turbulence models (Braginskii, Zhdanov)

Gyrokinetic model

Postprocessing
GENE-X: collision models for TCV-X21

No collisions  
Bhatnagar-Gross-Krook  
Lenard-Bernstein/Dougherty

Core dynamics of TCV dominated by trapped electron mode (TEM), which is not captured by fluid model

P. Ulbl et al., in preparation, 2023
Summary

GRILLIX

- has a similar scope to BOUT++
- is more targeted and specific in its model and approach
- less generic and modular with smaller community
- written in Fortran, GPU extension in C++ under development

Applications

- Variety of complex geometries
- Validations of TCV and AUG

Ongoing extensions

- Stellarator geometries
- Landau Fluid closure
- ...

GENE-X

- Flux-coordinate independent approach applied to gyrokinetic model
- Shares common API PARALLAX