

Title: Hermes model, version 2 (hot ion)
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 Project:

1 Model equations

The plasma equations evolve the plasma (electron) density n , electron thermal pressure $p_e = nT_e$, ion thermal pressure $p_i = nT_i$, vorticity ω , parallel ion momentum $nv_{\parallel i}$ and a form of Ohm's law for the parallel electron velocity $v_{\parallel e}$. For now the thin layer (Boussinesq) approximation is made in calculating the potential from vorticity, which has some effects on the other equations.

The (electron) density equation is:

$$\frac{\partial n}{\partial t} = -\nabla \cdot (n\mathbf{V}_{E \times B} + n\mathbf{V}_{mag,e}) \quad (1a)$$

$$-\nabla_{\parallel} (n_e v_{\parallel e}) \quad (1b)$$

$$+\nabla \cdot \left(\frac{\rho_e^2}{\tau_e T_e} \left[(T_e + T_i) \nabla_{\perp} n + n \left(\nabla_{\perp} T_i - \frac{1}{2} \nabla_{\perp} T_e \right) \right] \right) \quad (1c)$$

$$+\nabla \cdot (D_A \nabla_{\perp} \langle n \rangle) \quad (1d)$$

$$+S_n - S \quad (1e)$$

where the terms correspond to a) the $E \times B$ and magnetic drifts; b) the parallel flow; c) the classical cross-field transport¹; d) anomalous cross-field diffusion with fixed coefficient D_A ; e) external sources and exchange with neutrals. $\rho_e = \sqrt{eT_e/m_e}/\Omega_e$ is the electron Larmor radius, τ_e is the electron collision time. The anomalous diffusion term only acts on the axisymmetric profile, so here $\langle n \rangle$ denotes the toroidal average of n . The cross-field $E \times B$, electron and ion magnetic drifts are given by:

$$\mathbf{V}_{E \times B} = \frac{\mathbf{b} \times \nabla \phi}{B} \quad \mathbf{V}_{mag,e} = -T_e \nabla \times \frac{\mathbf{b}}{B} \quad \mathbf{V}_{mag,i} = T_i \nabla \times \frac{\mathbf{b}}{B} \quad (2)$$

The vorticity is given by

$$\omega = \nabla \cdot \left[\frac{1}{B^2} (n_0 \nabla_{\perp} \phi + \nabla_{\perp} p_i) \right] \quad (3)$$

where the density has been replaced with a constant value, the normalisation density n_0 (the

¹J.Madsen, V.Naulin, A.H.Nielsen, J.Juul Rasmussen "Collisional transport across the magnetic field in drift-fluid models" 2015

Boussinesq approximation). The evolution equation is:

$$\frac{\partial \omega}{\partial t} = \nabla \cdot \left[(p_e + p_i) \nabla \times \frac{\mathbf{b}}{B} \right] \quad (4a)$$

$$+ \nabla_{\parallel} j_{\parallel} \quad (4b)$$

$$- \nabla \cdot \left[\frac{1}{2B^2} \nabla_{\perp} (\mathbf{V}_{E \times B} \cdot \nabla p_i) + \frac{\omega}{2} \mathbf{V}_{E \times B} + \frac{n_0}{2B^2} \nabla_{\perp}^2 \phi (\mathbf{V}_{E \times B} + \mathbf{V}_{di}) \right] \quad (4c)$$

$$+ \nabla \cdot \left(\frac{3T_i}{10\tau_i B^2} \nabla_{\perp} \omega \right) \quad (4d)$$

$$+ \nabla \cdot \left[\frac{\pi_{ci}}{2} \nabla \times \frac{\mathbf{b}}{B} - \frac{1}{3} \frac{\mathbf{b} \times \nabla \pi_{ci}}{B} \right] \quad (4e)$$

$$+ \nabla \cdot (\nu_A \nabla_{\perp} \langle \omega \rangle) \quad (4f)$$

$$- \nabla \cdot \left(\frac{F_{\perp}}{nB^2} \nabla_{\perp} \phi \right) \quad (4g)$$

where in this equation the ion diamagnetic velocity $\mathbf{V}_{di} = \frac{\mathbf{b} \times \nabla p_i}{n_0 B}$ uses a constant density n_0 . The terms correspond to a) diamagnetic current; b) parallel current; c) polarisation current; d) cross-field collisional diffusion (viscosity); e) parallel collisional viscosity; f) anomalous perpendicular viscosity with fixed coefficient ν_A ; g) friction with neutrals. The scalar π_{ci} is

$$\begin{aligned} \pi_{ci} \simeq & \frac{3m_i}{4p_i T_i} [0.20 q_{\parallel i}^2 - 0.085 q_i^2] + 0.96 \frac{p_i}{\nu_i} \left\{ \kappa \cdot \left[\mathbf{V}_E + \mathbf{V}_{di} + 1.61 \frac{\mathbf{b} \times \nabla T_i}{B} \right] \right. \\ & \left. - \frac{2}{\sqrt{B}} \partial_{\parallel} (\sqrt{B} V_{\parallel i}) - \frac{1.42}{p_i \sqrt{B}} \partial_{\parallel} (\sqrt{B} q_{\parallel i}) - \frac{0.49 q_{\parallel i}}{p_i} (2.27 \partial_{\parallel} \ln T_i - \partial_{\parallel} \ln p_i) \right\} \quad (5) \end{aligned}$$

The electron pressure equation is:

$$\frac{3}{2} \frac{\partial p_e}{\partial t} = - \nabla \cdot \left(\frac{3}{2} p_e \mathbf{V}_{E \times B} + p_e \frac{5}{2} \mathbf{V}_{mag,e} \right) - p_e \nabla \cdot \mathbf{V}_{E \times B} \quad (6a)$$

$$- \nabla \cdot \left(\frac{3}{2} p_e v_{\parallel e} \right) - p_e \nabla_{\parallel} v_{\parallel e} \quad (6b)$$

$$+ \nabla_{\parallel} (\kappa_{e\parallel} \partial_{\parallel} T_e) \quad (6c)$$

$$+ 0.71 \nabla_{\parallel} (T_e j_{\parallel}) - 0.71 j_{\parallel} \partial_{\parallel} T_e + \frac{\nu}{n} j_{\parallel}^2 \quad (6d)$$

$$+ \nabla \cdot \left(\frac{\rho_e^2}{\tau_e} \left[\nabla_{\perp} p_e + \nabla_{\perp} p_i + \frac{11}{12} n \nabla_{\perp} T_e \right] \right) \quad (6e)$$

$$+ \nabla \cdot (D_A \langle T_e \rangle \nabla_{\perp} \langle n \rangle) + \nabla \cdot (\chi_A \langle n \rangle \nabla_{\perp} \langle T_e \rangle) \quad (6f)$$

$$+ S_{pe} - Q_e - W_i \quad (6g)$$

where the terms correspond to a) perpendicular drifts, including compression of $\mathbf{E} \times \mathbf{B}$ flow; b) parallel flow including compression; c) parallel heat conduction; d) Ohmic heating, including thermal force and thermal current; e) collisional cross-field transport; f) anomalous transport; g) sources, and energy exchange with neutrals and ions. The ion-electron transfer term W_i is given by the standard Braginskii expression:

$$W_i = \frac{3m_e n (T_e - T_i)}{m_i \tau_e} \quad (7)$$

Note that the divergence of the $E \times B$ velocity is written in the form

$$\nabla \cdot \left(\frac{\mathbf{b} \times \nabla \phi}{B} \right) = \nabla \cdot \left(\phi \nabla \times \frac{\mathbf{b}}{B} \right)$$

is used, so that the same form of the curvature is used in both the vorticity and pressure equations.

The ion pressure equation is:

$$\frac{3}{2} \frac{\partial p_i}{\partial t} = -\nabla \cdot \left(\frac{3}{2} p_i \mathbf{V}_{E \times B} + \frac{5}{2} p_i \mathbf{V}_{mag,i} \right) - p_i \nabla \cdot \mathbf{V}_{E \times B} \quad (8a)$$

$$-\nabla \cdot \left(\frac{3}{2} p_i \mathbf{b} v_{||i} \right) - p_i \nabla_{||} v_{||i} \quad (8b)$$

$$-\frac{j_{||}}{n_0} \partial_{||} p_i + \frac{p_i}{n_0} \nabla \cdot \left[(p_e + p_i) \nabla \times \frac{\mathbf{b}}{B} \right] \quad (8c)$$

$$+ v_{||i} \frac{2}{3} B^{3/2} \partial_{||} \left(\frac{\pi_{ci}}{B^{3/2}} \right) \quad (8d)$$

$$+ \nabla_{||} (\kappa_{i||} \partial_{||} T_i) + \nabla \cdot (\kappa_{i\perp} \nabla_{\perp} T_i) \quad (8e)$$

$$+ \frac{5}{2} \nabla \cdot \left(\frac{T_i}{T_e} \frac{\rho_e^2}{\tau_e} \left[\nabla_{\perp} p_e + \nabla_{\perp} p_i - \frac{3}{2} n \nabla_{\perp} T_e \right] \right) \quad (8f)$$

$$- \frac{3T_i}{10\tau_i B^2} \nabla_{\perp} \omega \cdot \nabla \left(\phi + \frac{p_i}{n_0} \right) - \left[\frac{\pi_{ci}}{2} \nabla \times \frac{\mathbf{b}}{B} - \frac{1}{3} \frac{\mathbf{b} \times \nabla \pi_{ci}}{B} \right] \cdot \nabla \left(\phi + \frac{p_i}{n_0} \right) \quad (8g)$$

$$+ S_{pi} - Q_i + W_i \quad (8h)$$

where the terms are a) cross-field $E \times B$ and magnetic drifts including compression; b) parallel flow including compression; c) energy exchange with diamagnetic flows; d) parallel viscous heating; e) parallel and perpendicular collisional heat conduction; f) collisional resistive drift; g) heating due to perpendicular viscosity; h) external sources, and exchange with neutrals and electrons. Note the appearance of n_0 in terms c), due to the use of the Boussinesq approximation in the vorticity. The ion heat conduction coefficients are

$$\kappa_{i||} = 3.9 \frac{p_i \tau_i}{m_i} \quad \kappa_{i\perp} = 2n \rho_i^2 / \tau_i \quad (9)$$

Note that the advection by magnetic drifts ($T_i \nabla \times \frac{\mathbf{b}}{B}$) includes the gyro-viscous cancellation, since this is the gyro-centre drift rather than the diamagnetic drift. The diamagnetic and stress tensor terms appear in Simakov-Catto as:

$$\begin{aligned} \nabla \cdot (m_i n_e v_{||i} \mathbf{V}_{di}) + \mathbf{b} \cdot (\nabla \cdot \Pi) &\simeq \nabla \cdot \left(m_i n_e v_{||i} \frac{\mathbf{b} \times \nabla p_i}{enB} \right) + \frac{2}{3} B^{3/2} \partial_{||} \left(\frac{\pi_{ci}}{B^{3/2}} \right) + \nabla \cdot \left(\frac{p_i}{\Omega_i} \mathbf{b} \times \nabla p_i \right) \\ &= \left[\frac{1}{\Omega_i} \mathbf{b} \times \nabla (p_i v_{||i}) \right] + \frac{2}{3} B^{3/2} \partial_{||} \left(\frac{\pi_{ci}}{B^{3/2}} \right) \\ &= \nabla \cdot \left[m_i n_e v_{||i} T_i \nabla \times \frac{\mathbf{b}}{B} \right] + \frac{2}{3} B^{3/2} \partial_{||} \left(\frac{\pi_{ci}}{B^{3/2}} \right) \end{aligned} \quad (10)$$

where we have used the identity

$$\nabla \cdot \left(\frac{\mathbf{b} \times \nabla \alpha}{B} \right) = \nabla \cdot \left[\alpha \nabla \times \frac{\mathbf{b}}{B} \right] \quad (11)$$

The ion parallel momentum equation is:

$$\frac{\partial}{\partial t} (n_e v_{||i}) = -\nabla \cdot [n_e v_{||i} (\mathbf{V}_{E \times B} + \mathbf{b} v_{||i} + \mathbf{V}_{mag,i})] \quad (12a)$$

$$-\partial_{||} p_e - \partial_{||} p_i \quad (12b)$$

$$-\frac{2}{3} B^{3/2} \partial_{||} \left(\frac{\pi_{ci}}{B^{3/2}} \right) \quad (12c)$$

$$+\nabla \cdot \left(v_{||i} \frac{\rho_e^2}{\tau_e T_e} \left[(T_e + T_i) \nabla_{\perp} n + n \left(\nabla_{\perp} T_i - \frac{1}{2} \nabla_{\perp} T_e \right) \right] \right) \quad (12d)$$

$$+\nabla \cdot (D_A \langle v_{||i} \rangle \nabla_{\perp} \langle n \rangle) \quad (12e)$$

$$-F_{||} \quad (12f)$$

where the terms are a) advection due to $\mathbf{E} \times \mathbf{B}$ flow, parallel flow, and ion magnetic drift; b) parallel pressure; c) parallel ion viscosity; d) collisional cross-field transport; e) anomalous cross-field transport; f) friction with neutrals

The parallel Ohm's law is:

$$\frac{\partial}{\partial t} \left[\frac{m_e}{m_i} (v_{||e} - v_{||i}) + \frac{1}{2} \beta_e \psi \right] = \partial_{||} \phi - \frac{1}{n_e} \partial_{||} p_e - 0.71 \partial_{||} T_e \quad (13a)$$

$$+\nu j_{||}/n_e \quad (13b)$$

$$+\frac{m_e}{m_i} (\mathbf{V}_{E \times B} + \mathbf{b} v_{||i}) \cdot \nabla (v_{||i} - v_{||e}) \quad (13c)$$

where $\psi = -2A_{||}/(B_0 \beta_e \rho_s)$ is the normalised electromagnetic potential. The dimensionless factor $\beta_e = en_0 T_0 / (B^2 / (2\mu_0))$ is an electron plasma beta.

The notation used for parallel derivatives is

$$\partial_{||} f \equiv \mathbf{b} \cdot \nabla f \quad \nabla_{||} f \equiv \nabla \cdot (\mathbf{b} f) \quad (14)$$

Note that these two operators are conjugate, and combine to form a divergence:

$$\nabla \cdot (\mathbf{b} f g) = f \partial_{||} g + g \nabla_{||} f$$

and this identity is important in deriving energy conservation. The plasma model is cast in conservative form, conserving particle number, and an energy

$$E = \int dv \frac{m_i n_0}{2} \left| \frac{\nabla_{\perp} \phi}{B} + \frac{\nabla_{\perp} p_i}{en_0 B} \right|^2 + \frac{1}{2} m_i n V_{||i}^2 + \frac{3}{2} p_e + \frac{3}{2} p_i + \frac{1}{4} \beta_e |\nabla_{\perp} \psi|^2 + \frac{m_e}{m_i} \frac{1}{2} \frac{j_{||}^2}{n} \quad (15)$$

where the terms correspond to the ion perpendicular kinetic energy ($\mathbf{E} \times \mathbf{B}$ and diamagnetic flow), ion parallel kinetic energy, electron and ion thermal energy, and electromagnetic field energy. Details are given in section 3. Differential operators are discretised using flux-conservative Finite Volume methods, details of which are given in section 12.

Several models for neutral gas evolution are available, described in section 8, including a model which is fluid-like along the magnetic field, and diffusive across the magnetic field (neutral model 4). This evolves neutral gas density n_n , pressure p_n and parallel velocity $v_{||n}$:

$$\frac{\partial n_n}{\partial t} = -\nabla \cdot (n_n \mathbf{b} v_{||n} + n_n \mathbf{v}_{\perp n}) + S \quad (16)$$

$$\frac{\partial}{\partial t} (n_n v_{||n}) = -\nabla \cdot (n_n v_{||n} \mathbf{b} v_{||n} + n_n v_{||n} \mathbf{v}_{\perp n}) - \partial_{||} p_n + \nabla_{||} (D_{nn} n_n \partial_{||} v_{||n}) + F_{||} \quad (17)$$

$$\frac{\partial p_n}{\partial t} = -\nabla \cdot (p_n \mathbf{b} v_{||n} + p_n \mathbf{v}_{\perp n}) - \frac{2}{3} p_n \nabla \cdot (\mathbf{b} v_{||n}) + \nabla \cdot (D_{nn} n_n \nabla_{\perp} T_n) + \frac{2}{3} Q \quad (18)$$

2 Code inputs and outputs

2.1 Input options

These switches control the terms included in the plasma evolution equations. They are grouped so that switching on or off a term maintains energy conservation, though the form of the conserved energy may change. See section ?? for details.

Setting	Default	Description
evolve_plasma	true	Enables/disable plasma evolution
electromagnetic	true	Include $A_{ }$ in Ohm's law
FiniteElMass	true	Electron inertia in Ohm's law
j_diamag	true	Diamagnetic drifts
j_par	true	Parallel current
parallel_flow	true	Evolve ion parallel momentum
pe_par	true	Electron pressure in Ohm's law
resistivity	true	Resistivity in Ohm's law
thermal_flux	true	
thermal_force	true	
electron_viscosity	true	
ion_velocity	true	
thermal_conduction	true	Parallel heat conduction
boussinesq	false	Use Boussinesq approximation in vorticity
ion_model	0	Ion temperature model 0 = Cold ions 1 = Evolve ion pressure p_i (INCOMPLETE) 2 = Evolve ion energy (INCOMPLETE)

The normalisations are controlled by:

Setting	Default	Description
Tnorm	100	Reference temperature [eV]
Nnorm	10^{19}	Reference density [m^{-3}]
Bnorm	1.0	Reference magnetic field [T]
AA	2	Ion atomic mass

The following settings are for dissipation terms. Some are described in section 11.

Setting	Default	Description
density_diffusion	true	Collisional particle diffusion
thermal_diffusion	true	Collisional energy diffusion
ion_viscosity	true	
neoclassical_q	true	Enhances collisional diffusion by $\sim q^2$
anomalous_D	true	Cross-field particle diffusion [m^2/s]
anomalous_chi	true	Cross-field energy diffusion [m^2/s]
numdiff	true	parallel diffusion of electron and ion momentum
hyper	-1	Hyper-resistivity
ExBdiff	-1	2^{nd} -order perpendicular dissipation
ADpar	-1	4^{th} -order parallel dissipation
resistivity_multiply	true	
ion_neutral	0.0	
flux_limit_alpha	-1	Flux limiter on heat conduction

The sheath boundary conditions are described in section 10 and controlled by:

Setting	Default	Description
<code>sheath_yup</code>	<code>true</code>	Apply sheath at upper Y boundaries?
<code>sheath_ydown</code>	<code>true</code>	Apply sheath at lower Y boundaries?
<code>sheath_model</code>	0	Sheath model to use 0 = Bohm, zero gradient density 1 = Loizu 2 = Bohm, free density
<code>sheath_gamma</code>	6.5	sheath heat transmission coefficient γ_{sh} $q = \gamma_{sh} n T c_s$

The neutral gas models are described in section 8 and is controlled by the following:

Setting	Default	Description
<code>neutral_model</code>	0	Neutral gas model to use 0 = No neutrals 1 = 2D (X-Z) simple diffusion 2 = Recycling (along y) 3 = 2D (X-Y) axisymmetric Navier-Stokes 4 = 3D UEDGE-like model: fluid along Y, diffusion in X-Z
<code>freecycle</code>	0.9	Neutral recycling fraction
<code>neutral_gamma</code>	5/4	Heat transmission to surface
<code>neutral_vwall</code>	1/3	Speed along the magnetic field at which neutrals are born (Fraction of Franck-Condon energy)
<code>Eionize</code>	30	Effective ionisation energy [eV]
<code>Lmax</code>	1.0	Maximum mean free path, limits diffusion in low density regions

Some settings control details of how operators are implemented

Setting	Default	Description
<code>staggered</code>	<code>false</code>	Use staggered differencing for parallel flows
<code>magnetic_drift</code>	<code>true</code>	Use magnetic drift rather than diamagnetic current
<code>ne_bndry_flux</code>	<code>true</code>	Allow density flux through radial boundaries?
<code>pe_bndry_flux</code>	<code>true</code>	Allow energy flux through radial boundaries?
<code>vort_bndry_flux</code>	<code>false</code>	Allow currents through radial boundaries?
<code>phi3d</code>	<code>false</code>	Use Laplace3D to calculate ϕ
<code>split_n0</code>	<code>false</code>	Solve axisymmetric ϕ separately
<code>newXZsolver</code>	<code>false</code>	If <code>split_n0=true</code> use LaplaceXZ rather than Laplacian

Sources are controlled using:

Setting	Default	Description
<code>startprofiles</code>	<code>true</code>	Add profiles from grid file
<code>Ne:source</code>	0.0	Density source. Units of Nnorm/s
<code>Pe:source</code>	0.0	Pressure (energy) source. Units of $e \times \text{Nnorm} \times \text{Tnorm/s}$
<code>adapt_sources</code>	<code>false</code>	
<code>source_p</code>	$1e-2$	
<code>source_i</code>	$1e-6$	
<code>core_sources</code>	<code>true</code>	Only allow sources in closed flux-surface regions
<code>energy_source</code>	<code>true</code>	
<code>ramp_mesh</code>	<code>true</code>	Adds a source to density and pressure $\frac{\partial n}{\partial t} = n_0 / \tau_{\text{ramp}}$ where n_0 is from the grid file
<code>ramp_timescale</code>	$1e4$	Timescale τ_{ramp}

Additional output variables:

Setting	Default	Description
<code>verbose</code>	<code>true</code>	Outputs additional fields, mainly for debugging
<code>output_ddt</code>	<code>true</code>	Output time derivatives

2.2 Outputs

Output quantities are normalised, with the normalisation factors stored in the output files:

Name	Description	Units
<code>Nnorm</code>	Density	m^{-3}
<code>Tnorm</code>	Temperature	eV
<code>Cs0</code>	Speed	m/s
<code>Omega_ci</code>	Time	1/s
<code>rho_s0</code>	Length	m

The following variables are stored in the output file if they are evolved:

Name	Description	Normalisation
<code>Ne</code>	Plasma density	$\text{Nnorm} [\text{m}^{-3}]$
<code>NVi</code>	Plasma flux	$\text{Nnorm} \times \text{Cs0} [\text{m}^{-2} \text{s}^{-1}]$
<code>Pe</code>	Electron pressure	$e \times \text{Nnorm} \times \text{Tnorm} [\text{Pascals}]$
<code>Nn</code>	Neutral density	$\text{Nnorm} [\text{m}^{-3}]$
<code>NVn</code>	Neutral flux	$\text{Nnorm} \times \text{Cs0} [\text{m}^{-2} \text{s}^{-1}]$
<code>Pn</code>	Neutral pressure	$e \times \text{Nnorm} \times \text{Tnorm} [\text{Pascals}]$

The following rates and coefficients are also stored:

Name	Description	Normalisation
<code>S</code>	Sink of plasma density	$\text{Nnorm} \times \text{Omega_ci} [\text{m}^{-3} \text{s}^{-1}]$
<code>F</code>	Sink of plasma momentum	$m_i \times \text{Nnorm} \times \text{Cs0} \times \text{Omega_ci} [\text{Nm}^{-3}]$
<code>R</code>	Radiative loss of energy	$e \times \text{Nnorm} \times \text{Tnorm} \times \text{Omega_ci} [\text{Wm}^{-3}]$
<code>E</code>	Sink of plasma energy	$e \times \text{Nnorm} \times \text{Tnorm} \times \text{Omega_ci} [\text{Wm}^{-3}]$
<code>kappa_epar</code>	Plasma thermal conduction	

Note that the `R` term is energy which is lost from the system, whilst `E` is energy which is transferred between plasma and neutrals. For all transfer terms (`S`, `F`, `R`) a positive value means a transfer from plasma to neutrals.

3 Conservation properties

To calculate energy conservation, multiply the vorticity equation by $\phi + p_i/n_0$, Ohm's law by $j_{||}$, and ion parallel momentum by $v_{||i}$, then integrate over all space. Starting with the vorticity equation:

$$\begin{aligned} \left(\phi + \frac{p_i}{n_0}\right) \frac{\partial \omega}{\partial t} &= \nabla \cdot \left[\frac{\phi + p_i/n_0}{B^2} \frac{\partial}{\partial t} (n_0 \nabla_{\perp} \phi + \nabla_{\perp} p_i) \right] \\ &\quad - \frac{1}{B^2} \frac{\partial}{\partial t} (n_0 \nabla_{\perp} \phi + \nabla_{\perp} p_i) \cdot \left(\phi + \frac{p_i}{n_0}\right) \end{aligned}$$

The first term integrates over space to give a flux through the boundary, whilst the second term is the ion perpendicular kinetic energy:

$$\left(\phi + \frac{p_i}{n_0}\right) \frac{\partial \omega}{\partial t} = -\frac{\partial}{\partial t} \left[\frac{1}{2} n_0 \left| \frac{\nabla_{\perp} \phi}{B} + \frac{\nabla_{\perp} p_i}{n_0 B} \right|^2 \right] + \text{Boundary}$$

This is the kinetic energy contained in the sum of the perpendicular ion $E \times B$ and diamagnetic velocities.

Exchange of energy with othe forms arises from the terms on the RHS of the vorticity equation. Equations 4a and 4b are quite straightforward, and directly give energy exchange terms. Equation 4c is a little more complicated: The second term of equation 4c, $E \times B$ advection of vorticity, produces:

$$\begin{aligned} \left(\phi + \frac{p_i}{n_0}\right) \nabla \cdot \left(\frac{\omega \mathbf{b} \times \nabla \phi}{2B} \right) &= \nabla \cdot \left(\left(\phi + \frac{p_i}{n_0}\right) \frac{\omega \mathbf{b} \times \nabla \phi}{2B} \right) \\ &\quad - \frac{\omega \mathbf{b} \times \nabla \phi}{2B} \cdot \nabla \phi \\ &\quad - \frac{\omega}{2} \mathbf{V}_{E \times B} \cdot \nabla \frac{p_i}{n_0} \end{aligned} \tag{19}$$

The first term gives a boundary flux, the second term is zero by vector identity, and the last term in equation 19 is cancelled by a contribution from the first term of equation 4c:

$$\begin{aligned} \left(\phi + \frac{p_i}{n_0}\right) \nabla \cdot \left[\frac{1}{2B^2} \nabla_{\perp} (\mathbf{V}_{E \times B} \cdot \nabla p_i) \right] &= \nabla \cdot \left[\frac{1}{2B^2} \left(\phi + \frac{p_i}{n_0}\right) \nabla_{\perp} \left(\frac{\mathbf{b} \times \nabla \phi}{B} \cdot \nabla p_i \right) \right] \\ &\quad - \nabla_{\perp} \cdot \left[\frac{\mathbf{V}_{E \times B} \cdot \nabla p_i}{2B^2} \nabla \left(\phi + \frac{p_i}{n_0} \right) \right] \\ &\quad + (\mathbf{V}_{E \times B} \cdot \nabla p_i) \underbrace{\frac{1}{2} \nabla_{\perp} \cdot \left[\frac{1}{B^2} \nabla \left(\phi + \frac{p_i}{n_0} \right) \right]}_{\omega/n_0} \end{aligned}$$

Note that this term is slightly modified from the Simakov-Catto expression, moving the B^2 factor out of the inner gradient. If this is not done then non-uniform B leads to spurious energy sources.

The third term of equation 4c does not contribute to energy exchange: A useful identity is that any divergence involving advection by the sum of $E \times B$ and ion diamagnetic velocities

does not contribute to transfer channels:

$$\begin{aligned}
 \left(\phi + \frac{p_i}{n_0}\right) \nabla \cdot \left[f \left(\frac{\mathbf{b} \times \nabla \phi}{B} + \frac{\mathbf{b} \times \nabla p_i}{n_0 B} \right) \right] &= \nabla \cdot \left[f \left(\phi + \frac{p_i}{n_0} \right) \left(\frac{\mathbf{b} \times \nabla \phi}{B} + \frac{\mathbf{b} \times \nabla p_i}{n_0 B} \right) \right] \\
 &\quad - f \left(\frac{\mathbf{b} \times \nabla \phi}{B} + \frac{\mathbf{b} \times \nabla p_i}{n_0 B} \right) \cdot \nabla \left(\phi + \frac{p_i}{n_0} \right) \\
 &= \nabla \cdot (\cdot) - f \left(\frac{\mathbf{b} \times \nabla \phi}{n_0 B} \cdot \nabla p_i + \frac{\mathbf{b} \times \nabla p_i}{n_0 B} \cdot \nabla \phi \right)
 \end{aligned}$$

The first term is a divergence which integrates to give a surface flux, whilst the second term is zero by vector identity.

Equation 4d, perpendicular viscosity, leads to an energy exchange with ion pressure: Collisions randomise the ions, turning kinetic energy into heat.

$$\begin{aligned}
 \left(\phi + \frac{p_i}{n_0}\right) \nabla \cdot \left(\frac{3T_i}{10\tau_i B^2} \nabla_{\perp} \omega \right) &= \nabla \cdot \left(\left[\phi + \frac{p_i}{n_0} \right] \frac{3T_i}{10\tau_i B^2} \nabla_{\perp} \omega \right) \\
 &\quad - \frac{3T_i}{10\tau_i B^2} \nabla_{\perp} \omega \cdot \nabla \left(\phi + \frac{p_i}{n_0} \right)
 \end{aligned} \tag{20}$$

The transfer channels now become:

$$\begin{aligned}
 \frac{\partial}{\partial t} \left[\frac{1}{2} n_0 \left| \frac{\nabla_{\perp} \phi}{B} + \frac{\nabla_{\perp} p_i}{n_0 B} \right|^2 \right] &= -\phi \nabla_{\parallel} j_{\parallel} - p_i \nabla_{\parallel} \left(\frac{j_{\parallel}}{n_0} \right) \\
 &\quad - \phi \nabla \cdot \left(p_e \nabla \times \frac{\mathbf{b}}{B} \right) \\
 &\quad - \phi \nabla \cdot \left(p_i \nabla \times \frac{\mathbf{b}}{B} \right) - \frac{p_i}{n_0} \nabla \cdot \left[(p_e + p_i) \nabla \times \frac{\mathbf{b}}{B} \right] \\
 &\quad + \frac{3T_i}{10\tau_i B^2} \nabla_{\perp} \omega \cdot \nabla \left(\phi + \frac{p_i}{n_0} \right)
 \end{aligned} \tag{21}$$

$$\frac{\partial}{\partial t} \left(\frac{1}{4} \beta_e |\nabla_{\perp} \psi|^2 \right) = -j_{\parallel} \partial_{\parallel} \phi + v_{\parallel i} \partial_{\parallel} p_e - \nu \frac{j_{\parallel}^2}{n_e} - v_{\parallel e} \partial_{\parallel} p_e + 0.71 j_{\parallel} \partial_{\parallel} T_e \tag{22}$$

$$\frac{\partial}{\partial t} \left(\frac{1}{2} n v_{\parallel i}^2 \right) = -v_{\parallel i} \partial_{\parallel} p_e - v_{\parallel i} \partial_{\parallel} p_i - v_{\parallel i} \frac{2}{3} B^{3/2} \partial_{\parallel} \left(\frac{\pi c_i}{B^{3/2}} \right) \tag{23}$$

$$\frac{3}{2} \frac{\partial p_e}{\partial t} = -p_e \nabla \times \left(\frac{\mathbf{b}}{B} \right) \cdot \nabla \phi + \nu \frac{j_{\parallel}^2}{n_e} + v_{\parallel e} \partial_{\parallel} p_e - 0.71 j_{\parallel} \partial_{\parallel} T_e \tag{24}$$

$$\begin{aligned}
 \frac{3}{2} \frac{\partial p_i}{\partial t} &= -p_i \nabla \times \left(\frac{\mathbf{b}}{B} \right) \cdot \nabla \phi + \frac{p_i}{n_0} \nabla \cdot \left[(p_e + p_i) \nabla \times \frac{\mathbf{b}}{B} \right] \\
 &\quad + v_{\parallel i} \partial_{\parallel} p_i - \frac{j_{\parallel}}{n_0} \partial_{\parallel} p_i \\
 &\quad - \frac{3T_i}{10\tau_i B^2} \nabla_{\perp} \omega \cdot \nabla \left(\phi + \frac{p_i}{n_0} \right) \\
 &\quad + v_{\parallel i} \frac{2}{3} B^{3/2} \partial_{\parallel} \left(\frac{\pi c_i}{B^{3/2}} \right)
 \end{aligned} \tag{25}$$

4 Collisional terms

4.1 Heat conduction and flux limiter

The parallel heat conduction coefficients $\kappa_{||e}$, $\kappa_{||i}$ are the Braginskii expressions

$$\kappa_{||e} = 3.2n_e v_{th,e}^2 \tau_e \quad \kappa_{||i} = 3.9n_e v_{th,i}^2 \tau_i \quad (26)$$

These can be limited using the method adopted by SOLPS²:

$$\kappa_{||} = \frac{\kappa_{SH}}{1 + |q_{SH}/q_{fl}|} \quad (27)$$

where κ_{SH} is the Spitzer-Härm (Braginskii) heat conductivity given by equations 26. The classical heat flux is

$$q_{SH} = -\kappa_{SH} \partial_{||} T \quad (28)$$

and the flux limit is

$$q_{fl} = \alpha n_e T^{3/2} \sqrt{m_e} \quad (29)$$

where $\alpha \simeq 0.2$ for electrons from comparison with kinetic calculations.

4.2 Resistivity

Resistivity is implemented in Ohm's law (equation 13c) as a collision frequency. In normalised units this is:

$$\nu_{ei} = \frac{R}{1.96\tau_e m_i / m_e}$$

where τ_e is the electron-ion collision frequency. The constant R is an input parameter `resistivity_multiply` which is 1 by default.

In addition, electron-neutral collisions are included if `electron_neutral` is set to `true` (the default).

$$\nu_{nn} = v_{th,e} n_n a_0$$

where $v_{th,e} = \sqrt{eT_e/m_e}$ is the electron thermal velocity, and $a_0 = \pi (5.29 \times 10^{-11})^2 \text{m}^2$ is the cross-section of a neutral Hydrogen atom.

The total electron collision rate is then

$$\nu = \nu_{ei} + \nu_{nn} \quad (30)$$

4.3 Ion viscosity

The ion collisional stress in equation 5 is taken from [Simakov and Catto 2003], omitting a final term proportional to plasma β . It reduces to the simple forms used elsewhere in the following limit:

First drop all terms involving the heat flux, keeping only these terms:

$$\pi_{ci} \simeq 0.96 \frac{p_i}{\nu_i} \left\{ \kappa \cdot \left[\mathbf{V}_E + \mathbf{V}_{di} + 1.61 \frac{\mathbf{b} \times \nabla T_i}{B} \right] - \frac{2}{\sqrt{B}} \partial_{||} \left(\sqrt{B} V_{||i} \right) \right\} \quad (31)$$

²R.Schneider et al. Contrib. Plasma Phys. 46, No. 1-2, 3-191 (2006) doi: 10.1002/ctpp.200610001

Rewrite the curvature terms:

$$\kappa \cdot \mathbf{V}_E = -\frac{1}{B} (\mathbf{b} \times \kappa) \cdot \nabla \phi \quad (32)$$

and similarly for the p_i and T_i terms, so

$$\kappa \cdot \left[\mathbf{V}_E + \mathbf{V}_{di} + 1.61 \frac{\mathbf{b} \times \nabla T_i}{B} \right] = -\frac{1}{B} (\mathbf{b} \times \kappa) \cdot \left[\nabla \phi + \frac{\nabla p_i}{en} + 1.61 \frac{\nabla T_i}{e} \right] \quad (33)$$

which if we assume ϕ , p_i and T_i are all flux functions becomes:

$$\begin{aligned} \kappa \cdot \left[\mathbf{V}_E + \mathbf{V}_{di} + 1.61 \frac{\mathbf{b} \times \nabla T_i}{B} \right] &\simeq -\frac{1}{B} (\mathbf{b} \times \kappa) \cdot \nabla \psi \left[\frac{\partial \phi}{\partial \psi} + \frac{1}{en} \frac{\partial p_i}{\partial \psi} + \frac{1.61}{e} \frac{\partial T_i}{\partial \psi} \right] \\ &= \frac{1}{B} (\mathbf{b} \times \kappa) \cdot \nabla \psi F(\psi) \end{aligned} \quad (34)$$

where

$$F(\psi) = - \left[\frac{\partial \phi}{\partial \psi} + \frac{1}{en} \frac{\partial p_i}{\partial \psi} + \frac{1.61}{e} \frac{\partial T_i}{\partial \psi} \right] \quad (35)$$

Using the approximation

$$\mathbf{b} \times \kappa \cdot \nabla \psi \simeq -RB_\zeta \partial_{||} \ln B \quad (36)$$

we get

$$\pi_{ci} \simeq 0.96 \frac{p_i}{\nu_i} \left\{ \frac{RB_\zeta}{B} F(\psi) \partial_{||} \ln B - \frac{2}{\sqrt{B}} \partial_{||} \left(\sqrt{B} V_{||i} \right) \right\} \quad (37)$$

The second term can be expanded as

$$\frac{2}{\sqrt{B}} \partial_{||} \left(\sqrt{B} V_{||i} \right) = 2 \partial_{||} V_{||i} + V_{||i} \ln B \quad (38)$$

which neglecting parallel gradients of $V_{||i}$ gives

$$\pi_{ci} \simeq 0.96 \frac{p_i}{\nu_i} \left[\frac{RB_\zeta}{B} F(\psi) - V_{||i} \right] \partial_{||} \ln B \quad (39)$$

The term in the parallel ion momentum is therefore approximately:

$$\mathbf{b} \cdot (\nabla \cdot \Pi_{ci}) \simeq \frac{2}{3} B^{3/2} \partial_{||} \left[0.96 \frac{p_i}{\nu_i B^{3/2}} \left(\frac{RB_\zeta}{B} F(\psi) - V_{||i} \right) \partial_{||} \ln B \right] \quad (40)$$

which acts to damp the net poloidal flow given by the combination of parallel and perpendicular velocities.

4.4 Electron parallel viscosity

This term is turned on and off using

`electron_viscosity = true`

The stress tensor in the electron momentum equation is usually dropped, as being proportional to the electron mass and hence small [Biskamp “Magnetic Reconnection in Plasmas”]. The friction between ions and electrons is usually kept, but the parallel viscosity is usually dropped. For numerical simulations however, retaining the electron parallel viscosity is important in providing dissipation at small (grid) scales, and reducing oscillations in the parallel direction.

The Braginskii stress tensor [Fitzpatrick lecture notes]

$$\Pi_{\alpha\beta}^{i,e} = -\eta_0^{i,e} \left(\frac{\partial V_\alpha}{\partial r_\beta} + \frac{\partial V_\beta}{\partial r_\alpha} - \frac{2}{3} \nabla \cdot \mathbf{V} \delta_{\alpha\beta} \right)$$

where

$$\begin{aligned} \eta_0^e &= 0.73 n \tau_e e T_e \\ \eta_0^i &= 0.96 n \tau_i e T_i \end{aligned}$$

which appears in the momentum equation

$$m_{i,e} n \frac{d\mathbf{V}_{i,e}}{dt} + \nabla p_{i,e} + \nabla \cdot \Pi^{i,e} \mp e n (\mathbf{E} + \mathbf{V}_{i,e} \times \mathbf{B}) = 0$$

Rearranging, the form for the parallel electron velocity diffusion becomes:

$$\frac{dV_{||e}}{dt} = \frac{1}{n} \nabla_{||} \left(n 0.97 \tau_e \frac{e T_e}{m_e} \partial_{||} V_{||e} \right)$$

where the diffusion of parallel momentum along the field is comparable to the heat conduction:

$$\Xi = 0.97 \tau_e \underbrace{\frac{e T_e}{m_e}}_{v_{th,e}^2} \simeq 10^7 m^2/s$$

5 Electrostatic potential

Most development and tests have been done using the Boussinesq approximation. This is enabled with the switch

`boussinesq = true`

If this is true, then the `split_n0` setting can be used to solve the axisymmetric ($n = 0$) component of ϕ separately. Note however that this uses LaplaceXY, which depends on PETSc.

6 Sheath boundary conditions

Several models are implemented

0. Bohm sheath boundary condition, zero gradient on other fields

$$V_{||i} \geq C_s \quad \partial_{||} T_e = 0 \quad \partial_{||} n_e = 0 \quad \partial_{||} \phi = 0$$

If $V_{||i} > C_s$ in front of the sheath, then the velocity at the sheath is set to this supersonic value

1. Loizu boundary conditions. This model assumes constant parallel flux in order to set a boundary condition on density

$$V_{||} = C_s \quad \partial_{||} (nV_{||i}) = 0$$

In this case the velocity is fixed at the sound speed

2. Bohm sheath with free density. The density is extrapolated using two points, so constant gradient boundary condition.

$$V_{||i} \geq C_s \quad \partial_{||}^2 n_e = 0$$

3. Insulating Bohm sheath with free density. This is to model cases where an insulator is placed at the sheath, so that no current flows:

$$j_{||} = 0$$

Otherwise the same as model 2.

7 External sources

Whether sources are adaptive or fixed is controlled by the `adapt_source` switch.

7.1 Adaptive sources

To adapt sources, a Proportional-Integral (PI) controller is used. The sources in the density and electron pressure equations `Sn` and `Sp` are then evolved:

$$S_n = -PE_n - I \int E_n dt \quad (41)$$

$$S_p = -PE_p - I \int E_p dt \quad (42)$$

where the errors in the density and pressure profiles are averaged over Y (parallel) and Z directions:

$$E_n = \langle n - n_0 \rangle_{YZ} \quad (43)$$

$$E_p = \langle p - p_0 \rangle_{YZ} \quad (44)$$

The P and I coefficients are constants from the input options `source_p` and `source_i`. Note that a nonzero I coefficient is needed in order for the profiles to converge to the specified profile n_0 . An example of the convergence of a source to achieve a target density is shown in figure 1.

NB: At the moment the sources are restricted to be always positive

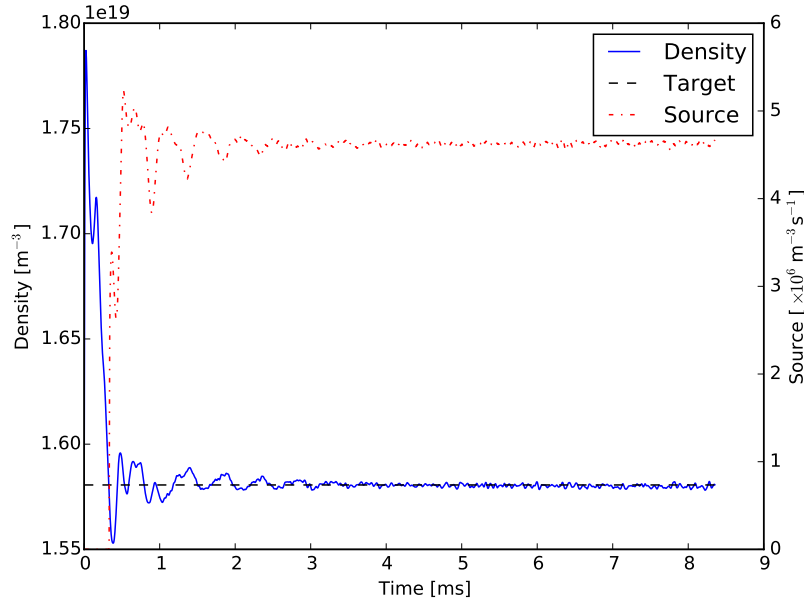


Figure 1: An example of density feedback in the `neutrals-d3d` test case

7.2 Fixed sources

Fixed sources are read from the options

```
[Ne]
source = ...
```

```
[Pe]
source = ...
```

which are read into the variables S_n and S_p then divided by `Omega_ci`.

Terms is then added to the density and pressure equations:

$$\frac{\partial n}{\partial t} = \dots + \begin{cases} S_n & \text{if } S_n > 0 \\ nS_n & \text{if } S_n < 0 \end{cases} \quad (45)$$

$$\frac{\partial p_e}{\partial t} = \dots + \begin{cases} S_p & \text{if } S_p > 0 \\ p_e S_p & \text{if } S_p < 0 \end{cases} \quad (46)$$

$$(47)$$

The purpose of the switch is so that neither density nor pressure can be forced negative due to a sink term.

8 Neutral model

The model used is controlled by the switch

```
neutral_model
```

This can have the following values:

Value	Meaning
0	No neutrals
1	Diffusive model in X-Z
2	Recycling model
3	Fluid model in X-Y
4	Diffusive in X-Z, fluid in Y (UEDGE-like)

8.1 Diffusive neutral model

In the simplest neutral model, neutral gas is modelled as a fluid with a density n_n which diffuses with a diffusion coefficient D_n :

$$\frac{\partial n_n}{\partial t} = \nabla \cdot (D_n \nabla n_n) + S - n_n/\tau_n \quad (48)$$

The temperature of the neutrals is assumed to be the same as the ions $T_n = T_i$. Diffusion of neutrals depends on the neutral gas temperature, and on the collision rate:

$$D_n = v_{th,n}^2 / (\nu_{cx} + \nu_{nn}) \quad (49)$$

where $v_{th,n} = \sqrt{eT_n/m_i}$ is the thermal velocity of a neutral atom; $\nu_{cx} = n\sigma_{cx}$ is the charge-exchange frequency, and $\sigma_{nn} = v_{th,n}n_n a_0$ is the neutral-neutral collision frequency where $a_0 \simeq \pi (5.29 \times 10^{-11})^2 \text{ m}^2$ is the cross-sectional area of a neutral Hydrogen atom. In order to prevent divide-by-zero problems at low densities, which would cause D to become extremely large, the mean free path of the neutrals is limited to 1m.

An additional loss term is required in order to prevent the particle inventory of the simulations becoming unbounded in detached simulations, where recycling no longer removes particles from the system. This represents the residence time for neutral particles in the divertor region, which in [Togo 2013] was set to around 10^{-4} s.

8.2 Recycling model

This recycling model assumes that the neutral density exponentially falls away from the divertor plate.

$$n_n = n_{n0} e^{-y/\lambda} \quad (50)$$

where n_{n0} is a constant that will need to be calculated and λ is the mean-free path of a neutral Deuterium atom. This mean-free path is a combination of charge exchange and ionization mean free paths,

$$\lambda = \sqrt{\lambda_{cx}\lambda_{is}} = \frac{v_{th}}{\sqrt{\langle\sigma v\rangle_{cx}\langle\sigma v\rangle_{is}}} \quad (51)$$

where $\langle\sigma v\rangle$ is the cross-section rate for the charge-exchange (cx) and ionisation (is) reactions, and v_{th} is the thermal speed, which is determined by assuming the neutral temperature is the Frank-Condon energy (3.5eV). This approach should allow the simulations to be much faster than including a full neutral fluid model in the next section.

The goal of this method is to conserve a fraction, f_r , of the particles that hit the divertor, assuming that they are recycled back and re-ionised.

$$\frac{\partial N_{\text{rec}}}{\partial t} = f_r \frac{\partial N_{\text{lost}}}{\partial t} \quad (52)$$

The rate at which particles are lost can be defined as the flux out (at the divertor plate) times the surface area:

$$\frac{\partial N_{\text{lost}}}{\partial t} = n v_{i\parallel} A \quad (53)$$

where A is the area on the divertor plate, which is *not* perpendicular to the magnetic field line, so it is important to scale this by the square root of the covariant metric tensor term, $\sqrt{g_{22}}$. The source term, which is the rate of particle recycling, can be defined using the ionisation cross-section, neutral density, and plasma density.

$$S_n = \frac{\partial N_{\text{rec}}}{\partial t} = \int n_e n_n \langle \sigma v \rangle_{is} dV \quad (54)$$

where $\langle \sigma v \rangle_{is}$ is the ionisation cross-section rate and the integral is over the entire volume of the simulation. By substituting equation this becomes

$$\frac{\partial N_{\text{rec}}}{\partial t} = n_{n0} \int n_e e^{-y/\lambda} \langle \sigma v \rangle_{is} dV. \quad (55)$$

Now, substituting equations and into results in an equation for the neutral density constant, n_{n0} that will give the proper recycling rate.

$$n_{n0} = \frac{f_r n v_{i\parallel} A}{\int n \langle \sigma v \rangle_{is} e^{-y/\lambda} dV} \quad (56)$$

The neutral density will evolve such that the recycling rate f_r is maintained along each field line individually. The flux of particles lost to the divertor on a single field line will be recycled to the same field line.

8.3 Fluid neutral model

This model evolves the equations for a neutral fluid, assuming axisymmetry (constant in Z), for the density n_n , velocity \mathbf{v}_n and pressure p_n .

$$\begin{aligned} \frac{\partial n_n}{\partial t} &= -\nabla \cdot (n_n \mathbf{v}_n) \\ \frac{\partial \mathbf{v}_n}{\partial t} &= -\mathbf{v}_n \cdot \nabla \mathbf{v}_n - \frac{1}{n_n} \nabla p_n + \frac{1}{n_n} \nabla \cdot (\mu \nabla \mathbf{v}) + \frac{1}{n_n} \nabla \left[\left(\frac{1}{3} \mu + \zeta \right) \nabla \cdot \mathbf{v}_n \right] \\ \frac{\partial p_n}{\partial t} &= -\nabla \cdot (p_n \mathbf{v}_n) - (\gamma - 1) p_n \nabla \cdot \mathbf{v}_n + \nabla \cdot (\kappa_n \nabla T_n) \end{aligned} \quad (57)$$

where the dissipation parameters μ , ζ and κ are constants set in the `[neutral]` section of the options:

Variable	Option	Meaning
μ	viscosity	Dynamic viscosity
ζ	bulk	Bulk (volume) viscosity
κ_n	conduction	Thermal conduction

The contravariant components of \mathbf{v}_n are evolved in the same (x, y, z) field-aligned coordinate system as the plasma. To evaluate the nonlinear advection term, whilst avoiding the use of noisy Christoffel symbols coming from derivatives of basis vectors, these components are transformed into (R, Z, ϕ) cylindrical coordinates, advected, then transformed back. This is done using matrices which are calculated in the initialisation stage by finite differences of the input mesh:

$$\begin{pmatrix} \nabla R \\ \nabla Z \end{pmatrix} = \begin{pmatrix} \frac{\partial R}{\partial x} & \frac{\partial R}{\partial y} \\ \frac{\partial Z}{\partial x} & \frac{\partial Z}{\partial y} \end{pmatrix} \begin{pmatrix} \nabla x \\ \nabla y \end{pmatrix} \quad (58)$$

$$= \begin{pmatrix} \text{Urx} & \text{Ury} \\ \text{Uzx} & \text{Uzy} \end{pmatrix} \begin{pmatrix} \nabla x \\ \nabla y \end{pmatrix} \quad (59)$$

These components are calculated by finite differences of the Rxy and Zxy arrays in the input, then adjusted to match the given values of hthe and Bpxy :

$$\sqrt{\left(\frac{\partial R}{\partial y}\right)^2 + \left(\frac{\partial R}{\partial x}\right)^2} = h_\theta$$

$$\sqrt{\left(\frac{\partial R}{\partial x}\right)^2 + \left(\frac{\partial R}{\partial y}\right)^2} = 1/(RB_\theta)$$

(Note that this second equality only works if x and y are orthogonal).

This matrix is then inverted, to give:

$$\begin{pmatrix} \nabla x \\ \nabla y \end{pmatrix} = \begin{pmatrix} \text{Txr} & \text{Tyr} \\ \text{Txz} & \text{Tyx} \end{pmatrix} \begin{pmatrix} \nabla R \\ \nabla Z \end{pmatrix} \quad (60)$$

The components of \mathbf{v}_n are evolved in covariant form:

$$\mathbf{v}_n = v_x \nabla x + v_y \nabla y + v_z \nabla z \quad (61)$$

which is then transformed to v_r and v_z :

$$v_r = \mathbf{v}_n \cdot \nabla R = \frac{\partial x}{\partial R} v_x + \frac{\partial y}{\partial R} v_y$$

$$v_z = \mathbf{v}_n \cdot \nabla Z = \frac{\partial x}{\partial Z} v_x + \frac{\partial y}{\partial Z} v_y$$

which are implemented as

```
Field2D vr = Txr * Vn2D.x + Tyr * Vn2D.y;
Field2D vz = Txz * Vn2D.x + Tyx * Vn2D.y;
```

These components are then advected as scalars for the $\mathbf{v}_n \cdot \nabla \mathbf{v}_n$ term, and are diffused for the $\nabla \cdot (\mu \nabla \mathbf{v})$ dynamic viscosity term. The quantity $(\frac{1}{3}\mu + \zeta) \nabla \cdot \mathbf{v}_n$ is treated as a pressure (with the same boundary conditions as p_n), and calculated in field-aligned coordinates.

At boundaries neutral thermal energy is lost at a rate controlled by the option

```
neutral_gamma = 5./4
```

This sets the flux of power to the wall to:

$$q = \gamma n_n T_n c_s$$

Currently this is only done at target boundaries, not radial boundaries.

8.4 Diffusive fluid model

This model (`neutral_model = 4`) solves fluid equations along y , and uses diffusive transport in X and Z. It was adopted from the approach used in UEDGE and this paper [Journal of Nuclear Materials, vol. 313-316, pp. 559-563 (2003)].

$$\begin{aligned}\frac{\partial n_n}{\partial t} &= -\nabla \cdot (n_n \mathbf{b} v_{||n} + n_n \mathbf{v}_{\perp n}) + S \\ \frac{\partial}{\partial t} (n_n v_{||n}) &= -\nabla \cdot (n_n v_{||n} \mathbf{b} v_{||n} + n_n v_{||n} \mathbf{v}_{\perp n}) - \partial_{||} p_n + \nabla_{||} (D_{nn} n_n \partial_{||} v_{||n}) + F \\ \frac{\partial p_n}{\partial t} &= -\nabla \cdot (p_n \mathbf{b} v_{||n} + p_n \mathbf{v}_{\perp n}) - \frac{2}{3} p_n \nabla \cdot (\mathbf{b} v_{||n}) + \nabla \cdot (D_{nn} n_n \nabla_{\perp} T_n) + \frac{2}{3} Q\end{aligned}$$

The parallel momentum is evolved, so that it can be exchanged with the plasma parallel momentum, but the mass is neglected for perpendicular motion. In the perpendicular direction, therefore, the motion is a balance between the friction (primarily with the plasma through charge exchange) and the pressure gradient:

$$\mathbf{v}_{\perp n} = -D_{nn} \frac{1}{p_n} \nabla_{\perp} p_n \quad (62)$$

At the moment there is no attempt to limit these velocities, which has been found necessary in UEDGE to get physical results in better agreement with kinetic neutral models [Discussion, T.Rognlien].

The perpendicular diffusion terms use a Laplacian operator which includes y derivatives, `Div_Perp_Lap_XYZ`

8.5 Transfer terms

Plasma fluid and neutral models are coupled through sources and sinks of particles, momentum and energy. In addition there are external sources:

- S_n = Source of plasma ions
- S_p = Source of pressure, related to energy source $S_E = \frac{3}{2} S_p$

In the simulations carried out so far, these source functions are both constant between mid-plane and X-point, and zero from X-point to target.

There are several transfer channels and sinks for particles, energy and momentum due to rates of recombination, ionisation and charge exchange:

$$\begin{aligned}\mathcal{R}_{rc} &= n^2 \langle \sigma v \rangle_{rc} & (\text{Recombination}) \\ \mathcal{R}_{iz} &= n n_n \langle \sigma v \rangle_{iz} & (\text{Ionisation}) \\ \mathcal{R}_{cx} &= n n_n \langle \sigma v \rangle_{cx} & (\text{Charge exchange})\end{aligned}$$

where n is the plasma density, and n_n is the neutral gas density. These all have units of $\text{m}^{-3} \text{s}^{-1}$.

- S = Net recombination i.e neutral source (plasma particle sink). Calculated as Recombination - Ionisation:

$$S = \mathcal{R}_{rc} - \mathcal{R}_{iz}$$

- R = Cooling of the plasma due to radiation, and plasma heating due to 3-body recombination at temperatures less than 5.25eV.

$$\begin{aligned} R &= (1.09T_e - 13.6\text{eV}) \mathcal{R}_{rc} && \text{(Recombination)} \\ &+ E_{iz} \mathcal{R}_{iz} && \text{(Ionisation)} \end{aligned}$$

The factor of 1.09 in the recombination term, together with factor of 3/2 in E below, is so that recombination becomes a net heat source for the plasma at $13.6/2.59 = 5.25\text{eV}$. E_{iz} is the average energy required to ionise an atom, including energy lost through excitation. Following Togo *et al.*, E_{iz} is chosen to be 30eV.

- E = Transfer of energy to neutrals.

$$\begin{aligned} E &= \frac{3}{2} T_e \mathcal{R}_{rc} && \text{(Recombination)} \\ &- \frac{3}{2} T_n \mathcal{R}_{iz} && \text{(Ionisation)} \\ &+ \frac{3}{2} (T_e - T_n) \mathcal{R}_{cx} && \text{(Charge exchange)**} \end{aligned}$$

(**) Note that if the neutral temperature is not evolved, then $T_n = T_e$ is used to calculate the diffusion coefficient D_n . In that case, T_n is set to zero here, otherwise it would cancel and leave no CX energy loss term.

- F = Friction, a loss of momentum from the ions, due to charge exchange and recombination. The momentum of the neutrals is not currently modelled, so instead any momentum lost from the ions is assumed to be transmitted to the walls of the machine.

$$\begin{aligned} F &= m_i V_{||} \mathcal{R}_{rc} && \text{(Recombination)} \\ &+ m_i V_{||} \mathcal{R}_{cx} && \text{(Charge exchange)} \end{aligned}$$

Where σ_{cx} is the cross-section for charge exchange, σ_{rc} is the cross-section for recombination, and σ_{iz} is the cross-section for ionisation. Each of these processes' cross-section depends on the local density and temperatures, and so changes in time and space as the simulation evolves.

8.6 Atomic cross sections

Cross sections are approximated with semi-analytic expressions. For the purposes of calculating these cross-sections, any temperatures below 1eV are set to 1eV. The charge exchange cross-section is approximated as:

$$\sigma_{iz} = \begin{cases} 10^{-14} T^{1/3} & \text{if } T \geq 1\text{eV} \\ 10^{-14} & \text{if } T < 1\text{eV} \end{cases} \quad (63)$$

with units of $[\text{m}^3/\text{s}]$. Ionisation is calculated as

$$\sigma_{cx} = \begin{cases} 5.875 \times 10^{-12} \cdot T^{-0.5151} \cdot 10^{-2.563/\log_{10} T} & \text{if } T \geq 20\text{eV} \\ 10^{-6} \cdot T^{-3.054} \cdot 10^{-15.72 \exp(-\log_{10} T) + 1.603 \exp(-\log_{10}^2 T)} & \text{if } 1\text{eV} < T < 20\text{eV} \\ 7.638 \times 10^{-21} & \text{if } T \leq 1\text{eV} \end{cases} \quad (64)$$

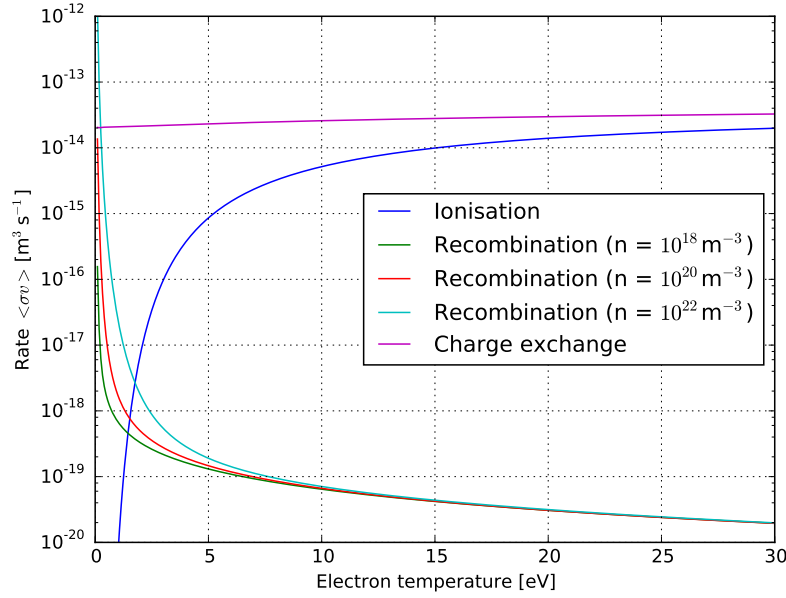


Figure 2: Cross-sections [Thanks to H.Willett]

Recombination rates are calculated using a 9×9 table of coefficients so is not reproduced here.

Plots of these cross-sections are shown in figure 2. There are a few anomalies with this: charge exchange always has the highest cross-section of any process, and ionisation has a jump at 20eV. The ionisation and charge exchange rates do not depend on density, but recombination does so a typical range of values is shown.

8.7 Impurities

A fixed carbon fraction can be added by using the setting

```
carbon_fraction = 0.01 # 1% carbon fraction
```

This only affects the plasma pressure, by adding a radiation loss term. At the moment the analytic carbon cooling curve from Hutchinson's paper (shown in figure 3) is used. A negative value indicates that there is no carbon, so the default is -1. This is only different from 0.0 in efficiency; if negative then the radiation will not be calculated.

9 Simulation startup procedure

Obtaining a steady state can require long simulation times, particularly if the initial conditions are not a good guess for what the final state looks like. To avoid violent transients and excessive simulation time evolving a large system of equations from an unphysical starting point, a step-by-step startup procedure can be followed:

1. Start without any neutrals (`neutral_model = 0`), specifying sources of particles near the target plates. Run for a timescale of $\text{few} \times 10^3 / \Omega_{ci}$, then adjust the sources and run for a bit longer. The idea is not to reach equilibrium, but to get past the initial

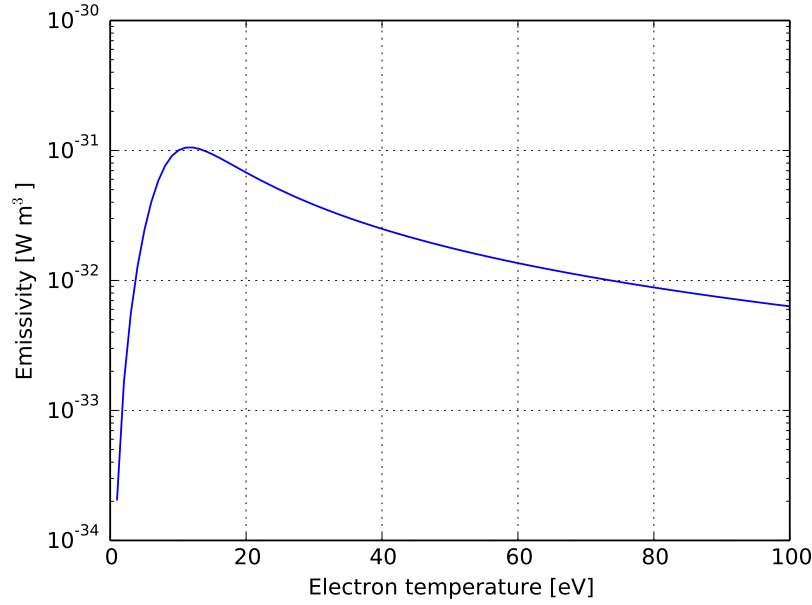


Figure 3: Carbon cooling rate [Hutchinson]

transients when the flow into the sheath begins, which can lead to problems for the neutral gas models.

2. Switch on the neutral model with a small recycling fraction (say 10%)
3. Increase the recycling fraction whilst decreasing the plasma particle source
4. Once the desired recycling fraction is reached, turn off the external particle source, and run for as long as needed to get an equilibrium
5. Turn on plasma currents to evolve the electric field
6. Add points in Z...

10 Boundary conditions

The current through the sheath is described in terms of electron and ion current

$$j_{sh} = en_{sh} (v_{sh,i} - v_{sh,e})$$

The ion current is just determined by the ion sheath velocity $v_{sh,i}$. The electron velocity is given by

$$v_{sh,e} = \begin{cases} \sqrt{\frac{eT_e}{m_e} \frac{1}{4\pi}} e^{-\phi/T_e} & \text{If } \phi \geq 0 \\ \sqrt{\frac{eT_e}{m_e} \frac{1}{4\pi}} & \text{If } \phi < 0 \end{cases} \quad (65)$$

If $\phi < 0$ at the sheath, the electron current saturates. This prevents unphysically large electron flows at the sheath.

10.1 Heat flux

The heat flux is more complicated to impose, since it involves both the thermal energy (P_e) and parallel momentum ($nV_{||}$) equations.

Terms which could transport energy out of the system at the sheath in the pressure (thermal energy) equation are

$$\frac{\partial P_e}{\partial t} = -\frac{5}{3}\nabla \cdot (P_e V_{||e}) \quad (66)$$

$$+\frac{2}{3}\nabla \cdot (\kappa \partial_{||} T_e) \quad (67)$$

$$+0.71\frac{2}{3}\nabla \cdot (T_e j_{||}) \quad (68)$$

$$-0.71\frac{2}{3}j_{||}\partial_{||} T_e \quad \text{Thermal force} \quad (69)$$

$$+\frac{2}{3}v_{||e}\partial_{||} P_e \quad (70)$$

In the SimCat code these appear as:

```
if(parallel_flow)
  ddt(Pe) -= (5./3)*Div_parP_LtoC(Pe,Ve);
if(thermal_conduction)
  ddt(Pe) += (2./3)*Div_Par_Diffusion(kappa_epar, Te);
if(thermal_flux)
  ddt(Pe) += (2./3)*0.71*Div_parP_LtoC(Te,Jpar);
if(thermal_force)
  ddt(Pe) -= (2./3)*0.71*Jpar*Grad_parP(Te);
if(pe_par) {
  ddt(Pe) += (2./3)* Ve * Grad_parP(Pe);
```

The final term transfers energy between pressure and momentum equations; the second from last (thermal force) term transfers energy to electromagnetic energy. If temperature and pressure are set to zero gradient, then these terms are zero at the sheath and so the energy flux is

$$\Gamma_E = \frac{5}{2}P_e V_{||e} - 0.71T_e j_{||} \quad (71)$$

In the momentum equation the parallel fluxes are due to:

$$\frac{\partial nV_{||}}{\partial t} = -\nabla \cdot (nV_{||}V_{||}) \quad (72)$$

$$-\partial_{||} P_e \quad (73)$$

and so the flux of energy from the system in the momentum equation is

$$\Gamma_E = \frac{1}{2}nV_{||,sh}^2 V_{||,sh} = \frac{1}{2}nT_e C_s \quad (74)$$

where $V_{||,sh} \geq c_s$ is the velocity at the sheath.

If currents are neglected, the energy flux through the boundary is therefore:

$$\Gamma_E = 3nT_e C_s$$

This amount should therefore be subtracted from the heat flux through the boundary

$$q = \gamma n T_e C_s$$

where $\gamma = 5.5 \rightarrow 7.8$ is the sheath energy transmission factor (default 6.5 in model currently).

At the midplane (upstream) boundary, no-flow boundaries are implemented:

$$\begin{aligned} \partial_{||} n &= 0 \\ \partial_{||} p &= 0 \\ V_{||} &= 0 \\ \partial_{||} n_n &= 0 \end{aligned} \tag{75}$$

and hence $\partial_{||} T = 0$ and $\mathbf{q} = 0$.

At the target plate, normal sheath boundary conditions are applied, so velocity at the sheath entrance is sonic:

$$V_{||}^{sheath} \geq C_s \tag{76}$$

If the velocity just in front of the sheath is supersonic, then a zero-gradient boundary condition is used, but if the flow in front of the sheath is subsonic then the sound speed is used. The flux of ions to the wall is therefore

$$\Gamma = n^{sheath} V_{||}^{sheath} \tag{77}$$

The temperature gradient is set using the sheath energy transmission factor γ_s so that the total power flux to the target is the sum of kinetic, convection and conduction:

$$\frac{1}{2} m_i n V_{||}^3 + \frac{5}{2} p V_{||} - \kappa_{||e} \partial_{||} T = \gamma_s n T C_s \tag{78}$$

This equation is then rearranged to calculate the gradient of T at the boundary. The temperature gradient is then limited so that temperature always decreases going towards the wall. Physically this means that the power to the target is allowed to exceed the sheath transmission factor.

The particle flux at the target depends on the recycling fraction η . The flux of neutrals from the target is

$$\Gamma_n = -\eta \Gamma$$

Typically values of $\eta = 0.9$ were used, i.e. 90% recycling.

11 Numerical dissipation

For numerical stability, and hence correct convergence, numerical schemes typically require some form of dissipation. This can be done in many different ways, though care must be taken not to affect the physics. Note that all numerical dissipation terms include factors of the mesh spacing, such that they converge to zero as the mesh is refined.

The terms which are available are currently:

- **numdiff** : Viscosities in both electron and ion parallel velocity equations.

$$\begin{aligned} \frac{\partial}{\partial t} (VePsi) &= \dots + \nabla_{||} (10 \times \text{numdiff} \delta y^2 g_{yy} \partial_{||} v_{||e}) \\ \frac{\partial}{\partial t} (NVi) &= \dots + \nabla_{||} (\text{numdiff} \delta y^2 g_{yy} \partial_{||} v_{||i}) \end{aligned}$$

- **ExBdiff** : Perpendicular dissipation on quantities advected by $E \times B$ velocity

$$\frac{\partial}{\partial t}(f) = \dots + \mathbf{ExBdiff} \times \nabla \cdot \left(\frac{\delta x^2}{g^{xx}} \nabla_{\perp} f \right)$$

where f is $\{Ne, Vort, NVi, Pe\}$

- **pardiff** : A parallel velocity driven by pressure gradients

$$v_{\parallel} = -\mathbf{pardiff} \times \delta y^2 g_{yy} \partial_{\parallel} \log p_e$$

Terms in the density, pressure and ion momentum equations appear as:

$$\frac{\partial}{\partial t}(f) = \dots + \nabla_{\parallel} (f \times \mathbf{pardiff} \times \delta y^2 g_{yy} \partial_{\parallel} \log p_e)$$

12 Operators

Several operators have been implemented for SimCat, so that

13 Simulation cases

13.1 2D simulations

To run 2D (drift-plane) simulations, set **sinks = true**. This switches on the following terms:

$$\frac{\partial n}{\partial t} = \dots - \frac{\sqrt{T_i}}{2L_{\parallel}} n \quad (79)$$

$$\frac{\partial p_e}{\partial t} = \dots - \frac{2}{3} \kappa_{\parallel e} \frac{T_e}{L_{\parallel}} - T_e \frac{\sqrt{T_i}}{2L_{\parallel}} n \quad (80)$$

In addition, closures are applied to the vorticity equation. If **sheath_closure = true** then sheath closure

$$\frac{\partial \omega}{\partial t} = \dots + \frac{1}{L_{\parallel}} n \sqrt{T_e} \left[1 - \sqrt{\frac{m_i}{m_e 4\pi}} \exp(-\phi/T_e) \right]$$

13.2 Fluid simulations without EM fields

Evolving the plasma equations without currents or electromagnetic fields reduces the model to a set of fluid equations for the parallel dynamics and perpendicular diffusion. Coupled to a neutral gas model, this allows long simulations on transport times. An example is the **neutrals-d3d** test case, which uses neutral model 4 and source feedback to produce the results in figure 4.

13.3 axisym

Axisymmetric ($n = 0$) simulation of Pfirsch-Schluter currents. Starts from a stationary input with a pressure gradient (and so diamagnetic current) but no parallel current. An $m = 1$ electric potential structure forms initially, oscillates and damps towards a quasi-steady state.

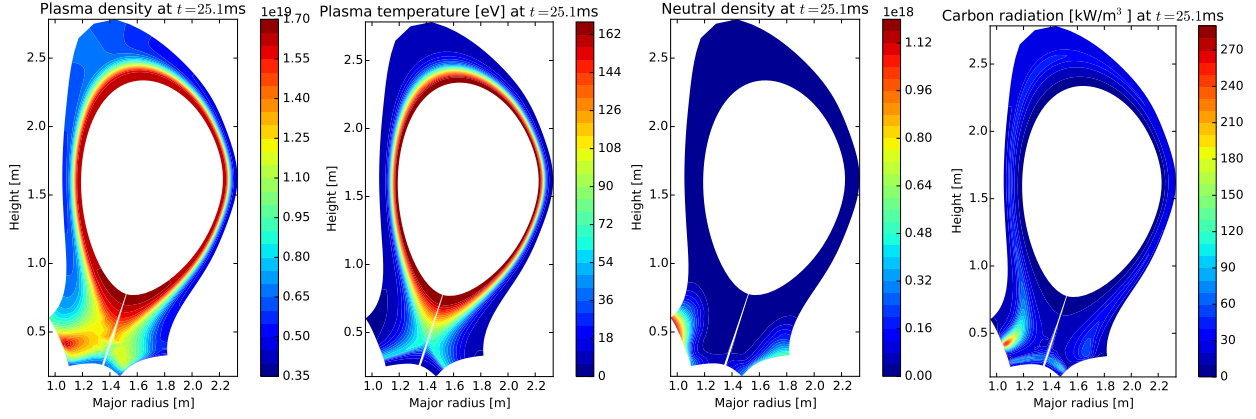


Figure 4: DIII-D fluid transport test case. From left to right are: plasma density, plasma temperature, neutral gas density, and carbon radiation

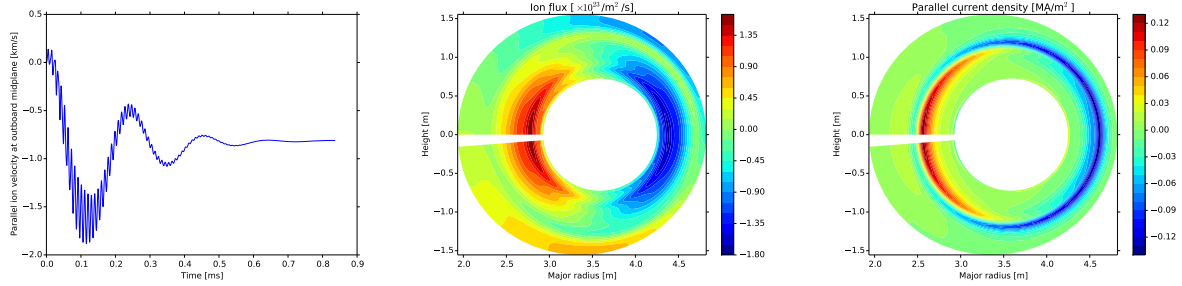


Figure 5: Axisym test case: Transient in parallel ion velocity (left); steady-state ion parallel flux (centre); steady-state parallel current (right)

13.4 ISTTOK

This is a simulation of the circular cross-section, poloidally limited device. The coordinate system is unusual for BOUT++, in using z as the poloidal angle, and y (parallel) as the toroidal angle.

Starting from an orthogonal toroidal coordinate system consisting of toroidal flux ψ_t , poloidal angle θ and toroidal angle ζ in which $\hat{\mathbf{e}}_{\psi_t} \times \hat{\mathbf{e}}_{\theta} = \hat{\mathbf{e}}_{\zeta}$. The magnitudes of the vectors are:

$$|\nabla\psi_t| = rB_{\zeta} \quad |\nabla\theta| = \frac{1}{r} \quad |\nabla\zeta| = \frac{1}{R}$$

The BOUT++ coordinate system is defined by

$$x = \psi_t \tag{81}$$

$$y = \zeta \tag{82}$$

$$z = \frac{1}{q}\zeta - \theta \tag{83}$$

(note the sign of z needed to maintain a right-handed coordinate system). For this to be a Clebsch coordinate system we need the identity:

$$\mathbf{B} = \nabla z \times \nabla x = \frac{1}{J}\mathbf{e}_y \tag{84}$$

Substituting we get

$$\nabla z \times \nabla x = \left(\frac{1}{q} \nabla \zeta - \nabla \theta \right) \times \nabla \psi_t \quad (85)$$

$$= B_\zeta \hat{\mathbf{e}}_\zeta + B_\theta \hat{\mathbf{e}}_\theta = \mathbf{B} \quad (86)$$

The Jacobian is given by

$$J^{-1} = (\nabla x \times \nabla y) \cdot \nabla z = \frac{B_\zeta}{R} \quad (87)$$

The curvature is assumed to be

$$\kappa = -\frac{1}{R} \nabla R \quad (88)$$

where from

$$R = R_0 + r \cos \theta$$

we get:

$$\nabla R = \cos \theta \nabla r - r \sin \theta = \cos \theta \frac{\nabla \psi_t}{r B_\zeta} - r \sin \theta \quad (89)$$

and so

$$\mathbf{b} \times \kappa = -\frac{B_\zeta}{BR} \sin \theta \hat{\mathbf{e}}_{\psi_t} - \frac{B_\zeta}{BR} \cos \theta \hat{\mathbf{e}}_\theta + \frac{B_\theta}{BR} \cos \theta \hat{\mathbf{e}}_\zeta \quad (90)$$

Taking the dot product with each of the coordinate basis vectors:

$$(\mathbf{b} \times \kappa) \cdot \nabla x = -\frac{r B_\zeta^2}{BR} \sin \theta \quad (91)$$

$$(\mathbf{b} \times \kappa) \cdot \nabla y = \frac{B_\theta}{RB^2} \cos \theta \quad (92)$$

$$(\mathbf{b} \times \kappa) \cdot \nabla z = \frac{1}{rR} \left(\frac{B_\zeta}{B} + \frac{B_\theta^2}{B_\zeta B} \right) \cos \theta \quad (93)$$

Since we have neglected the poloidal curvature, and are working in large aspect-ratio, the poloidal terms are dropped leaving only the x and z components:

$$(\mathbf{b} \times \kappa) \cdot \nabla x = -\frac{r B_\zeta^2}{BR} \sin \theta \quad (\mathbf{b} \times \kappa) \cdot \nabla z = \frac{B_\zeta}{BrR} \cos \theta \quad (94)$$

If θ is anticlockwise in the poloidal plane, and B_ζ is positive, then $\mathbf{b} \times \kappa$ points downwards everywhere.

From http://www.cfn.ist.utl.pt/eng/Prj_Tokamak_main_1.html#description

R	46cm
r	8.5cm
Bt	0.5T
I _p	7 kA
n _e (max)	5e18m ⁻³
T _e (max)	120eV
q(a)	5

To create the input grid:

```
>>> import circle
>>> circle.generate(68,16,512, R=0.46,
                    r=0.085, dr=0.02,
                    Bt=0.5, q=5.0,
                    ixseps=20,
                    file="isttok.nc")
```