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Towards a better edge description in gyrokinetic simulations: plasma–wall and plasma-neutral interaction

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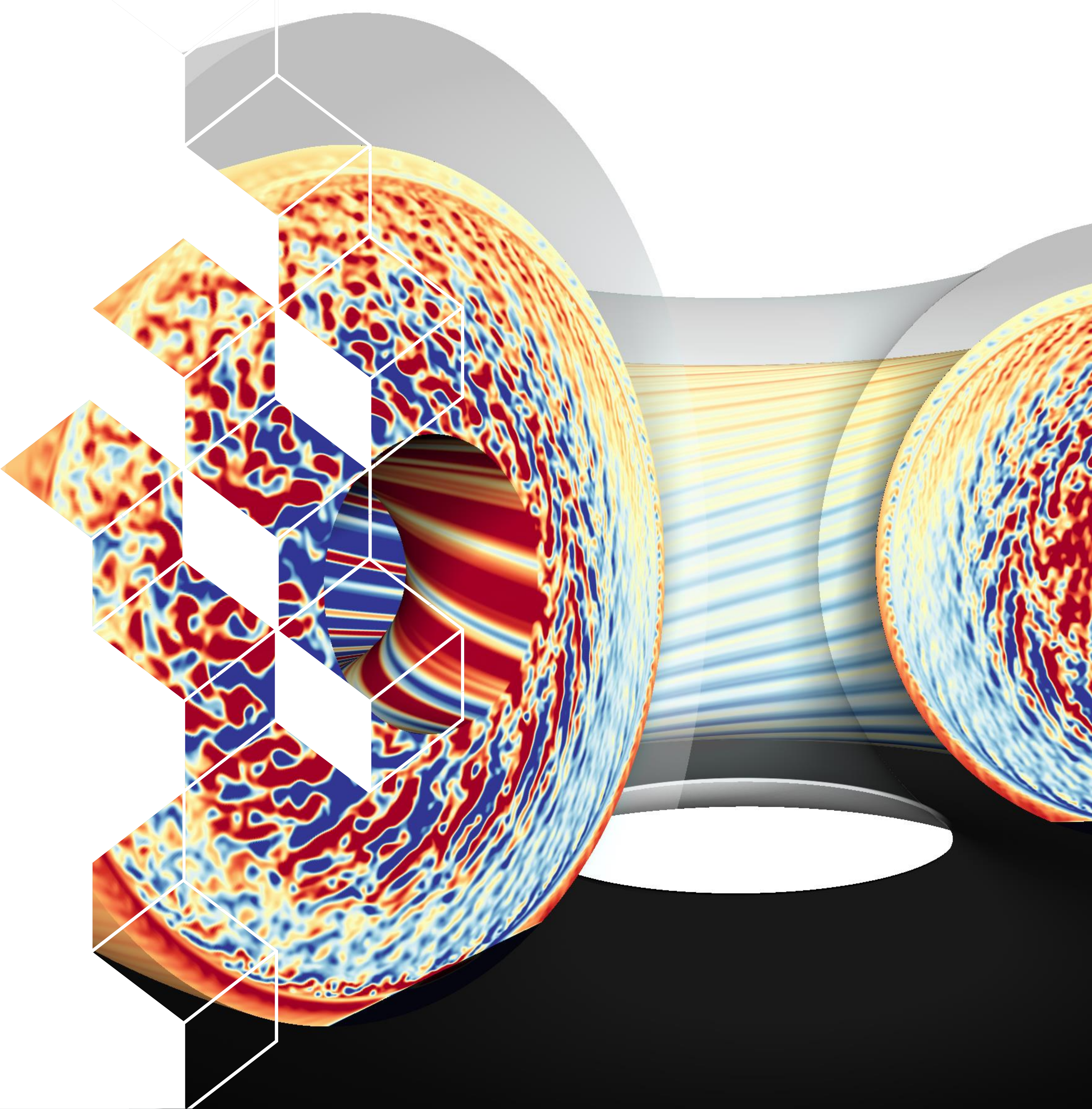
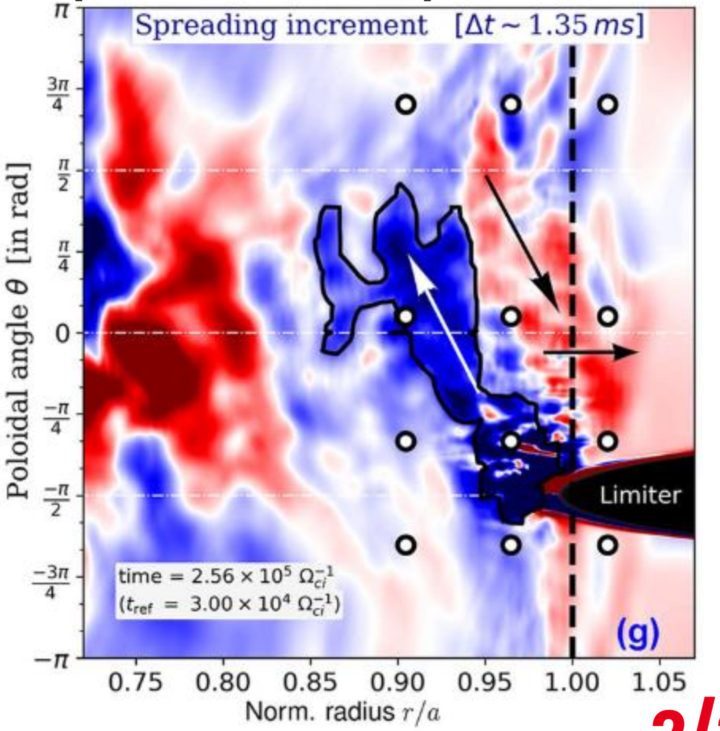
TSVV4 annual meeting – 17th October 2024



Motivation: Scrape-Off Layer conditions influence turbulence in edge plasmas

- Turbulence: main mechanism that degrades confinement in tokamaks [Wootton 1990]
- Turbulence can be regulated by ExB sheared flows in edge. Sheared flows are related to transport barrier formation [Diamond 2005] [Wagner 1982]
  → Importance of correct edge description
- Plasma-wall interaction influences SOL & edge conditions
  - Interplay between SOL, edge & core [Dif-Pradalier 2022]
  - SOL radial electric field $E_r \propto -\nabla T_e/e$ → **sheath** [Stangeby]
  - Recycling of 99% of incoming plasma particles at wall → **plasma-neutral interaction**
- Goal: include plasma-wall & plasma neutral interaction within gyrokinetic turbulent simulations

Interplay between SOL, edge and core turbulence in GK simulation [Dif-Pradalier 2022]



Outline

1. Plasma-neutral interaction
   - coupling of a **fluid neutral model** with **kinetic plasma** description
   - proof of principle in VOICE code (1D-1V kinetic Vlasov + Poisson)
   - Follow-up: integration in gyrokinetic GYSELA framework (PhD starting in November)

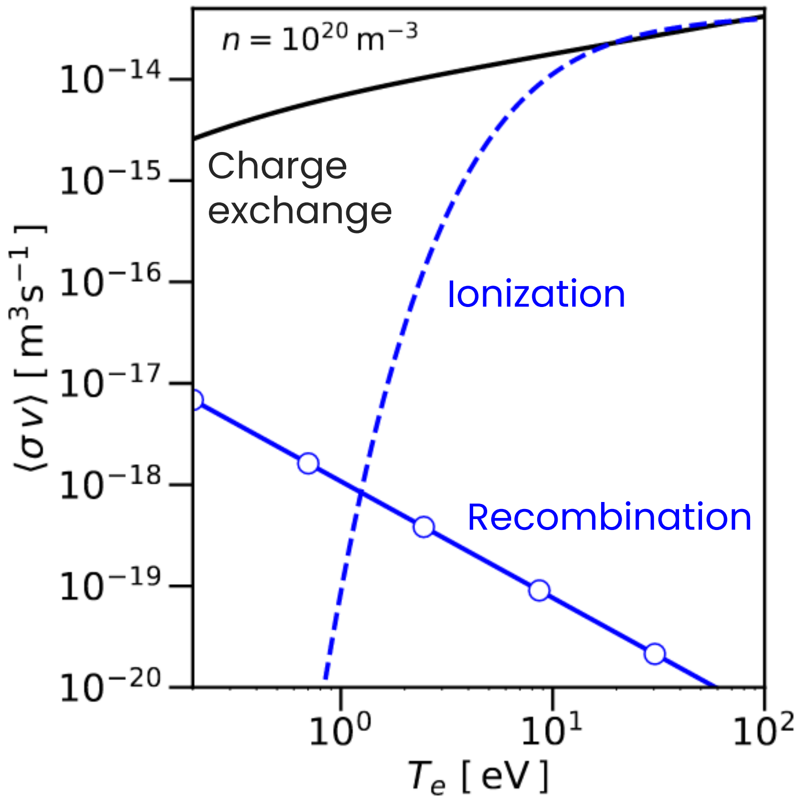
2. Plasma-wall interaction in gyrokinetics: two subgrid sheath models
   - **Axisymmetric limiter**
   - **Non-axisymmetric limiter**
   - Implementation in 5D (3D-3V) gyrokinetic code GYSELA

Plasma-neutral interaction reactions, and integration within (gyro) kinetic framework

- Fluid neutrals within gyrokinetic code: reduced computational time compared to kinetic neutrals
  - Validity of fluid model: neutral mean free path $\lambda_{\mathrm{mfp}} \ll L$ system length $(\mathrm{K_n} = \lambda_{\mathrm{mfp}}/L \ll 1)$
  - Plasma-neutral interaction in VOICE (1D-1V Vlasov-Poisson) prior to GK code GYSELA

- Plasma-neutral interaction physics
  - Considered reactions: **charge-exchange**, **ionization** & **recombination**
  - Reaction rates from ADAS database + polynomial fit

[ADAS Database; J. Blanco 2024]



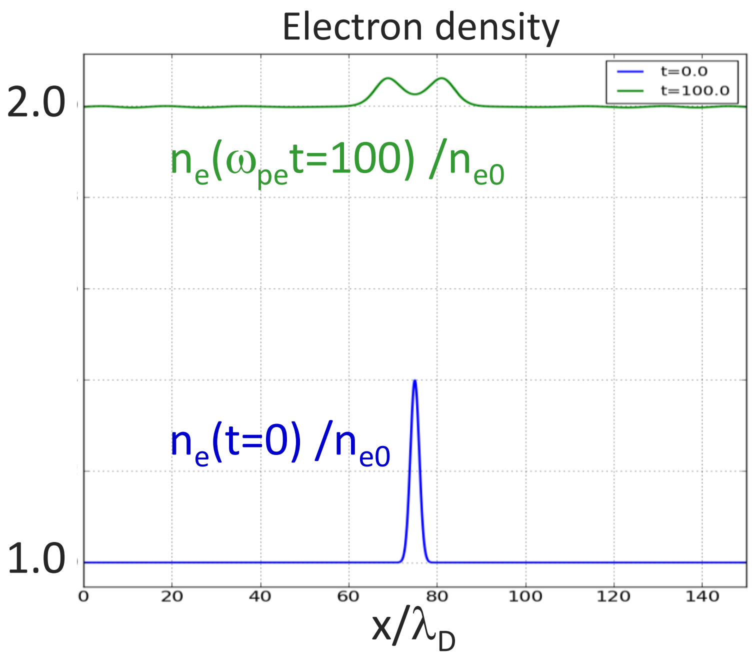
A fluid model for neutrals with an advective-diffusive transport term ("pressure-diffusion" model) [Horsten 2017] [Uytven 2022] [Quadri 2023]

- Pressure-diffusive model for neutrals (convective-diffusive transport)
  - No energy balance eq. solved for neutral $T_N = T_i$
  - Closure on pressure gradient $\nabla p_N = \underbrace{(n_N \langle \sigma v \rangle_{\mathrm{cx}} + n_e \langle \sigma v \rangle_{\mathrm{r}}) m_i n_i \boldsymbol{u}_i - (n_i \langle \sigma v \rangle_{\mathrm{cx}} + n_e \langle \sigma v \rangle_{\mathrm{i}}) m_N \boldsymbol{\Gamma}_N}_{\text{Momentum source term (charge exch, ion. \& recomb.)}}$

    Momentum source term (charge exch, ion. & recomb.)
  - Leads to $\boldsymbol{\Gamma}_N = n_{N,\mathrm{eq}}\, \boldsymbol{u}_i - D_{N,p} \nabla p_N$ with $n_{N,\mathrm{eq}} = \frac{n_i n_e \langle \sigma v \rangle_{\mathrm{r}} + n_N n_i \langle \sigma v \rangle_{\mathrm{cx}}}{n_i \langle \sigma v \rangle_{\mathrm{cx}} + n_e \langle \sigma v \rangle_{\mathrm{i}}}$ and $D_{N,p} = \frac{1}{m_N (n_i \langle \sigma v \rangle_{\mathrm{cx}} + n_e \langle \sigma v \rangle_{\mathrm{i}})}$
  - Eq. solved: neutral **particle balance** $\partial n_N + \nabla \cdot \boldsymbol{\Gamma}_N = S_{N,n} = n_i n_e \langle \sigma v \rangle_{\mathrm{r}} - n_N n_e \langle \sigma v \rangle_{\mathrm{i}}$
- Coupling to Vlasov equation (kinetic plasma)
  - Key point: "$1 \text{ neutral} \leftrightarrow 1 \text{ ion} + 1 \text{ electron}$" → $\frac{\mathrm{D}F_s}{\mathrm{D}t} = \cdots + S_N$ with $\int dv\, S_N = -S_{N,n}$
  - S_N pure source of density constructed using basis of Hermite polynomials [Sarazin 2011]

Proof of principle in 1D-1V Voice code, next: extension to GYSELA

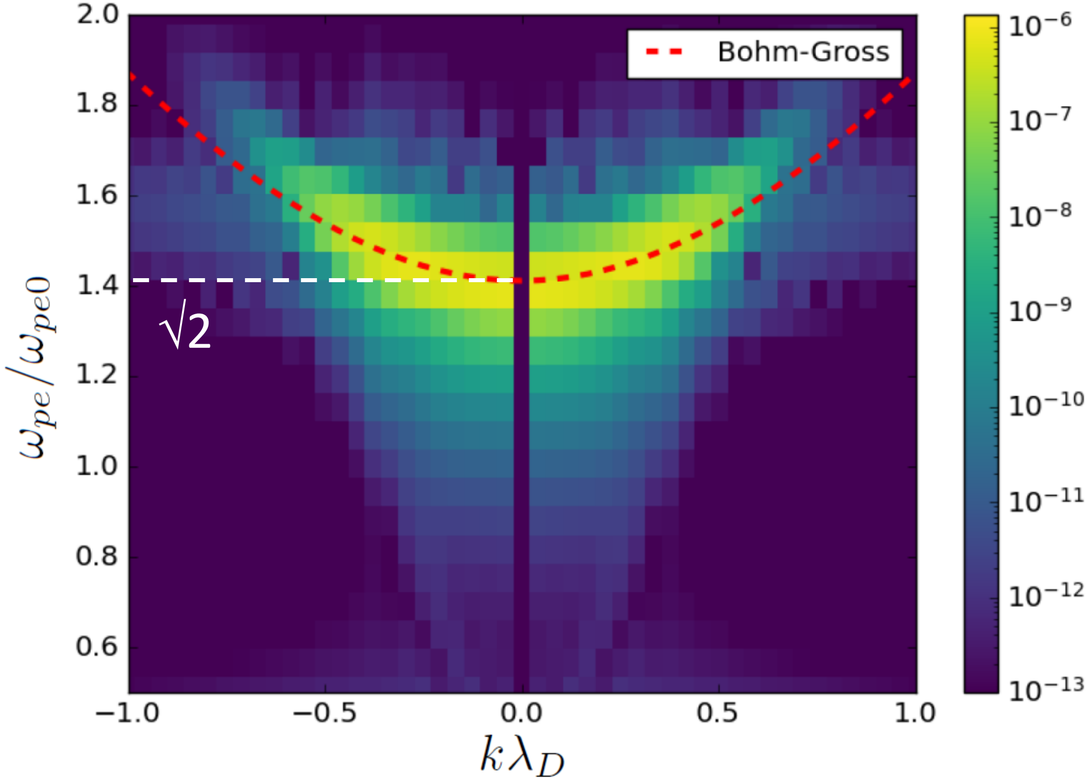
- Simulation settings
  - $\lambda_{\text{mfp}} = v_{T_N} / n_0 \langle \sigma v \rangle_{\text{cx}} \approx 10^4 \lambda_D$ → reaction rates artificially increased to that $\lambda_{\text{mfp}} \approx \lambda_D$ (keeping the **ratio between rates unchanged**)
  - Temperature ≈ 10 eV → ionization & charge exchange dominate
  - t=0: localized bump of ions & electrons ($\rightarrow$ Langmuir waves) + constant n_N
- Ionization of neutrals → higher freq. Langmuir waves



Bohm Gross:

$$\omega \approx \omega_{pe}(1 + 3(k\lambda_D)^2)^{1/2}$$

with $\omega_{pe} = \sqrt{\dfrac{e^2 n_e}{\varepsilon_0 m_e}}$



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Describing plasma-wall interaction in the gyrokinetic framework requires a subgrid model

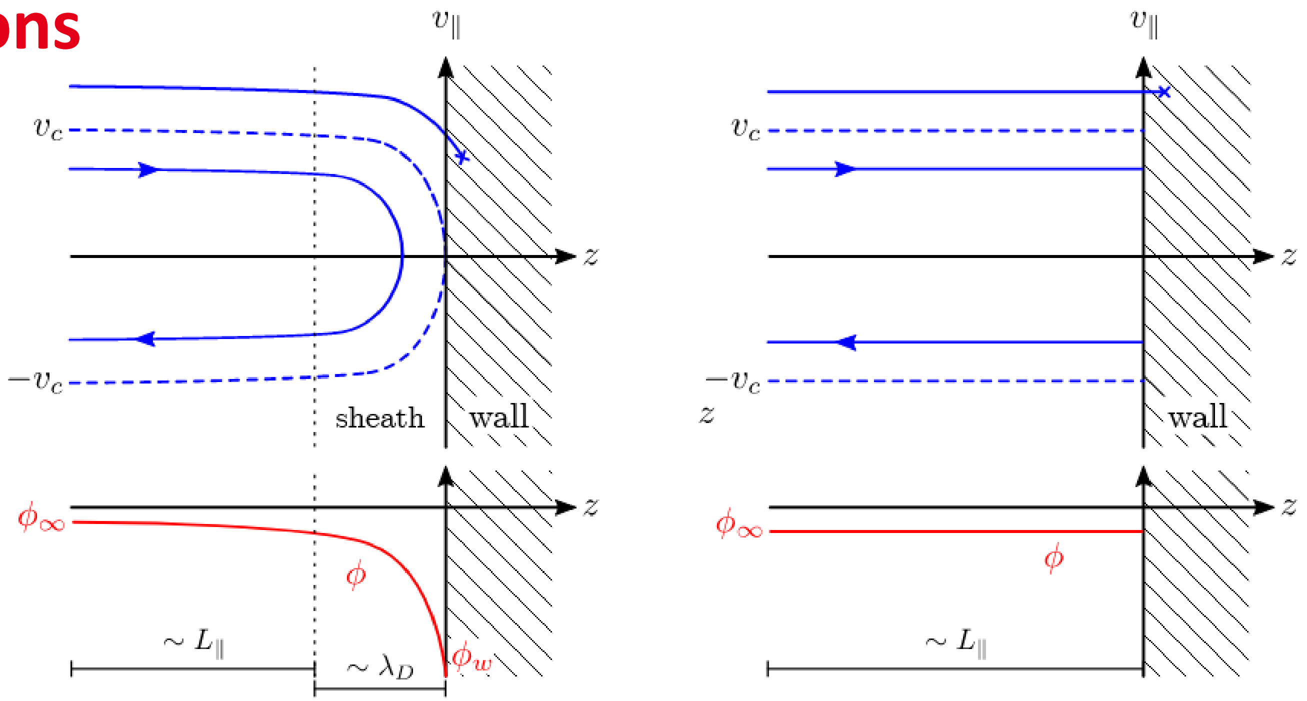
- Debye sheath: subgrid for gyrokinetics and is **positively charged**

	Debye sheath	Gyrokinetic plasma
Scale	$\lambda_D \approx 1\ \mu\mathrm{m}$	$\rho_i \approx 50\ \mu\mathrm{m}$
Frequency	$\omega_{pe} \approx 200\ \mathrm{GHz}$	$\Omega_{ci} \approx 100\ \mathrm{MHz}$

With typical SOL density & temperature $n_0 \approx 10^{19}\ \mathrm{m}^{-3}$ $T_0 \approx 30\ \mathrm{eV}$

- Directly resolving Debye sheath in a gyrokinetic code not possible → subgrid model
- Critical feature: plasma-wall interaction **ensures quasineutrality** on spatial scales $\mathbf{L} \gg \boldsymbol{\lambda_D}$ and time scales $\boldsymbol{\tau} \gg \boldsymbol{\omega_{pe}^{-1}}$
- Goal: retrieve this feature in gyrokinetic framework using **subgrid sheath model**

Subgrid sheath model components: absorption of ions & fast electrons, reflection of slow electrons



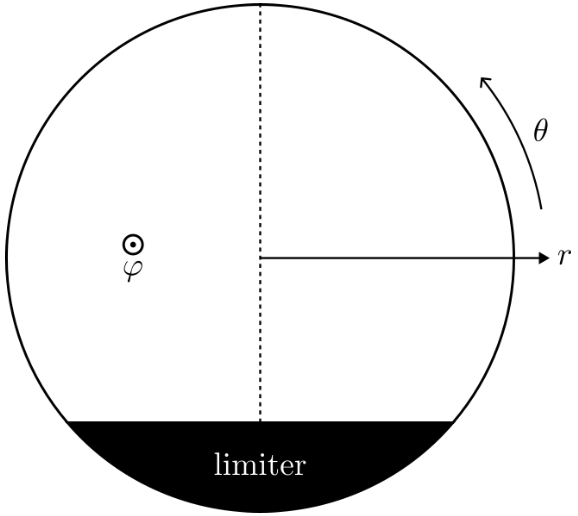
- Description in simplified $(z, v_\parallel)$ phase space
- Fast electrons $v_\parallel > v_c$ and ions: **absorbed**
- Slow electrons $v_\parallel < v_c$ **reflected**

- Key elements of a subgrid sheath model:
  1. Absorption of Ions & fast electrons
  2. Reflection of slow electrons → dependent of numerical scheme
  3. Definition of cutoff velocity v_c → *logical*, *conducting*, *flux-averaged* sheath models

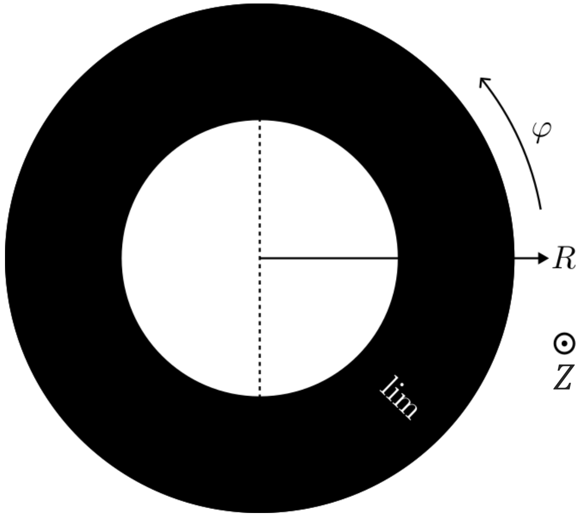
- Next slides: description of two subgrid sheath models valid for *backward semi-Lagrangian* schemes (GYSELA framework)

1.

Axisymmetric limiter with immersed boundary conditions & flux-averaged cutoff velocity



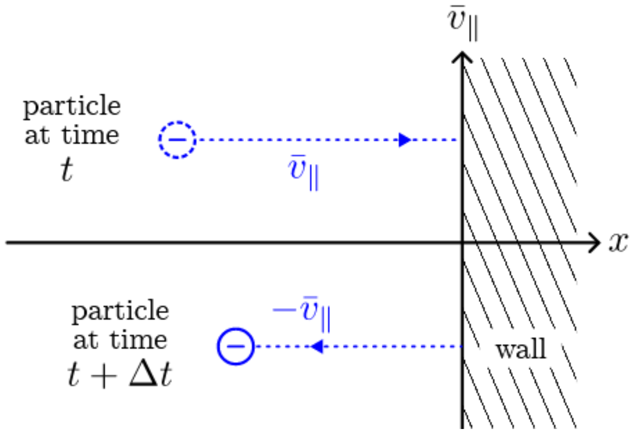
Poloidal plane



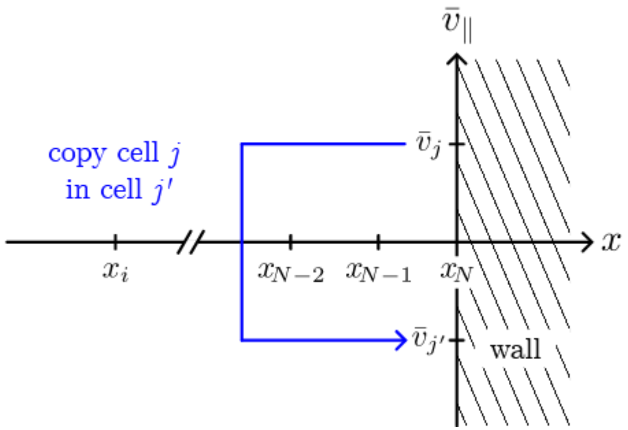
View from above

Implementation of electrons reflection depends on numerical scheme

- Lagrangian scheme

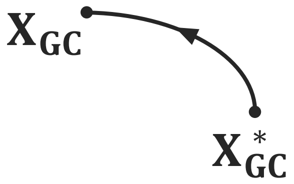


- Eulerian scheme



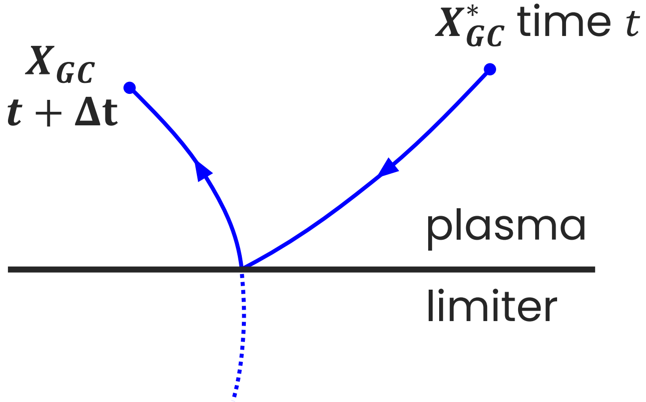
- Backward semi-Lagrangian scheme: characteristics traced back in time to update distribution function

$$F_e(\mathbf{X}_{GC}, t+\Delta t) = F_e(\mathbf{X}^*_{GC}, t)$$



$$\frac{d\mathbf{X}_{GC}}{dt} = v_\parallel + v_\perp$$

- Reflection of slow electrons: flip characteristics on wall limiter surface



- Absorption of fast electrons

$$F_e(t+\Delta t, \mathbf{X}_{GC}) = 0$$

for each fast electron that intercepts the wall

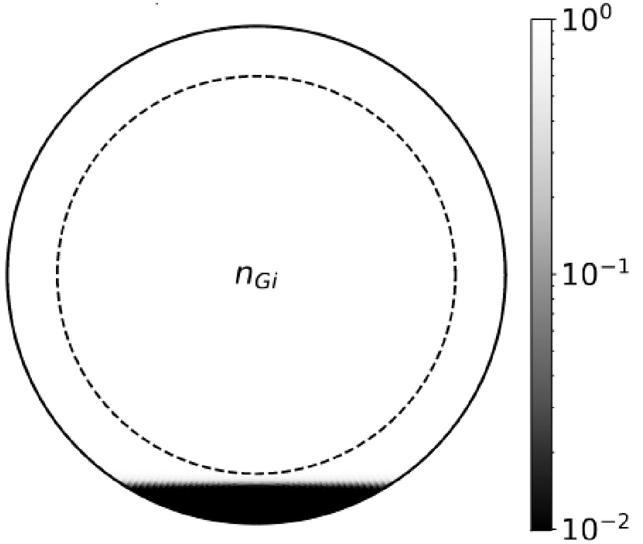
Immersed boundary conditions for ion absorption

- Limiter **immersed** in simulation domain $$\frac{DF_i}{Dt} = \mathcal{C} + \mathcal{S} + \mathcal{S}_{\text{lim}}, \qquad \mathcal{S}_{\text{lim}}(F_i) = -\nu \mathcal{M}_{\text{lim}} (F_i - F_{\text{lim}}).$$

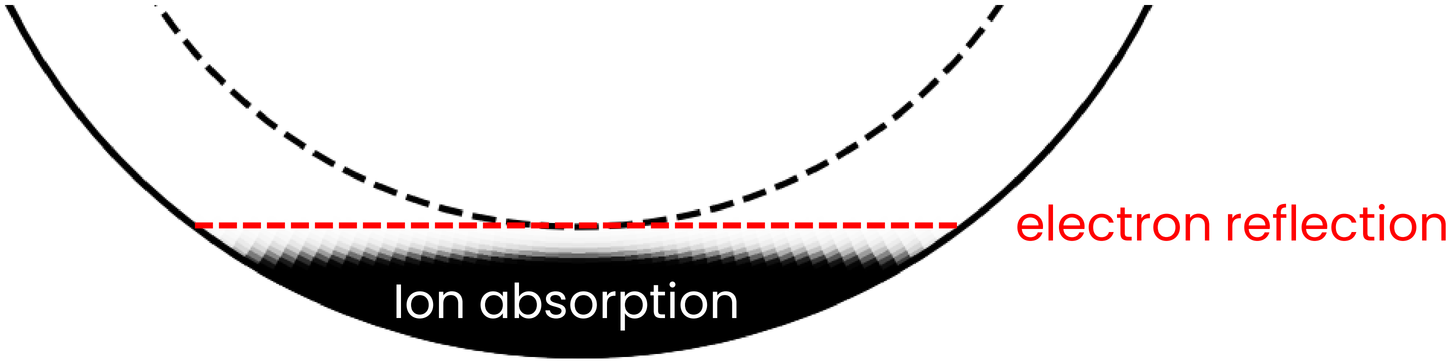
  F_{lim} : maxwellian of very low density

  M_{lim} : limiter mask (=1 in limiter, 0 in plasma, smooth transition)

- Example of uniform ion density profile with limiter



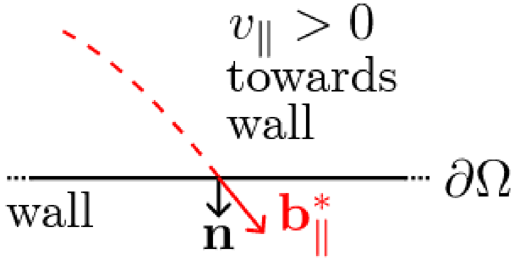
- Ion absorption & electron reflection do not coincide due to penalization



- Shift necessary for computing fluxes (next slide)

Flux-averaged sheath ensures plasma quasineutrality by matching ion & electron gyrocenter fluxes *on spatial average* over limiter

- Logical sheath: v_c such that $\Gamma_{GC} = \Gamma_e$ at **every position** on limiter surface
- Conducting sheath: $v_c = \sqrt{2e(\phi - \phi_w)/m_e}$ with ϕ_w limiter bias
- Flux averaged sheath model : definition of cutoff velocity v_c such that



Limiter ion gyrocenter flux $\langle \Gamma_{GC,i} \rangle_{\text{lim}}$

Limiter partial electron flux $\langle \Gamma_e \rangle_{\text{lim}}$

$$\int_{\partial\Omega} d^2S \int_{-\infty}^{+\infty} dv_\parallel \int_0^{+\infty} d\mu\, J_v\, J_0 F_i(\mathbf{x}, v_\parallel, \mu)\left(v_\parallel \mathbf{b}_\parallel^* + \mathbf{v}_E + \mathbf{v}_D\right)\cdot \mathbf{n} = \int_{\partial\Omega} d^2S \int_{-v_c}^{+\infty} d\bar{v}_\parallel \int_0^{+\infty} d\mu\, J_v\, F_e(\mathbf{x}, \bar{v}_\parallel, \mu)\left(\bar{v}_\parallel \mathbf{b}_\parallel^* + \mathbf{v}_E + \mathbf{v}_D\right)\cdot \mathbf{n},$$

Spatial average over limiter surface

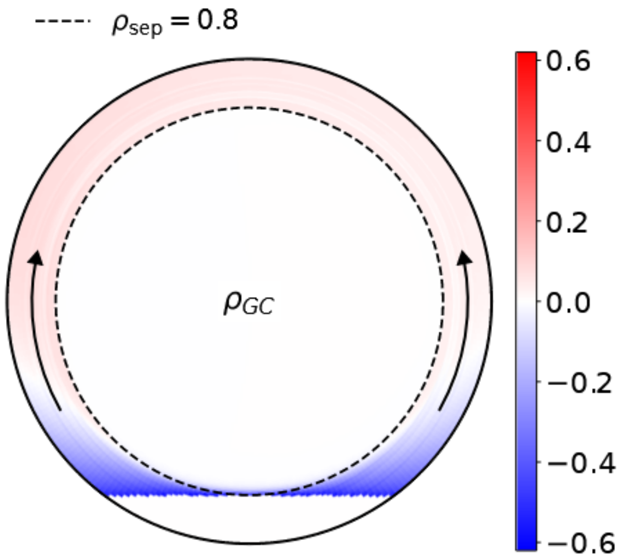
Normal vector to limiter surface

$v_\parallel \in [-\infty; -v_c]$ electrons are absorbed in limiter
→ no contribution to electron flux (?)

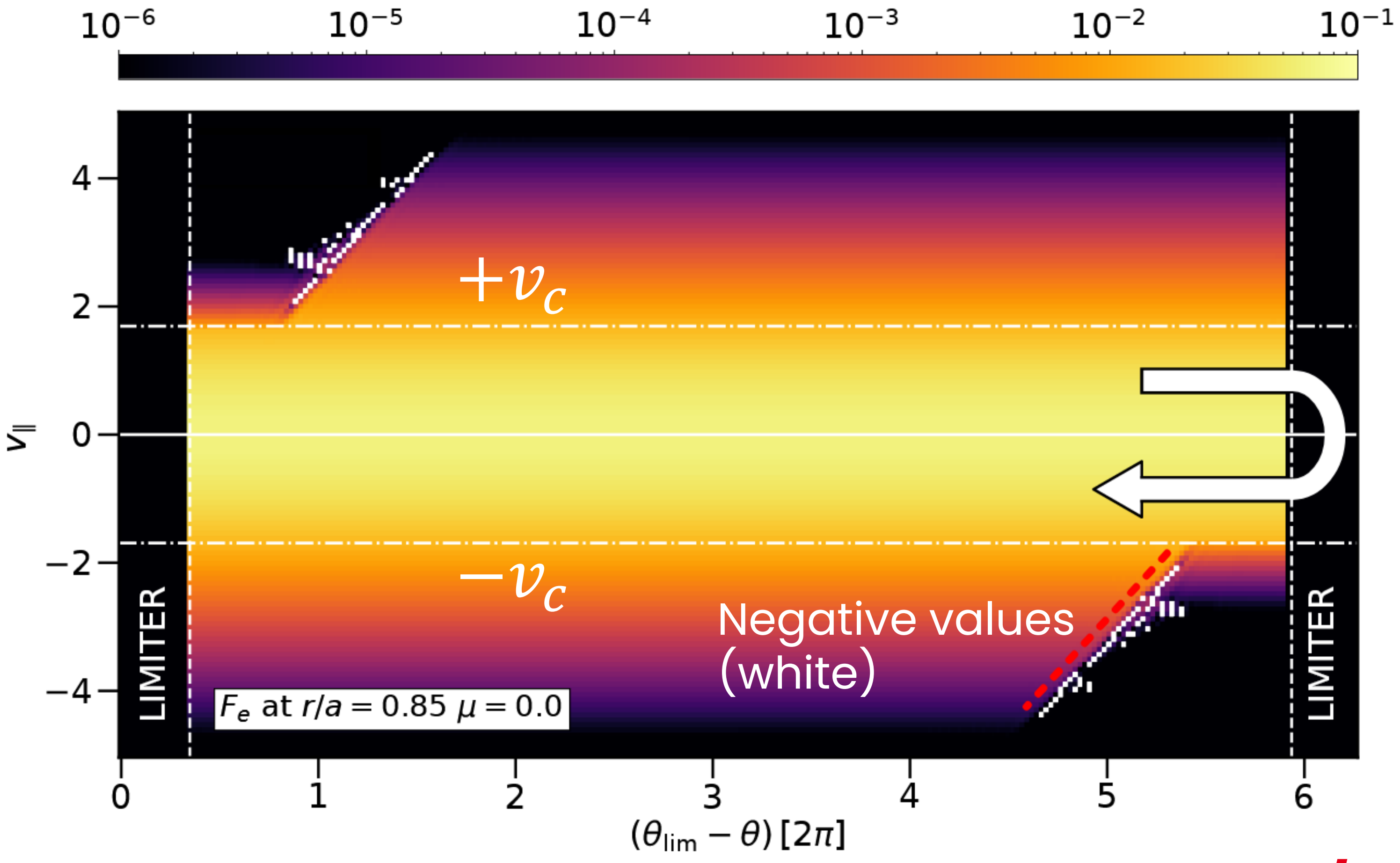
Conducting & flux averaged sheath models allow for current loops

Absorption of ions and fast electrons & refection of slow electrons work as expected

- Fast electron depletion propagates in SOL
- Depletion of ions visible close to limiter
- Large charge density when QN is not solved



Electron distribution function in SOL (no QN, fixed v_c, no collisions)

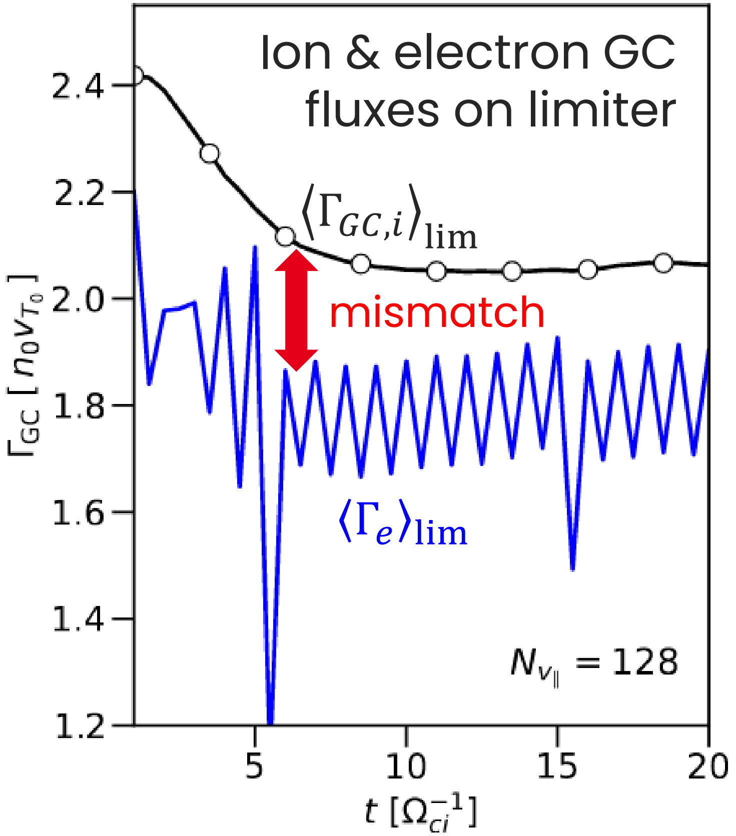


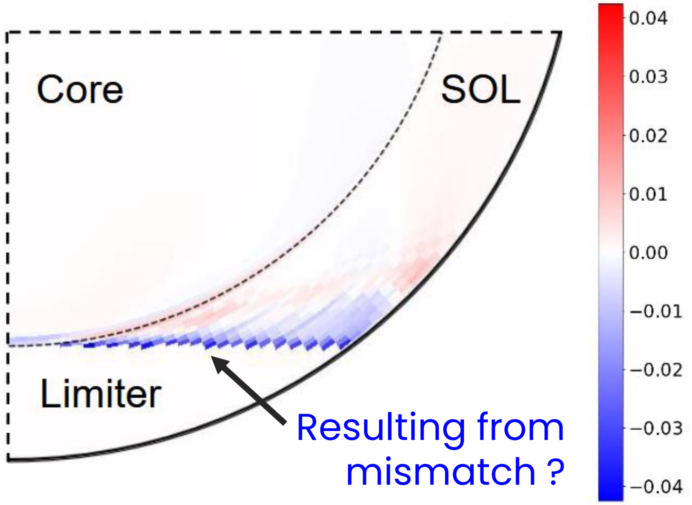
Electron & ion fluxes on limiter surface do not match: limiter surface is negatively charged

- Eventually leads to quasineutrality & simulation breakdown on very short timescales $t \approx 100\ \Omega_{ci}^{-1} \ll t_{\text{turb.}}$
- Independent of discretization
- Flux mismatch possible origins:
  - Limiter immersed in domain (QN solver)
  - $v_\parallel \in [-\infty; -v_c]$ electrons actually contribute to electron flux

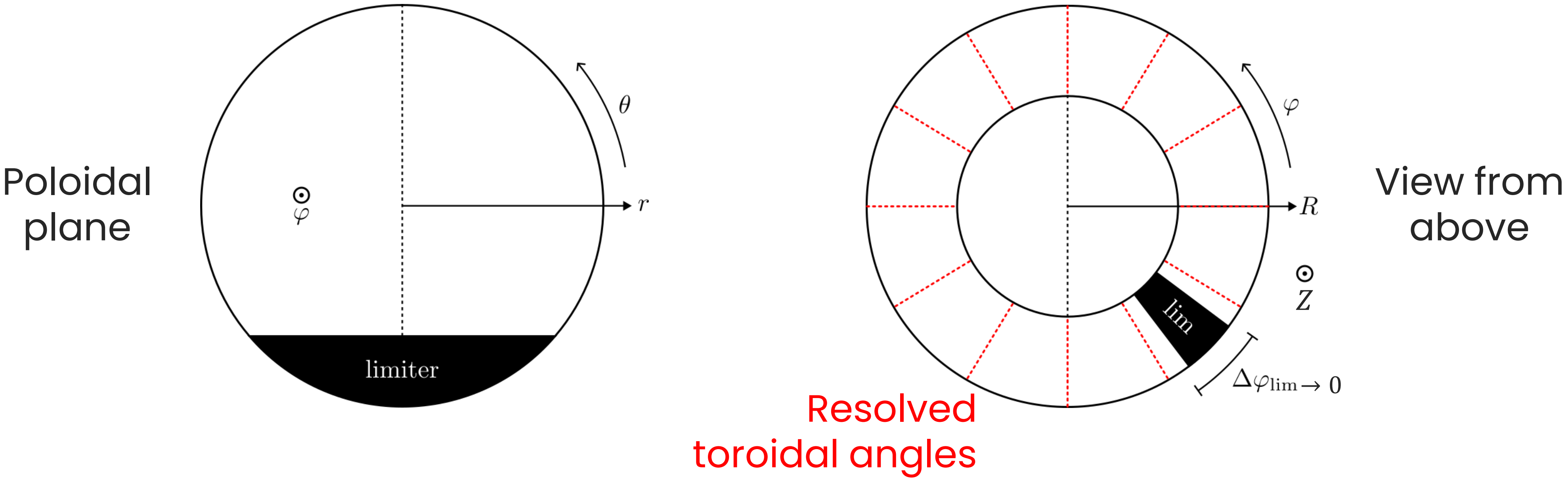
$$\langle \Gamma_{GC,i} \rangle_{\text{lim}} = \int_{\partial\Omega} d^2S \int_{-v_c}^{+\infty} d\bar{v}_\parallel \int_0^{+\infty} d\mu\, J_v\, F_e(\mathbf{x}, \bar{v}_\parallel, \mu)\, (\bar{v}_\parallel \mathbf{b}_\parallel^* + \mathbf{v}_E + \mathbf{v}_D) \cdot \mathbf{n},$$
$$+ \int_{\partial\Omega} d^2S \int_{-v_c}^{+\infty} d\bar{v}_\parallel \int_{-\infty}^{-v_c} d\mu\, J_v\, F_e(\mathbf{x}, \bar{v}_\parallel, \mu)\, (\bar{v}_\parallel \mathbf{b}_\parallel^* + \mathbf{v}_E + \mathbf{v}_D) \cdot \mathbf{n},$$

(to be checked in simulations)





2. Infinitely-thin toroidal limiter without penalization & with conducting cutoff velocity



- Unknowns: **Penalization**, **Backward semi-Lagrangian** scheme, **flux-averaged** cutoff velocity
  - Limiter located between two adjacted toroidal positions → not immersed in simulation
  - Cutoff velocity computed with conducting sheath model $v_c = \sqrt{2e\phi/m_e}$

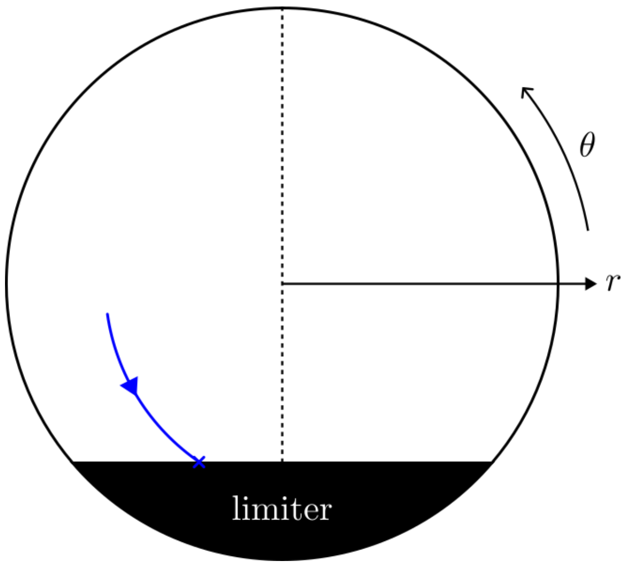
The thin toroidal limiter: a simple boundary condition embedded within toroidal advection step

- Strang splitting of gyrokinetic equation

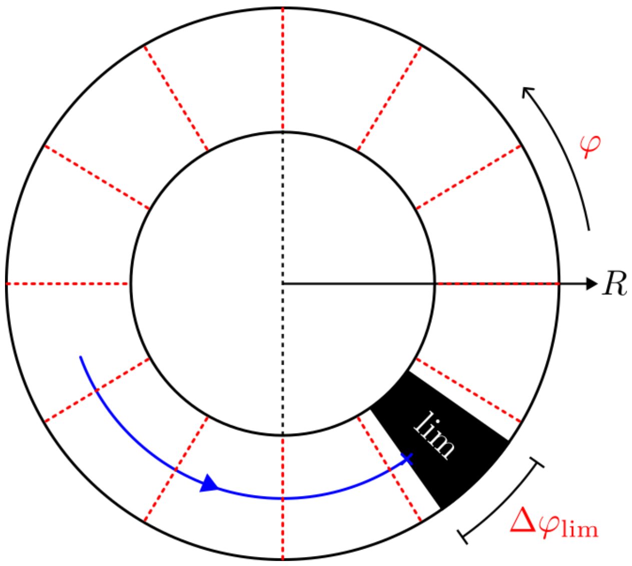
$$\frac{\partial F_s}{\partial t} + \frac{d\mathbf{x}}{dt} \cdot \nabla_{\mathbf{x}} F_s + \frac{dv_\parallel}{dt} \nabla_{v_\parallel} F_s = \mathcal{S}(F_s) + \mathcal{C}(F_s).$$

1. $v_\parallel$ advection on $\Delta t/2$
2. φ advection on $\Delta t/2$
3. (r, θ) advection on Δt

+ symmetric



Particles intercept **axisymmetric** limiter during (r,θ) advection

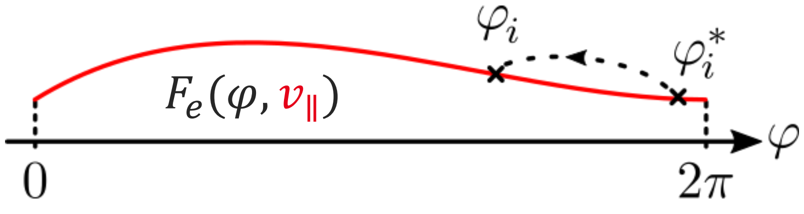


Particles intercept **thin** limiter during φ advection

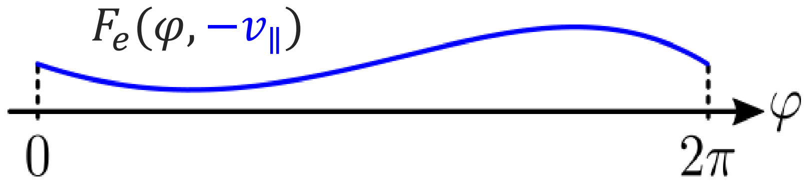
- Axisymmetric limiter is immersed in Vlasov **and** QN
- Thin limiter is located bewteen two toroidal mesh points
- Thus thin limier is immersed in **Vlasov only (not in QN)**

Absorptions & and reflections simple and efficient within 1D toroidal advection

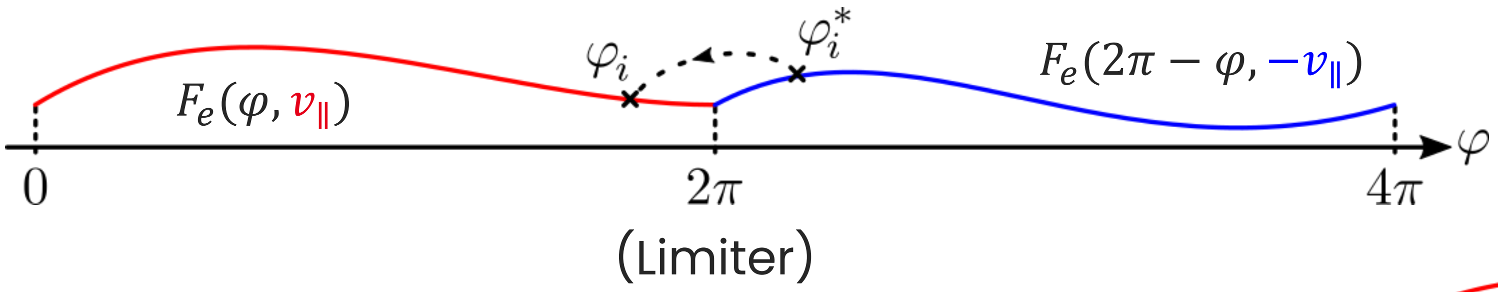
- Usual 1D toroidal advection at fixed (r, θ, μ) (periodic BC. at $\varphi = 2\pi$)



$$F_e(\varphi_i, v_\parallel, t + \Delta t) = F_e(\varphi_i^*, v_\parallel, t)$$

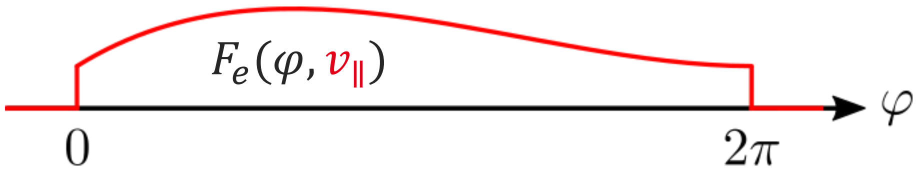


- With thin limiter: reflection on an **extended toroidal domain**



$$F_e(\varphi_i, v_\parallel, t + \Delta t) = F_e(2\pi - \varphi_i^*, -v_\parallel, t)$$

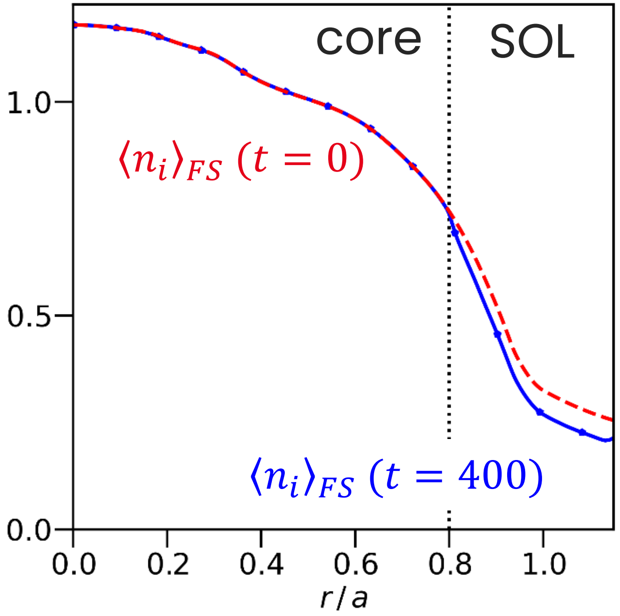
- Absorption: BC. Dirichlet at zero outside domain

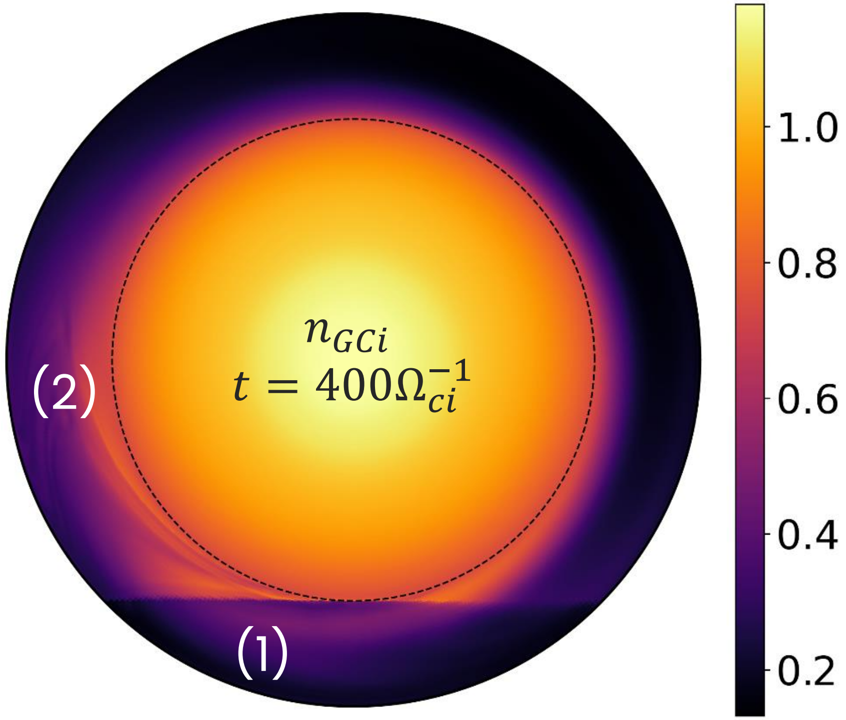


- Simple implementation: no computation of interception point for reflection

Thin toroidal limiter leads to a depletion of SOL density at early simulation times

- Thin lim. allows for reaching longer simulation times $t \approx 2000\ \Omega_{ci}^{-1}$
  - vs. $t \approx 100\ \Omega_{ci}^{-1}$ for axisymmetric lim.
  - WIP: reach turbulent times $t > 100{,}000\ \Omega_{ci}^{-1}$

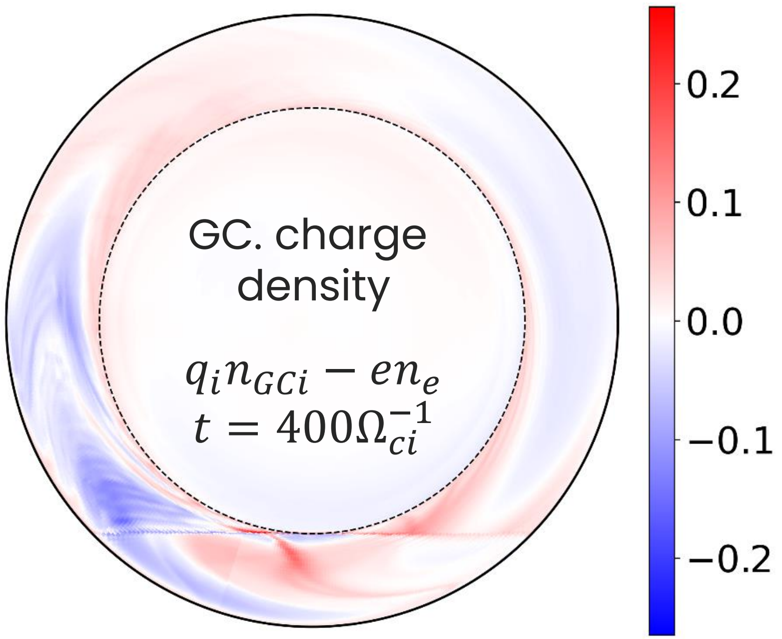




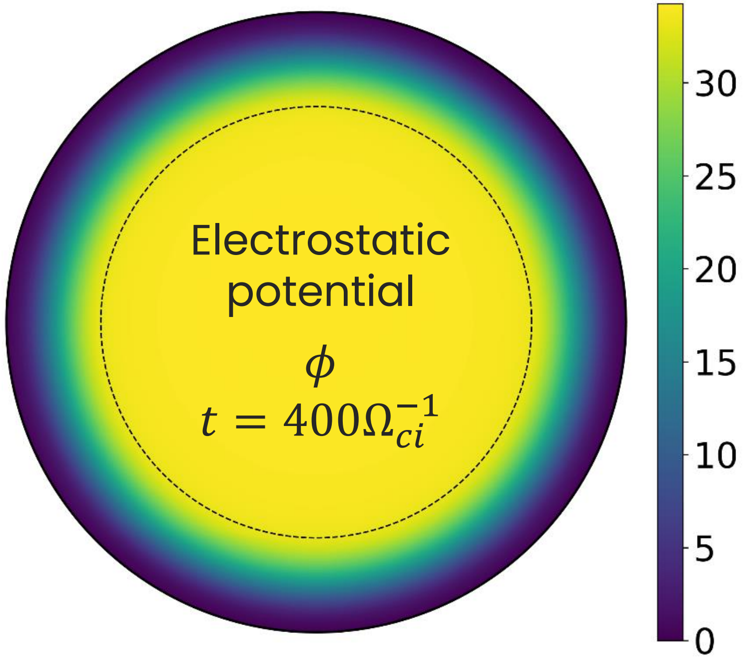
- (1) Ion density non-vanishing in « limiter » domain → different physics than with axi. lim ?
- (2) Complex reorganization features → need for overcoming initial transient $t > 2000\ \Omega_{ci}^{-1}$

Possible necessity of adapting the quasineutrality model for overcoming initial transient

$$-\nabla_\perp \cdot \left(\frac{m_i \bar{n}_{\mathrm{eq},i}}{e Z_i B^2} \nabla_\perp \phi \right) + \langle n_e^{\mathrm{pass.}} \rangle_{\mathrm{FS}} \frac{e(\phi - \langle \phi \rangle_{\mathrm{FS}})}{\langle T_e \rangle_{\mathrm{FS}}}$$
$$= Z_i n_{GI} - n_e^{\mathrm{trap.}} - \langle n_e^{\mathrm{pass.}} \rangle_{\mathrm{FS}}$$



Trapped kinetic electron model →



- Large (spurious?) GC charge density at early times
  - ➢ $\phi \approx \langle \phi \rangle_{FS} \gg 1$ in simulation
  - ➢ $\langle \phi \rangle_{FS}$ can't balance large charges with poloidal dependency
- BC for QN solver : $\phi = 0$ at $r = r_{max}$ → $v_c = 0$ absorption of all electrons in lim

Concluding remarks & perspectives

1. Plasma-neutral interaction
   - Pressure-diffusion fluid model for neutrals
   - Coupling to kinetic plasma description with moment approach for source
   - Proof of principle simulation in 1D-1V Voice code
   - Next: fluid model to be added in GK code GYSELA
2. Plasma-wall interaction
   - Description of two subgrid sheath models valid in gyrokinetic framework
   - Long (turbulent) simulation time not reached at the moment
   - Axisymmetric limiter: assess the origin of ion & electron flux mismatch
   - Thin toroidal limiter: overcome initial reorganization (QN BC modification)

Backup slides

Coupling fluid neutral & kinetic plasma neutral with Hermite polynomials

- Neutral-plasma coupling via source term in Vlasov equation $\frac{\mathrm{D}F_s}{\mathrm{D}t} = C(F_s) + S(F_s) + S_N(F_s, n_N, x, v)$
  - S_N = particle source only, no momentum/energy injection
  - Constraint: ensure "$1 \text{ neutral} \leftrightarrow 1 \text{ ion} + 1 \text{ electron}$" balance

- Construction of S_N by projection on Hermite polynomials [Sarazin 2011]

$$S_N(F_s, n_N, x, v) = \sum_{h=0}^{+\infty} c_h(n_N, F_s)\, H_h\left(\frac{v_s}{\sqrt{2T_N}}\right) \exp\left(-\frac{v_s^2}{2T_N}\right) = c_0\left(\frac{3}{2} - \frac{v_s^2}{2T_N}\right) \exp\left(-\frac{v_s^2}{2T_N}\right)$$

Pure density source

  - With $c_0 = \frac{S_{n,N}}{\sqrt{2\pi T_N}}$ and $S_{n,N} = n_N n_e \langle\sigma v\rangle_{\mathrm{i}} - (n_i n_e \langle\sigma v\rangle_{\mathrm{r}}$

- Number of particles (plasma + neutrals) conserved $\begin{cases} \partial_t n_N + \boldsymbol{\nabla} \cdot \boldsymbol{\Gamma}_N = -S_{N,n} \\ \frac{\mathrm{D}F_s}{\mathrm{D}t} = \cdots + S_N(F_s, n_N, x, v) \text{ and } \int dv\, S_N = S_{N,n} \end{cases}$