Development and application of BOUT++ for large scale turbulence simulation

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PPPL Theory seminar
28 February 2017
Outline

Numerical developments

New coordinate system
Flux-coordinate independent method

A new plasma model (Hermes)

2-fluid cold ion model in divergence form
Including neutral interactions

Turbulence and Neutral Simulations

Linear device
MAST-U
DIII-D
What is BOUT++

• Framework for solving systems of PDE’s

• Flexible numerical methods and geometries
  • Pvode, PETSc, grids from EFIT

• Easy to implement physics models
  • $\frac{ddt(N_i)}{} = - \text{Div}(N_i \times V_i)$

• Designed with tokamaks in mind
  • Axisymmetry
  • Parallelization

• Open source at:
  https://github.com/boutproject/BOUT-dev
Standard field-aligned coordinates

- Coordinate system should be **field-aligned**:
- Ease of parallel operations
- Perturbations tend to have low $k_{\parallel}$

Coordinates:

\[ x = \psi \]
\[ y = \theta \]
\[ z = \phi - \int_{\theta_0}^{\theta} \nu \, d\theta \]
Why new coordinates?

- Still desire field-aligned system
- But poloidal projection of $x$ and $y$ are constrained to be orthogonal
- With new coordinate system we can:
  - Match divertor geometry
  - Approach X-point more closely and evenly
Flexible field-aligned coordinates

\[ x = \psi \]
\[ y = \theta - \int_{\psi_0}^{\psi} \eta \, d\psi \]
\[ z = \phi - \int_{y_0}^{y} \nu \left(1 + \int_{\psi_0}^{\psi} \eta \, d\psi \right) \, dy \]

Can now calculate metric tensors for spatial operators
Numerical accuracy

- Tested via the method of manufactured solutions\(^1\)
- Nine combination of orthogonalities tested
- Implementation in BOUT++ is 2\(^{nd}\) order accurate

J Leddy *et al* (2017) *Computer Physics Communications*
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<table>
<thead>
<tr>
<th>Orthogonal ((\eta = 0))</th>
<th>Poloidal pitch ((\eta = \text{const}))</th>
<th>Poloidal shear ((\eta \neq \text{const}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>No pitch ((\nu = 0))</td>
<td>2.00</td>
<td>2.14</td>
</tr>
<tr>
<td>Constant pitch ((\nu = \text{const}))</td>
<td>2.02</td>
<td>2.04</td>
</tr>
<tr>
<td>Shear ((\nu \neq \text{const}))</td>
<td>2.14</td>
<td>2.14</td>
</tr>
</tbody>
</table>

J Leddy *et al* (2017) *Computer Physics Communications*
FCI method

- In irregular and stochastic magnetic fields, having a flux coordinate independent (FCI) system can be preferable
- Cartesian planes – follow field lines and interpolate to perform parallel derivatives
- Benefits:
  - No assumption of flux surfaces
  - Parallel derivative entirely in parallel direction so no singularities in metric
Straight stellarator test

- As a test of the FCI Method, a straight stellarator was constructed.

- Solved parallel diffusion equation to trace flux surfaces.

- Inherent perpendicular diffusion reduced to tolerable levels ($<10^{-8}$) for ~1mm resolution.

\[ d_t (f) = \nabla^2_\parallel f \]

P Hill et al (2017) *Computer Physics Communications*
B Shanahan et al (2016) Accepted by *JP;CS*
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Limiter boundary condition

- Recently implemented:
  - Grid generator which takes input from analytic functions, VMEC equilibria, etc.
  - Parallel boundary conditions/poloidal limiters
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Multi-fluid codes

The workhorse of plasma boundary studies (e.g. SOLPS, EDGE2D, UEDGE, SONIC, ...)

Include detailed physics of plasma-wall interaction
- Parallel transport of heat and particles
- Sheath physics
- Neutral gas recycling
- Impurities
- Divertor plates, baffles, ducts, slots, pumps, ...

But
- Simplified cross-field transport

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\[ \frac{D}{r - r_{\text{sep}}} \sim 3.6 \text{ mm} \]

\[ D_\perp = 0.3 \text{ m}^2\text{s}^{-1}, \ \chi_{\perp,i,e} = 1.0 \text{ m}^2\text{s}^{-1} \]

\[ \lambda_q (\text{omp}) = 3 - 4 \text{ mm} \]

R. Schneider et al. (2006) *Contributions to Plasma Physics*
S. Wiesen et al. (2015) *Journal of Nuclear Materials*
X. Bonnin et al. (2016) *Plasma Fusion Research*
Turbulence codes

Calculating the turbulent transport requires solving for the time-varying plasma currents and electric fields

- Drift waves, ballooning/interchange instabilities, small-scale structure
- Computationally demanding, timesteps < ion cyclotron time
- Several codes under development (e.g. GBS, TOKAM-X, HESEL, BOUT++)
- Have not previously included detailed geometry, impurities, neutrals, ...

F D Halpern et al. (2016) *Journal of Computational Physics*
P Tamain et al. (2016) *Journal of Computational Physics*
Combining models

- Several attempts to combine transport models with turbulence codes
- Difficulties include
  - Consistency of underlying models
  - Separation of scales
  - Nonlinearity of atomic processes with density, temperature

Here the aim is to combine everything into one simulation, modelling “transport” and turbulence together

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F. Guzman et al. (2015) PPCF
The Hermes model

Current status

- Cold ion drift-fluid model
- Fluid neutrals: Diffusive, full Navier-Stokes, and hybrid models
- New differential operators for particle and energy conservation
- New electric field solver for n=0 mode

Flux-driven edge fluid simulations in X-point geometry

Under development

- Hot ion model
- EIRENE coupling for kinetic neutrals
- Pre-conditioners for faster simulation

Based on BOUT++

https://github.com/boutproject/hermes

Dudson and Leddy (2017) Submitted to PPCF
Model equations (1/2)

Evolving (electron) density \(n\), electron pressure \(p\)

\[
\frac{\partial n_e}{\partial t} = -\nabla \cdot \left[ n_e \left( \mathbf{V}_{E \times B} + \mathbf{V}_{mag} + b v_{||e} \right) \right] \\
+ \nabla \cdot (D_\perp \nabla_\perp n_e) + S_n
\]

\[
\frac{3}{2} \frac{\partial p_e}{\partial t} = -\nabla \cdot \left( \frac{3}{2} p_e \mathbf{V}_{E \times B} + \frac{5}{2} p_e b v_{||e} + p_e \frac{5}{2} \mathbf{V}_{mag} \right) \\
- p_e \nabla \cdot \mathbf{V}_{E \times B} + v_{||e} \partial_{||} p_e + \nabla_{||} \left( \kappa_e \partial_{||} T_e \right) \\
+ 0.71 \nabla_{||} (T_e j_{||}) - 0.71 j_{||} \partial_{||} T_e + \frac{\nu}{n} j_{||}^2 \\
+ \nabla \cdot (D_\perp T_e \nabla_\perp n_e) + \nabla \cdot (\chi_\perp n_e \nabla_\perp T_e) + S_p
\]

With \(E\times B\) and magnetic drifts given by:

\[
\mathbf{V}_{E \times B} = \frac{\mathbf{b} \times \nabla \phi}{B} \\
\mathbf{V}_{mag} = -T_e \nabla \times \frac{\mathbf{b}}{B}
\]

Dudson and Leddy (2017) Submitted to PPCF
Model equations (2/2)

Flows and currents are evolved through the vorticity, ion parallel momentum, and vector potential

\[
\frac{\partial \omega}{\partial t} = -\nabla \cdot (\omega \mathbf{V}_{E \times B}) + \nabla || \mathbf{j}|| - \nabla \cdot (n \mathbf{V}_{mag}) + \nabla \cdot (\mu_\perp \nabla \perp \omega)
\]

\[
\frac{\partial}{\partial t} \left( n_e v_{||i} \right) = -\nabla \cdot \left[ n_e v_{||i} (\mathbf{V}_{E \times B} + b v_{||i}) \right] - \partial || p_e + \nabla \cdot (D_\perp v_{||i} \nabla \perp n) - F
\]

\[
\frac{\partial}{\partial t} \left[ \frac{1}{2} \beta_e \psi - \frac{m_e}{m_i} \frac{\mathbf{j}_{||}}{n_e} \right] = \nu \frac{\mathbf{j}_{||}}{n_e} + \partial || \phi - \frac{1}{n_e} \partial || p_e - 0.71 \partial || T_e + \frac{m_e}{m_i} (\mathbf{V}_{E \times B} + b v_{||i}) \cdot \nabla \frac{\mathbf{j}_{||}}{n_e}
\]

Finite electron mass, electromagnetic

Boussinesq approximation

\[
\omega = \nabla \cdot \left( \frac{n_0}{B^2} \nabla \perp \phi \right)
\]
Conservation properties

- Movement of particles and thermal energy done using finite volumes (fluxes through cell faces), so particles conserved to high precision

Conserved energy

\[ E = \int dv \left[ \frac{m_i n_0}{2B^2} |\nabla \perp \phi|^2 + \frac{1}{2} m_i n V_{||}^2 + \frac{3}{2} p_e + \frac{1}{4} \beta_e |\nabla \perp \psi|^2 + \frac{m_e}{m_i} \frac{1}{2} \frac{j_{||}^2}{n} \right] \]
Boundary conditions

Interaction with plasma sheath a complex problem. Here relatively simple boundary conditions are used (multiple options in code for boundary conditions)

Ion velocity goes to the sound speed

\[ v_{||i} \geq c_s \]
\[ c_s = \sqrt{eT_e/m_i} \]

Conducting wall

\[ \dot{j}_{||} = e n_e \left[ v_{||i} - \frac{c_s}{\sqrt{4\pi}} \exp\left(-\{\phi/T_e\}\right) \right] \]

Sheath heat flux transmission

\[ q = v_{||i} \left( \frac{1}{2} m_i n_e v_{||i}^2 + \frac{5}{2} p_e \right) - \kappa_{||e} \partial_{||} T_e = \gamma_s n_e T_e c_s \]

with \( \gamma_s = 6.5 \)

M U Siddiqui et al. (2016) Physics of Plasmas
New solver for electric potential

To calculate electrostatic potential we invert the vorticity:

$$\nabla \cdot \left( \frac{m_i n}{B^2} \nabla_\perp \phi \right) = \frac{1}{J} \frac{\partial}{\partial u^i} \left( \frac{J m_i n}{B^2} g^{ij} \left( \nabla_\perp \phi \right)_j \right)$$

For low-n modes the poloidal terms become important.

Around the X-point unphysical oscillations occur if poloidal terms are neglected.

→ New solver implemented using PETSc for axisymmetric (n=0) component.
Successfully evolve n=0 potential

- Initial Alfvénic oscillations f~500 kHz damp on ~20 μs timescale

→ First time this has been possible with BOUT / BOUT++ in X-point geometry
Radial electric field

- Quasi-steady state has large radial electric field in SOL, driven by sheath and parallel electron force balance
- Reversing toroidal field modifies $E_r$ near separatrix
- Poloidal rotation sensitive to subtle effects, missing e.g. ion pressure
Neutral gas model (1/2)

Neutral gas is modelled as a fluid

\[
\frac{\partial n_n}{\partial t} = -\nabla \cdot [\mathbf{V}_n n_n] + S
\]

\[
\frac{\partial}{\partial t} \left( \frac{3}{2} p_n \right) = -\nabla \cdot \mathbf{q}_n + \mathbf{V}_n \cdot \nabla p_n + E
\]

\[
\mathbf{q}_n = \frac{5}{2} p_n \mathbf{V}_n - \kappa_n \nabla T_n
\]

Where \( S \) and \( E \) represent transfer of particles and energy between plasma and neutrals.

- Long mean free path of neutrals means Monte-Carlo treatment necessary in many cases
- Molecules not included. Can be important in high density regions
- Fluid model allows qualitative analysis and interpretation
Neutral gas model (2/2)

Model follows approach used in UEDGE

- Parallel to the magnetic field the neutral momentum equation is:

\[
\frac{\partial}{\partial t} \left( m_i n_n V_{\parallel n} \right) = -\nabla \cdot \left[ m_i n_n V_{\parallel n} \mathbf{b} V_{\parallel n} \right] - \partial_{\parallel} p_n + F
\]

- Perpendicular to the magnetic field, neglect neutral inertia, and balance neutral pressure against friction:

\[
F_{\perp} \simeq -\nu V_{n\perp}
\]

\[
V_{n\perp} = -\frac{1}{\nu} \nabla_{\perp} p_n
\]

\[
\nu = \nu_{cx} + \nu_{iz} + \nu_{nn}
\]

Collision rate = Charge exchange, ionisation, neutral-neutral

M.Umansky et al. (2003) *Journal of Nuclear Materials*
Atomic physics

- No molecular processes, only atoms evolved
- Simple semi-analytic fits used for atomic processes: Ionisation, recombination and charge exchange
- Provide source/sinks of particles, momentum and energy

- Carbon impurity included using fixed ion fraction (1% typically)
- Analytic radiation curve from Hutchinson thermal fronts paper

I.H.Hutchinson, (1994) *Nuclear Fusion*
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Turbulence and Neutral Simulations
   Linear device
   MAST-U
   DIII-D
Combining turbulence + neutrals

- Linear devices have simple geometries, making them a nice test-bed for plasma-neutral interaction.

- We have simulated a small Magnum-PSI sized device with the following parameters:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Magnetic field</td>
<td>0.15 T</td>
</tr>
<tr>
<td>Length</td>
<td>1.2 m</td>
</tr>
<tr>
<td>Radius</td>
<td>10 cm</td>
</tr>
</tbody>
</table>
Combining turbulence + neutrals

- Strong turbulence leads to significant modification of profiles (aided by insulating sheath boundary condition)
- Peak density off-axis at times
- Affects interaction with neutrals: only sources of neutrals are recycling at the target, and volume recombination

J. Leddy et al. (2016) In Press *Journal of Nuclear Materials & Energy*
Particle source/sinks

- Ionisation mainly occurs in highest density and temperature regions of the plasma (centre of eddies)
- Recombination is localised to the high density but low temperature regions (edge of the eddies)
Charge-exchange

- Significant energy is only removed where the temperature difference is greatest ($T_e - T_n$)
- Energy removed from plasma in centre (hottest region)
- Energy transferred to plasma in the edge, where $T_n > T_e$

- Note: cold ion model, so electron temperature used for atomic processes
Effect of fluctuations

Averaged over $8000 \omega_{ci}^{-1}$ ($\sim0.17$ms)
• Consistently higher neutral source with turbulence than without
• Difference in source/sinks peaks off-axis
• $\sim10\%$ max difference in ionisation, $\sim50\%$ max difference in recombination

Local profiles
\[ n_e n_n \langle \sigma v \rangle (T_e) \]

Axially-averaged profiles
\[ \bar{n}_e \bar{n}_n \langle \sigma v \rangle (\bar{T}_e) \]
Including drifts is challenging

- Balance of diamagnetic, parallel and polarisation currents
- Sheath currents at divertor
- Electric fields modify flows, edge asymmetries

Introduces rapid timescales: Alfven waves, electron parallel dynamics
  - Typically reduces timestep by factor of $\sim 10$
  - Can lead to numerical instabilities

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R. Pitts (2015) IAEA TM on Divertor Concepts

T D Rognlien, et al. (1999) *Physics of Plasmas*
**MAST-Upgrade simulations**

Axisymmetric fluid simulation: No electric fields, no turbulence

- **Recycling fraction**: 80%
- **Carbon fraction**: 1%
- **$n_{e,sep}$**: $1.3 \times 10^{19} \, \text{m}^{-3}$
- **$T_{e,sep}$**: 63 eV
- **$D$**: 0.2 m$^2$/s
- **$X$**: 0.5 m$^2$/s

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E. Havlicova, et al. (2014) *Contributions to Plasma Physics*
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MAST-Upgrade simulations

- Obtained stable solutions in Super-X geometry
- Net volume recombination near target plates

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Input power</td>
<td>497 kW (thermal)</td>
</tr>
<tr>
<td></td>
<td>510 kW (total)</td>
</tr>
<tr>
<td>Input particles</td>
<td>$5.7 \times 10^{21}/s$</td>
</tr>
<tr>
<td>Carbon radiation</td>
<td>340 kW (67%)</td>
</tr>
<tr>
<td>Volumetric loss</td>
<td>56 kW (11%)</td>
</tr>
</tbody>
</table>

Future work

- Evolving axisymmetric electric field
- Simulate turbulent transport in Super-X geometry
Turbulence in X-point geometry

Extending the mesh in the toroidal direction, turn off anomalous cross-field transport, and add random noise to vorticity.
Turbulence in X-point geometry

Extending the mesh in the toroidal direction, turn off anomalous cross-field transport, and add random noise to vorticity.

Inboard midplane

Density at separatrix

Outboard midplane

Inner target

Outer target
Turbulence in X-point geometry

Extending the mesh in the toroidal direction, turn off anomalous cross-field transport, and add random noise to vorticity

- Fluctuations extended poloidally
- Observed in divertor region, including inner leg PF region
- Large n=0 oscillation in potential

![Graph showing radial electric field and potential over time](image_url)
Turbulence in X-point geometry

Extending the mesh in the toroidal direction, turn off anomalous cross-field transport, and add random noise to vorticity

- Fluctuations extended poloidally
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Conclusions

- Numerical methods improved for tokamak and non-axisymmetric geometries
- Hermes model being developed (using BOUT++) to study the interaction of transport and turbulence
- Improvements made to model equations and numerical methods allow stable evolution of n=0 electric fields and currents in X-point geometry for the first time in BOUT++
- Fluid neutral model allows study of high recycling regimes. Simulations in linear device demonstrate interaction between plasma turbulence and neutral gas
Extra slides
Example equilibrium (DIII-D like)

Hermes can be run as an axisymmetric transport code (e.g. SOLPS, EDGE2D, UEDGE, ...)

- Specify anomalous diffusion coefficients for cross-field transport
- Includes (optional) flux limiters as used in SOLPS
- Start a simulation without electric fields or drifts

Resolution: 48 x 128 (x 128)

Midplane profiles

$n = 9.2 \times 10^{18} \text{ m}^{-3}$

$T_{e,\text{sep}} = 58 \text{ eV}$

$e,\text{sep}$
Evolving axisymmetric profiles

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- Specify anomalous diffusion coefficients for cross-field transport
- Includes (optional) flux limiters as used in SOLPS
- Start a simulation without electric fields or drifts
Evolving axisymmetric potential

Initial Alfvenic oscillations f\sim 500 \ kHz damp on \sim 20 \ \mu s timescale

Followed by slower oscillation with f \sim 6.7 \ kHz

Shear Alfven wave
\[ f_A = \frac{v_A}{(2\pi R q)} \]
\[ \approx 550 - 1100 \text{kHz} \]

Geodesic Acoustic Mode
\[ f_{GAM} = \frac{c_s}{2\pi R} \sqrt{2 + \frac{1}{q^2}} \]
\[ \approx 3 - 11 \text{kHz} \]

Parallel sound wave
\[ f_s = \frac{c_s}{(2\pi R q)} \]
\[ \approx 0.5 - 2.3 \text{kHz} \]
Model includes Alfven waves

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Poloidal flows

A common way to represent the ExB flow is

\[ \nabla \cdot \left( n \frac{\mathbf{b} \times \nabla \phi}{B} \right) = \frac{\mathbf{b} \times \nabla \phi}{B} \cdot \nabla n + n \left[ \nabla \times \left( \frac{\mathbf{b}}{B} \right) \right] \cdot \nabla \phi \]

Particles added to some cells, removed from others

- In general does not conserve particle number
- Geometry (curvature) need to be restricted

Instead, poloidal flows treated in divergence form → Ensures conservation of particles

\[ \nabla \cdot \left( n \frac{\mathbf{b} \times \nabla \phi}{B} \right) \]

Drift-plane motion

\[ = \frac{1}{J} \frac{\partial}{\partial \psi} \left( J n \frac{\partial \phi}{\partial z} \right) - \frac{1}{J} \frac{\partial}{\partial z} \left( J n \frac{\partial \phi}{\partial \psi} \right) \]

\[ + \frac{1}{J} \frac{\partial}{\partial \psi} \left( J n \frac{g^{\psi \phi} g^{yz} \frac{\partial \phi}{\partial y}}{B^2} \right) - \frac{1}{J} \frac{\partial}{\partial y} \left( J n \frac{g^{\psi \phi} g^{yz} \frac{\partial \phi}{\partial \psi}}{B^2} \right) \]

Radial flow due to poloidal electric fields
Poloidal flow due to radial electric fields
Tokamaks: Particle conservation

- Conservation of particle number is important in high recycling regimes
- Since total density, pressure is evolved, numerical sources/sinks could affect fidelity of small-scale fluctuations

100% recycling test case

![Diagram showing particle density over time and height in a tokamak](image-url)