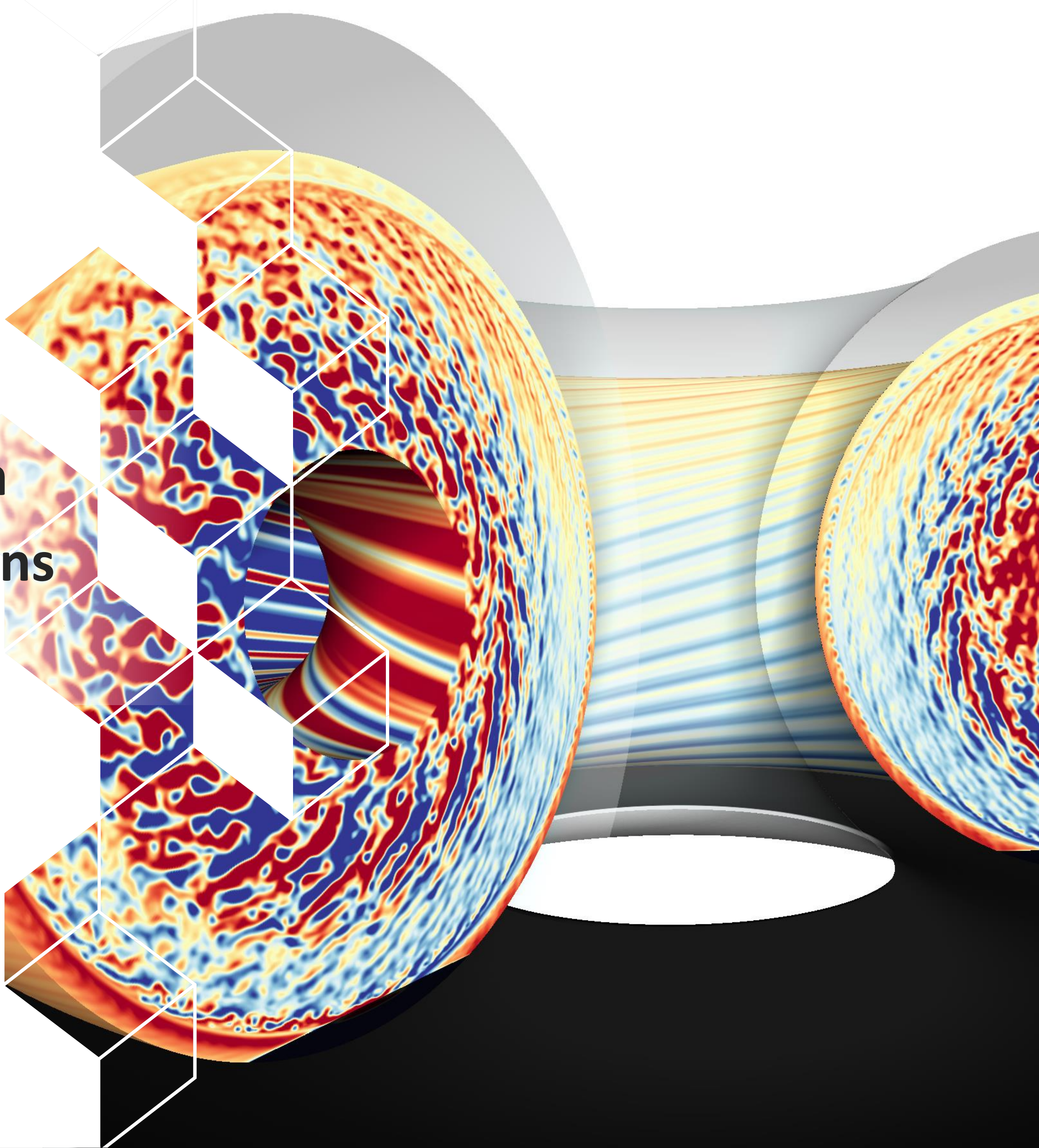
Debye sheath: comparison between fluid predictions & kinetic simulations

Towards a gyrokinetic modeling



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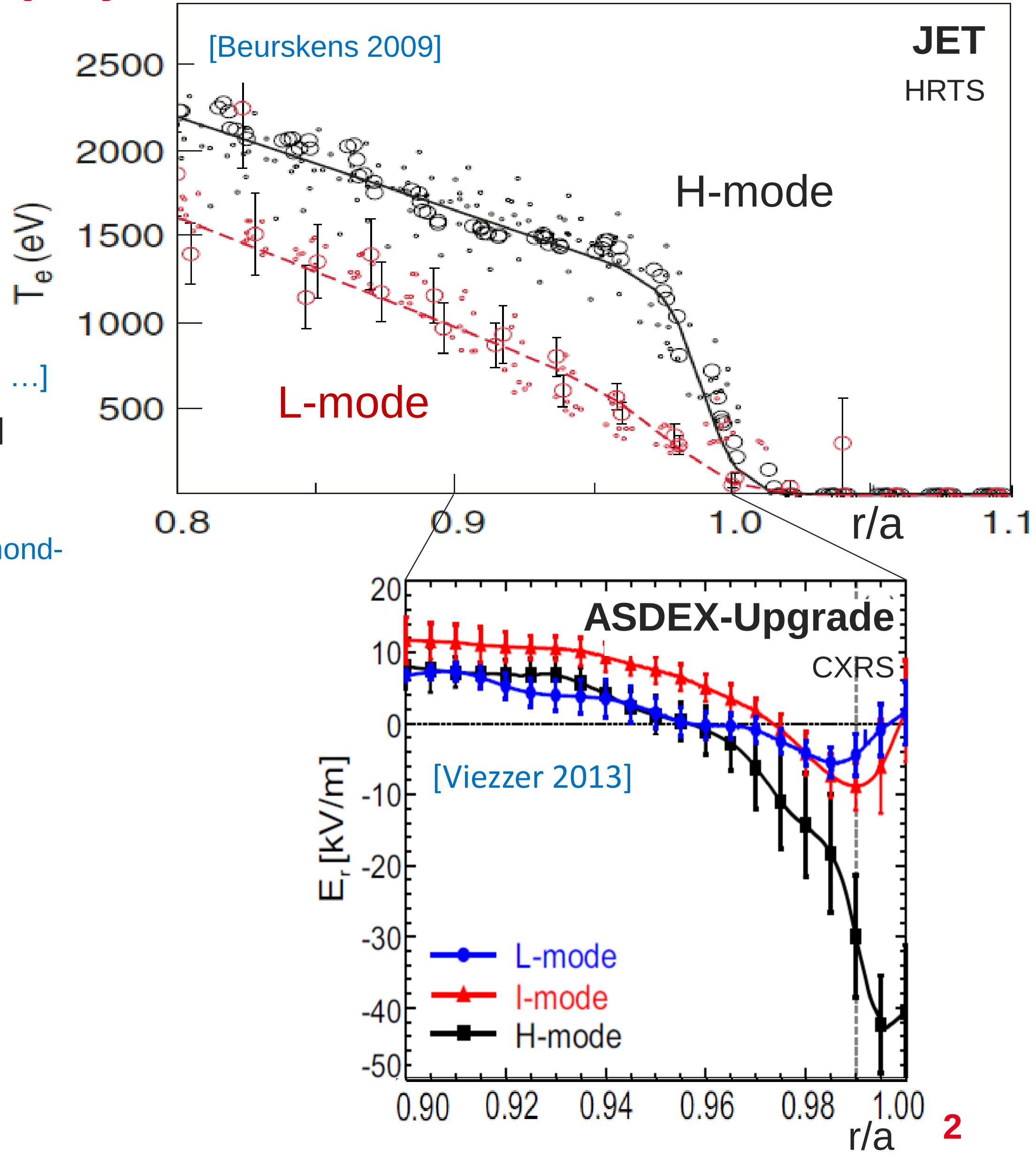
Physical context: improved confinement in tokamak plasmas largely governed by edge physics

- Energy confinement in tokamak plasmas governed by **turbulent transport** across magnetic field surfaces
- Most regimes of improved confinement characterized by **transport barriers** close to last closed field surface
  [Wagner 1982, Whyte 2010, …]
- Critical role of the **sheared radial electric field E_r** (→ sheared rotation of turb. eddies) in turbulence regulation
  [Itoh-Itoh 1988, Biglari-Diamond-Terry 1990, …]



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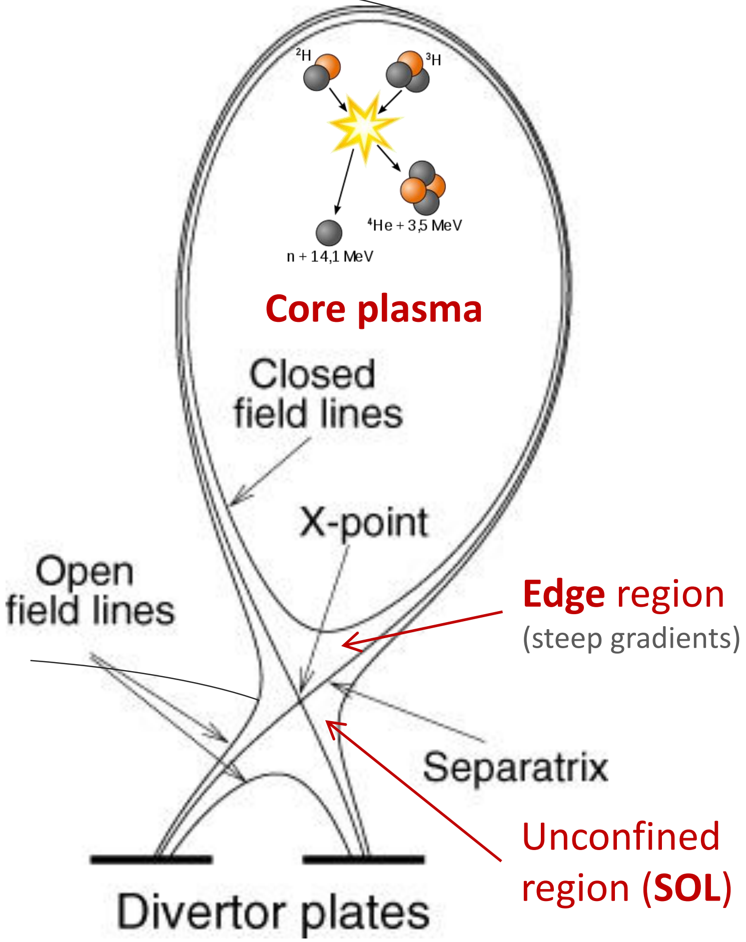
- Several players involved in **E_r profile**:
  - *Confined region*: radial force balance $E_r = \frac{\nabla_r p_{\perp i}}{en} - V_\theta B_\varphi + V_\varphi B_\theta$
  - *Edge*: ion orbit losses, collisional drag
  - *SOL*: plasma-wall interaction $E_r^{SOL} \approx -\frac{\Lambda}{e} \nabla_r T_e$
  - *All*: turbulence (Reynolds stress)



⇨ Need for **core-edge-SOL modeling** to understand & predict bifurcations toward improved confinement regimes

Outline

1. **Kinetics of plasma-wall interaction**: analogies with & departures from fluid predictions (VOICE)

2. Coupling **kinetic plasma species & fluid neutrals** – proof of principle (VOICE)

3. Towards the **implementation of plasma-wall interaction in 5D gyrokinetics** (GYSELA)

VOICE = (1D,1V) – fully kinetic electrons & ions – Poisson

GYSELA = (3D,2V) – GK ions, DK electrons – Quasi-Neutrality

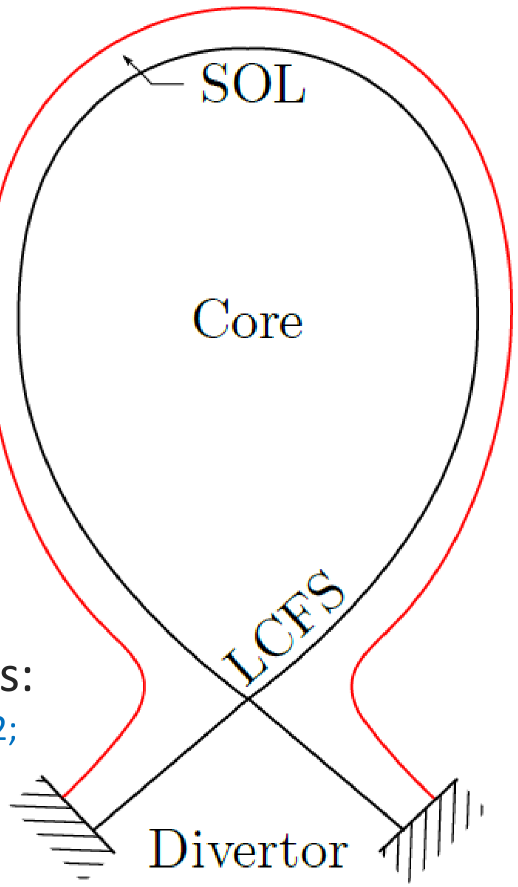
} Flux-driven, semi-Lagrangian

Objective

Understanding (1D,1V) VOICE results from a fluid perspective:

Plasma self-organization under the **balance of sources, collisions** and **parallel transport losses** mediated at the plasma-wall Debye sheath

[Munschy 2024 a & b]

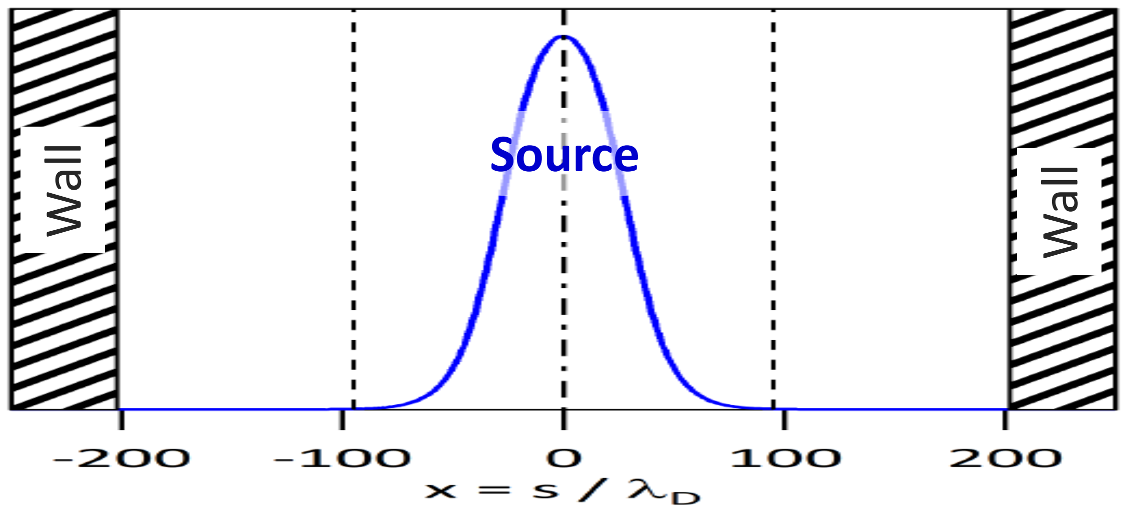


$$\begin{cases} \partial_t f_a + \sqrt{A_a}\left(v_a \partial_x f_a - Z_a \partial_x \phi \ \partial_{v_a} f_a\right) = \mathcal{C}(f_a) + \mathcal{S}(f_a) \\ \partial_x^2 \phi = -\rho_c \quad \text{with} \quad \rho_c = \sum_{\text{species}} Z_a n_a . \end{cases}$$

Refined sheath physics:
[Chodura 1982; Tskhakaya 2002; Geraldini 2018]

Review [Robertson 2013]

Normal incidence – single ion species



Coordinate along **B**-field line

Focus on numerical issues: semi-Lagrangian + non-equidistant mesh

- **Strang splitting** → solve Vlasov advections & Source/Collisions separately [Cheng-Knorr 1976, Strang 1968]

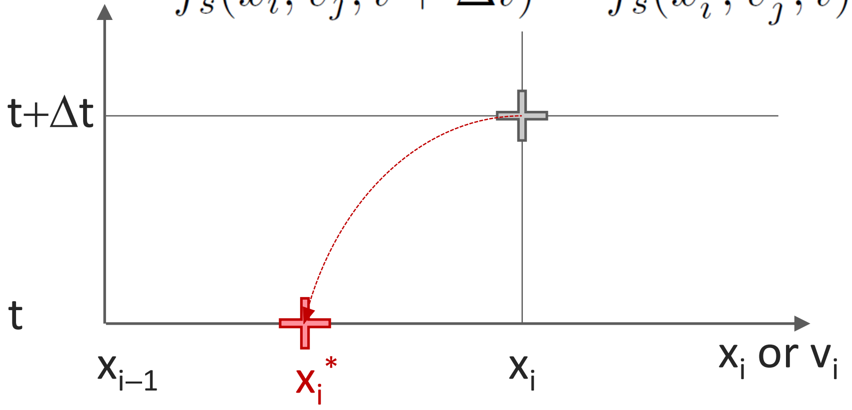
$$\partial_t f_a + \sqrt{A_a}\left(v_a \partial_x f_a - Z_a \partial_x \phi \; \partial_{v_a} f_a\right) = \mathcal{C}\left(f_a\right) + \mathcal{S}\left(f_a\right)$$

- **Semi-Lagrangian scheme** [Staniforth 1991, Sonnendrücker 1999]

Vlasov ⇒ f_s = Cst along trajectories

- Find foot print (x_i^*, v_i^*) of characteristics from (x_i, v_i)
- Interpolation (cubic splines) → $f_s(x_i^*, v_i^*, t)$

$$f_s(x_i, v_j, t+\Delta t) = f_s(x_i^\star, v_j^\star, t)$$

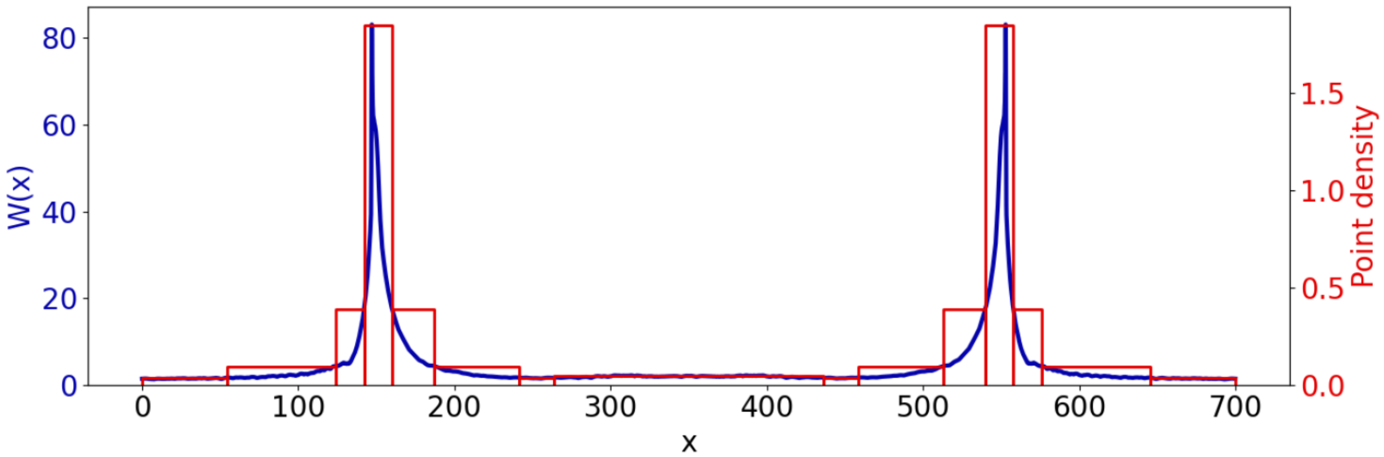


- **Refined mesh where strong gradient/curvature** [Bourne 2023]

Typical parameters:

$m_i/m_e = 400$	mass ratio
$L_x = 700\lambda_{D0}$	sim. box length
$N_x = 1500$	pts in x direction
$N_v = 700$	pts in v direction

~20h to reach steady state (NVIDIA Tesla V100, 5120 CUDA cores)



Focus on collision operator

$$\partial_t f_a + \sqrt{A_a}\left(v_a \partial_x f_a - Z_a \partial_x \phi \ \partial_{v_a} f_a\right) = \mathcal{C}\left(f_a\right) + \mathcal{S}\left(f_a\right)$$

- **Self collisions**

$$\mathcal{C}_{ss}(f_s) = \nu^{\star}_{\mathrm{D0}} \frac{\partial}{\partial v_s}\left\{ D_v f_{Ms} \frac{\partial}{\partial v_s}\left(\frac{f_s}{f_{Ms}}\right)\right\}$$

[Dif-Pradalier 2011, Estève 2015]

Magnitude

Velocity dependent diffusion coef. ~ v^{-3}

Maxwellian with space-time evolving N_{Ms}, U_{Ms} & T_{Ms} to conserve particles, momentum & energy

$$D_v = D_0 \frac{\Phi - G}{y_s}$$

$$\Phi(y_s) = \frac{2}{\sqrt{\pi}} \int_0^{y_s} e^{-z^2}\, dz$$

$$G(y_s) = \frac{\Phi - y_s \Phi'}{2 y_s^2}.$$

$$y_s = |v_s| / \sqrt{2 T_s}$$

- **Inter species coll.**

$$\mathcal{C}_{ss'}(f_s) = \nu^{\star}_{\mathrm{D0}} \left\{ \frac{C_{\mathcal{E}}^{ss'}}{n_s T_s}\left(\frac{(v_s - u_s)^2}{T_s} - 1\right) + \frac{C_{\Gamma}^{ss'}}{n_s T_s^{1/2}} \frac{v_s - u_s}{\sqrt{T_s}} \right\} F_{Ms}$$

$$C_{\mathcal{E}}^{ss'} = -3 n_s \frac{m_s}{m_s + m_{s'}} \nu_{ss'} \left(T_s - T_{s'}\right) - u_s C_{\Gamma}^{ss'}$$

$$C_{\Gamma}^{ss'} = -n_s m_s \nu_{ss'} \left(u_s - u_{s'}\right)$$

$\Rightarrow$ Simple fluid-like momentum & energy transfers

Focus on source/sink terms

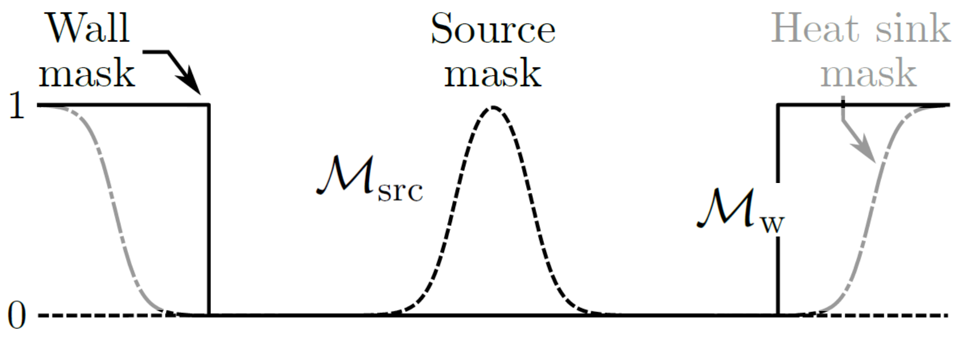
$$\partial_t f_a + \sqrt{A_a}\left(v_a \partial_x f_a - Z_a \partial_x \phi\ \partial_{v_a} f_a\right) = \mathcal{C}(f_a) + \mathcal{S}(f_a)$$

normalization to $\lambda_{D0}=(\varepsilon_0 T_0/e^2 n_0)^{1/2}$, $v_{T0s}=(T_0/m_s)^{1/2}$, $\omega_{p0s}= v_{T0s}/\lambda_{D0}$

❑ **Source** of **particles & heat** (convective) [Sarazin 2011]

$$\mathcal{S}_{\mathrm{src}}(f_s) = \frac{\mathcal{M}_{\mathrm{src}}(x)}{\int_0^{L_x} \mathcal{M}_{\mathrm{src}}(x)\,dx} \frac{s_{\mathrm{k}}}{\sqrt{2\pi T_{\mathrm{src}}/m_s}} \exp\left(-\frac{m_s v_s^2}{2T_{\mathrm{src}}}\right)$$

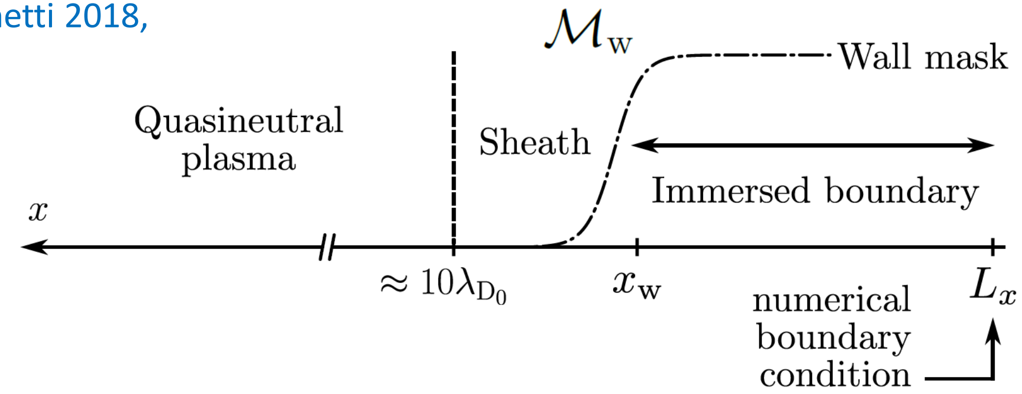
Spatial shape — Magnitude



❑ **Sink = immersed boundary** ("penalized wall") [Paredes 2014, Baschetti 2018, Dif-Pradalier 2022]

$$\mathcal{S}_{\mathrm{sink,n}}(f_s) = -\mathcal{M}_{\mathrm{w}} \nu_s (f_s - f_{\mathrm{w}s})$$

$$f_{\mathrm{w}s}(v) = \frac{n_{\mathrm{w}}}{\sqrt{2\pi T_{\mathrm{w}}/m_s}} \exp\left(-\frac{m_s v_s^2}{2T_{\mathrm{w}}}\right)$$ with $\mathbf{n_w \ll n_0}$

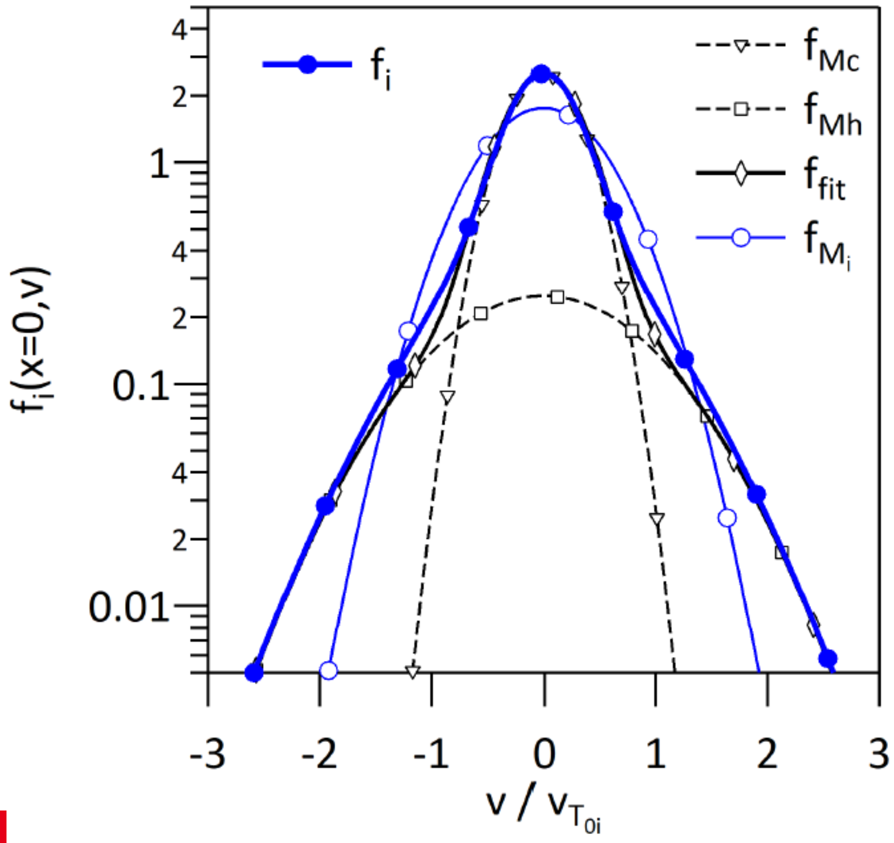


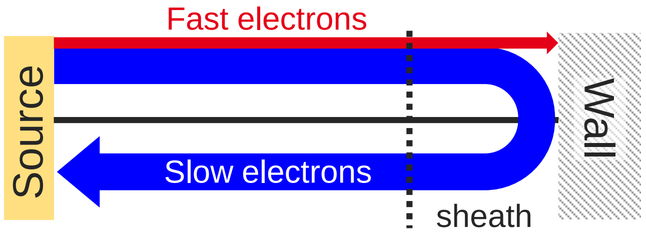
N.B.: $\mathcal{M}_{\mathrm{w}}$ does not precisely determine wall position x_{w}

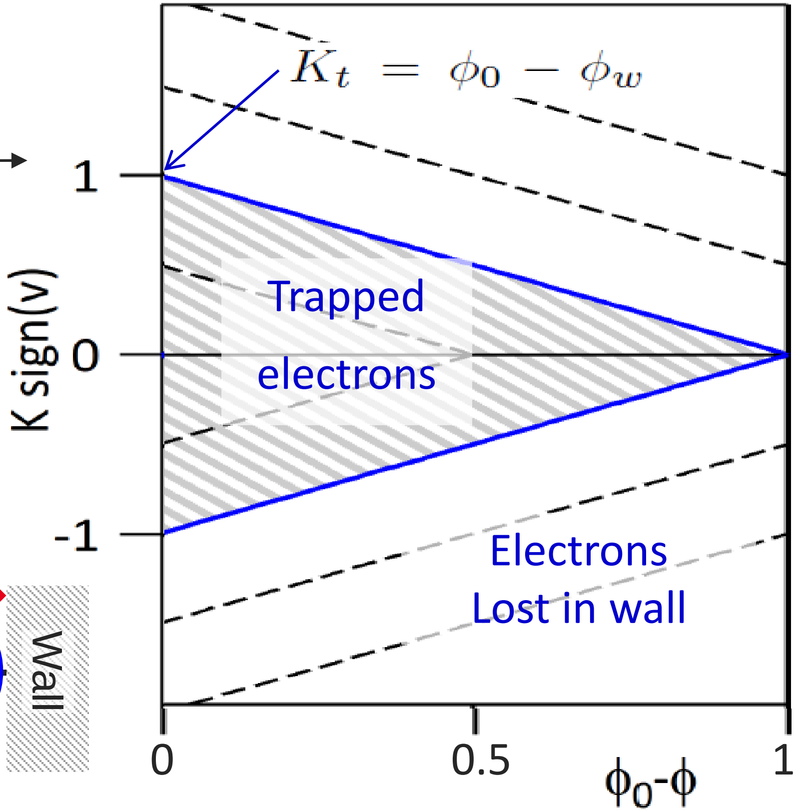
Collisions mandatory to reach steady-state

- Electron energy conservation at vanishing source & without collisions:

$$K = \frac{1}{2}v^2 = K_0 - (\phi_0 - \phi)$$







- Source continuously injects trapped electrons
- W/o coll., trapped/lost regions are decoupled

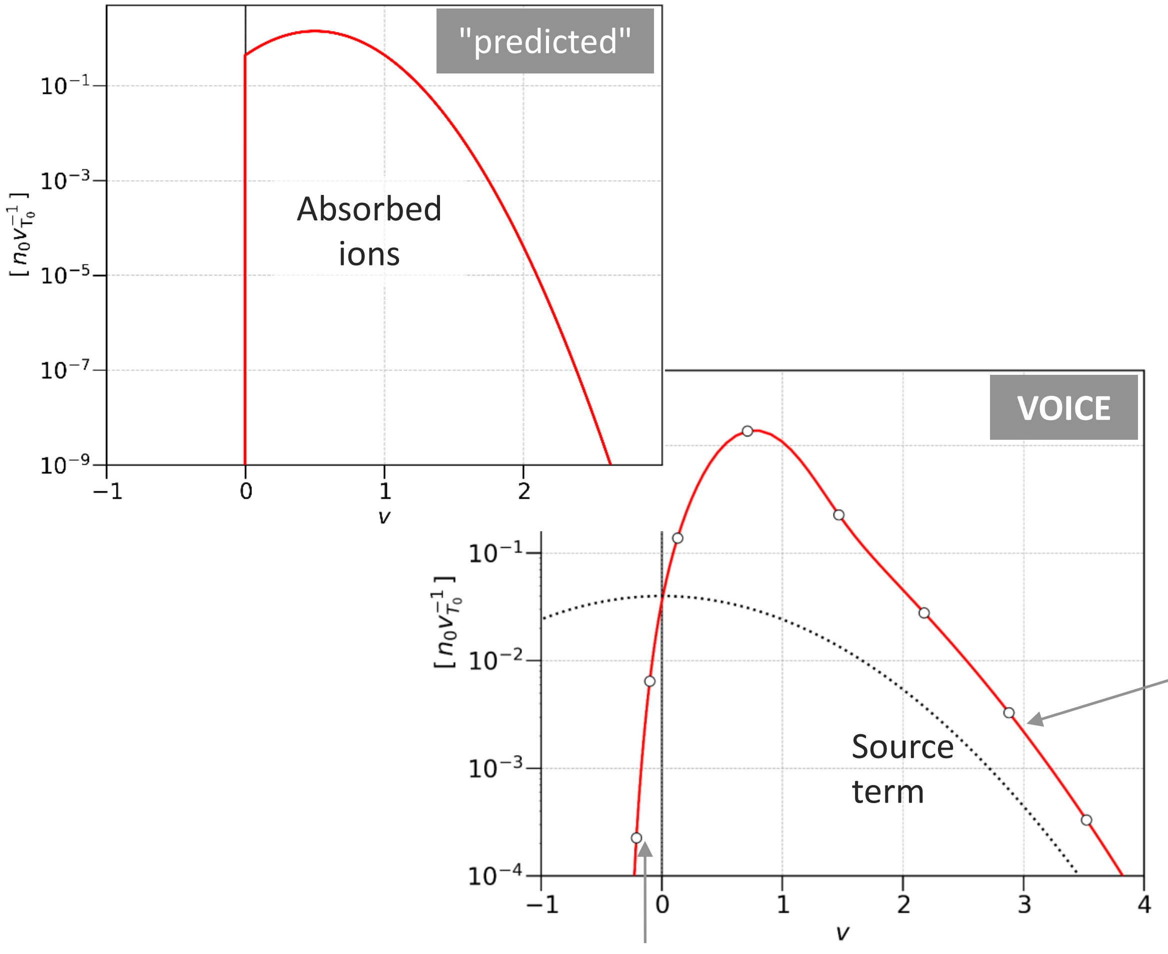
$\Rightarrow$ collisions mandatory

[Boyd 1951; Persson 1962]

Distribution functions @ sheath entrance ≠ truncated Maxwellians

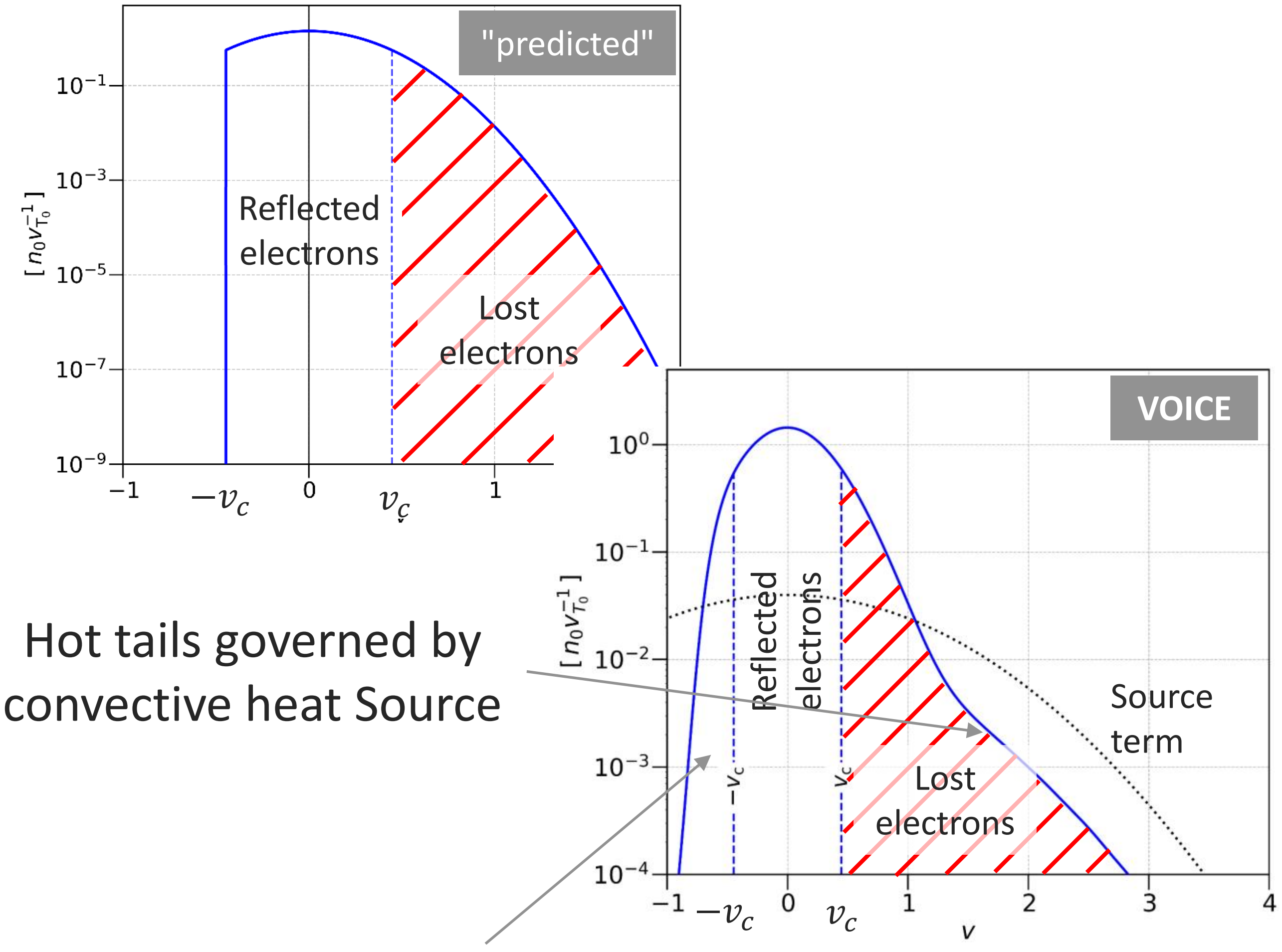
Plasma **self-organization** under the combined effects of **source**, **collisions** and **Debye sheath**

❑ **Ions:** "forbidden" region populated by collisions



Collisions

❑ **Electrons:** collisions + incomplete wall absorption



Hot tails governed by convective heat Source

Finite penalization strength + Collisions ("wall re-emission")

Recovery of potential drop & its expected dependencies

- **Potential drop in the sheath $\Delta\phi_{sh}$** governed by different electron-ion inertia

$$\Delta\phi_{\rm sh}^{\rm pred.} = \frac{T_{\rm e}^{\rm sh}}{e}\log\left(\frac{\Gamma_{\rm i}^{\rm sh}}{\Gamma_{\rm e}^{\rm sh+}}\right) = \frac{T_{\rm e}^{\rm sh}}{2e}\underbrace{\log\left(2\pi\frac{m_{\rm e}}{m_{\rm i}}M^2\left(1+\frac{T_{\rm i}^{\rm sh}}{T_{\rm e}^{\rm sh}}\right)\right)}_{2\Lambda \approx 2\times 3.8}$$

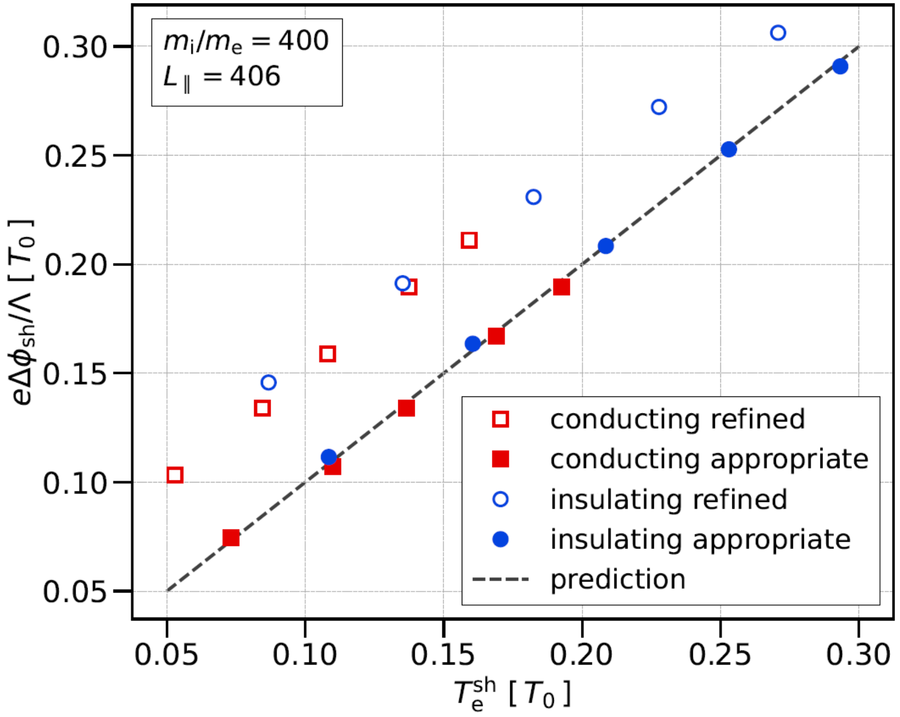
- **Recovered with VOICE** provided one accounts for "outgoing" electrons Γ_e^-

$$\Rightarrow \quad \Gamma_{\rm i}^{\rm sh} = \Gamma_{\rm e}^{+\rm pred.} - \Gamma_{\rm e}^{-}$$

With $\Gamma_{\rm e}^{+\rm pred.} = \int_{v_c}^{+\infty} dv\, v n_{\rm e}^{\rm sh}\sqrt{\frac{m_{\rm e}}{2\pi T_{\rm e}^{\rm sh}}}\, e^{-\frac{m_{\rm e}v^2}{2T_{\rm e}^{\rm sh}}}$

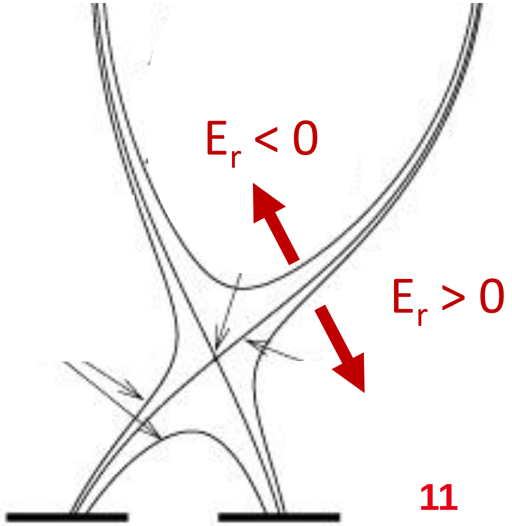
So that

$$\Delta\phi_{\rm sh}^{\rm pred,\,ref.} = \frac{T_{\rm e}^{\rm sh}}{e}\log\left(\sqrt{2\pi\frac{m_{\rm e}}{m_{\rm i}}M^2\left(1+\frac{T_{\rm i}^{\rm sh}}{T_{\rm e}^{\rm sh}}\right)}\left(1+\frac{\Gamma_{\rm e}^{-}}{\Gamma_{\rm i}^{\rm sh}}\right)\right)$$



- Important consequence for fusion plasmas:

Radial electric field positive in the Scrape-Off Layer (SOL) $E_r^{SOL} \approx -\frac{\Lambda}{e}\nabla_r T_e > 0$



Bohm criterion: depends on – not well defined – sound speed

- Fluid prediction for plasma-wall interaction:

Bohm criterion: $M = u_i/c_s \geq 1$ at sheath entrance

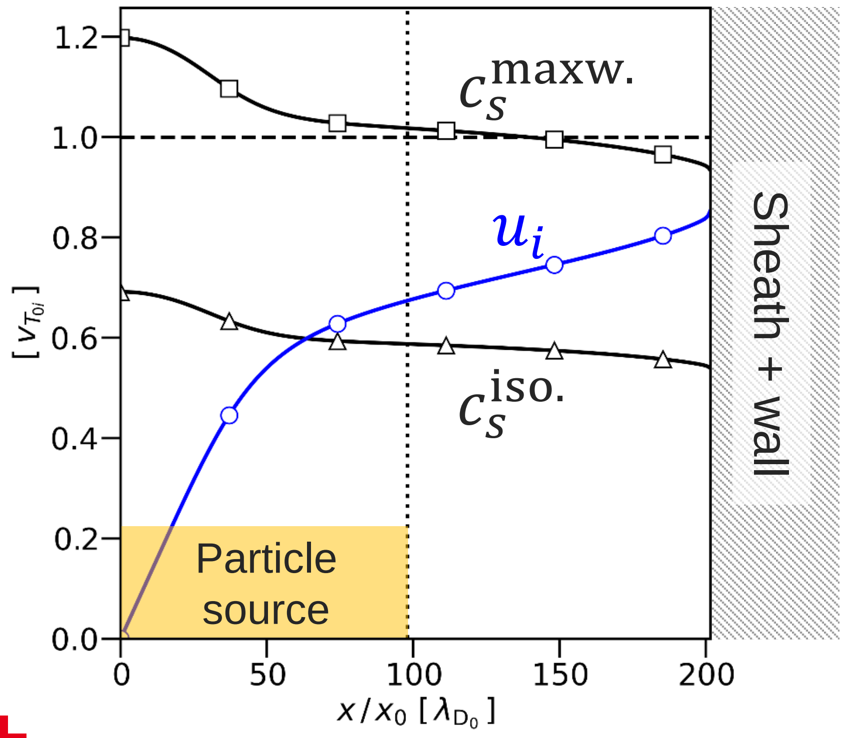
$\Rightarrow$ supersonic ion flow in Debye sheath

- Expression of c_s **depends on fluid closure**

From Fourier transform of fluid equations $\rightarrow$ dispersion relation for c_s

Closure	Isothermal	Maxwellian	Cold ions	Polytropic
Sound speed c_s	$\sqrt{\frac{T_i + T_e}{m_i}}$	$\sqrt{\frac{3(T_i + T_e)}{m_i}}$	$\sqrt{\frac{T_e}{m_i}}$	$\sqrt{\frac{\gamma_p (T_i + T_e)}{m_i}}$
Assumptions	$T_s = \text{cte.}$	$Q_s^{\text{heat}} = 0$	$T_i = 0$	$\frac{dp}{p} = \gamma_p \frac{dn}{n}$

$$Q_s^{heat} = \int_{-\infty}^{+\infty} dv \, \frac{1}{2} m_s (v - u_s)^3 f_s$$



- VOICE results: $Q_s^{\text{heat}} \neq 0$

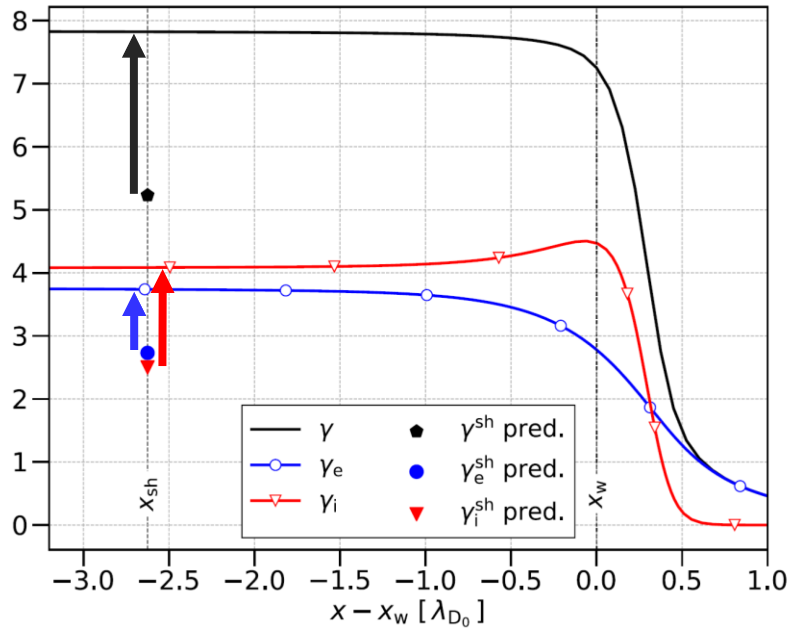
Bohm criterion M = ±1 is not operational to define Debye sheath entrance

Larger sheath *heat transmission factors* than predicted

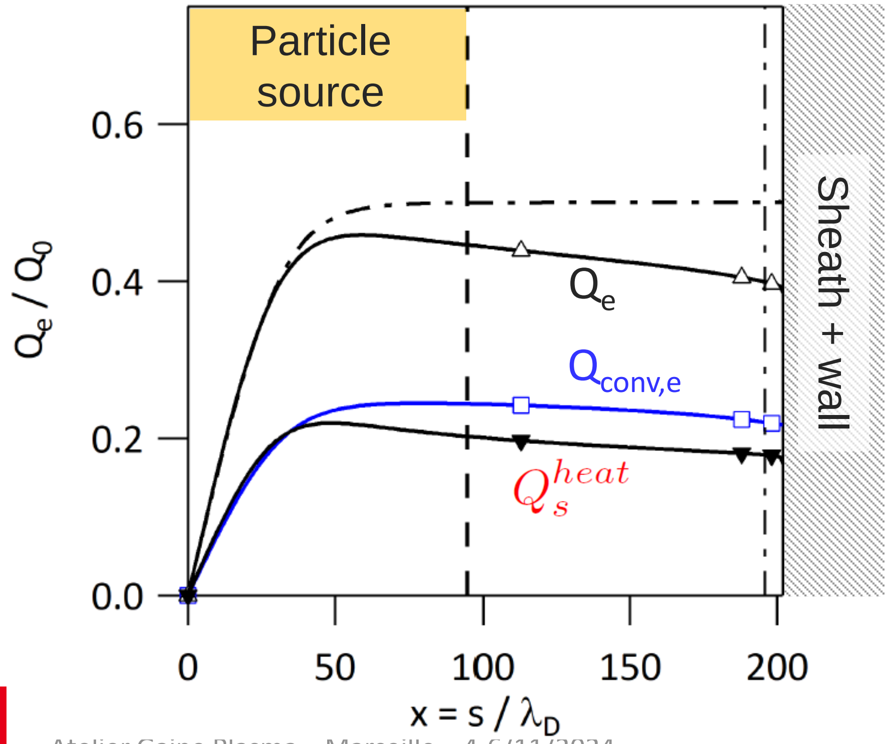
Total energy flux expressed as a function of convected flux:

$$Q_s = \gamma_s \Gamma_{sh} T_s$$

Heat transmission factor



- Fluid framework (Maxw. closure) → Prediction for γ_s
- **VOICE results: larger γ_i** (~60%) and **γ_e** (~35%)



- Kinetic results:
  - **Non vanishing heat flux** (not predicted in fluid)

$$Q_s = \underbrace{u_s \left(\frac{3}{2} n_s T_s + \frac{1}{2} m_s n_s u_s^2 \right)}_{Q_{conv,e}} + Q_s^{heat}$$

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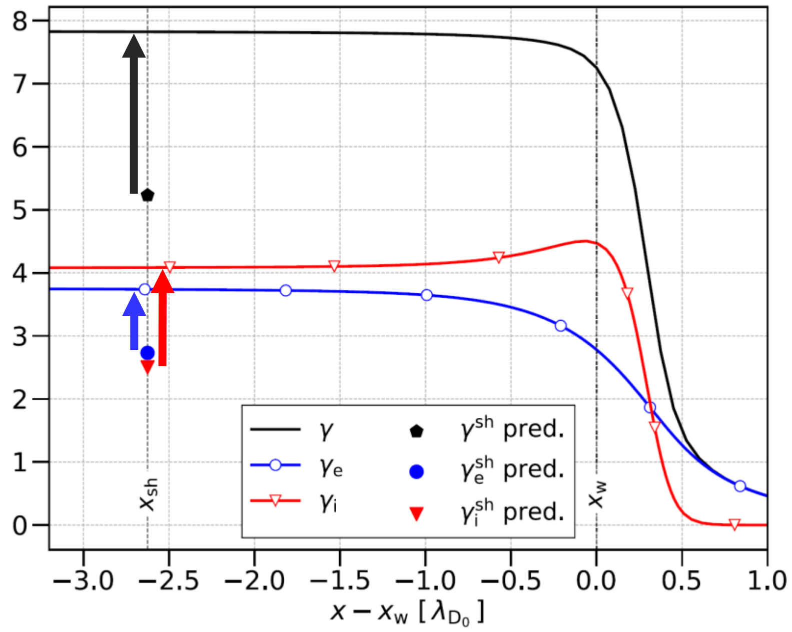

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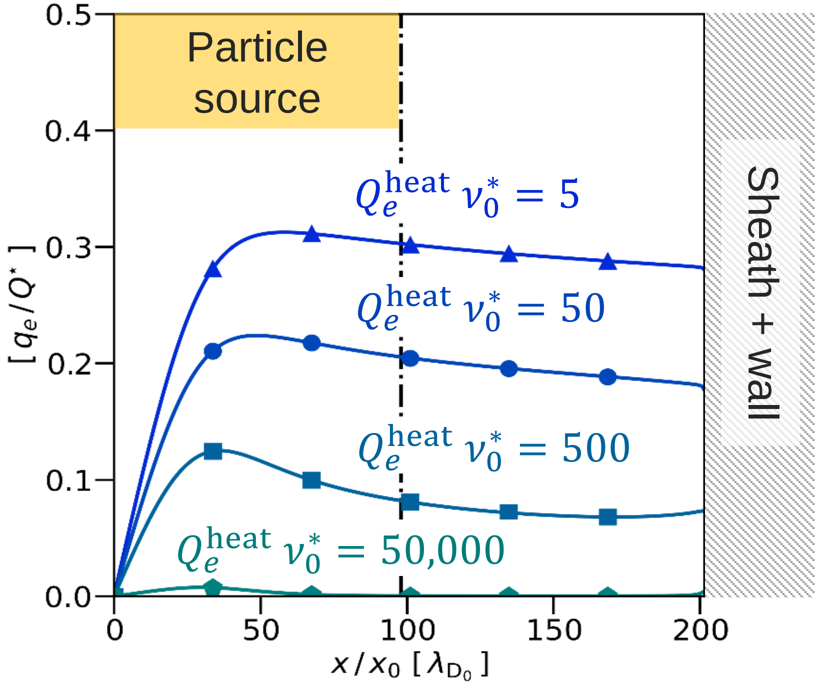

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  - Extremely slow convergence of Q_s^{heat} towards 0 when ν_0^* ↑

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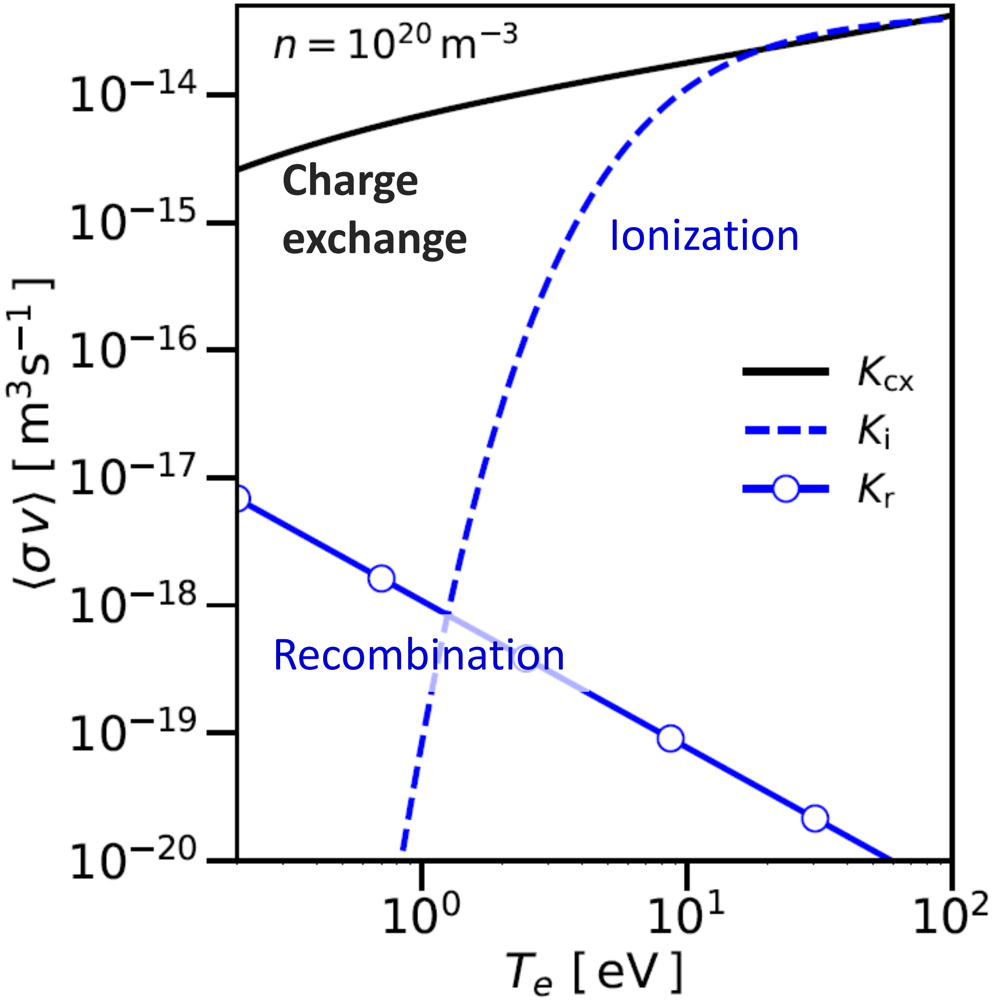
} Flux-driven, semi-Lagrangian

Accounting for a source of neutrals

Motivations

- Plasma-wall interaction: particles recycled by the wall as neutrals at a rate > 99% in W environment
- SOL turbulent dynamics mostly governed by convection
- Flux-driven GK simulations with kinetic electrons require a particle source

[ADAS Database; J. Blanco 2024]



Physics of the plasma-neutral interaction

- Considered reactions: **charge-exchange**, **ionization** & **recombination**
  - $\langle\sigma v\rangle_i$ strongly increases from 1 to 10eV $\Rightarrow$ threshold
  - $\langle\sigma v\rangle_r$ only relevant below T≈1eV
- Particle source/sink $\rightarrow \langle\sigma v\rangle_i$ & $\langle\sigma v\rangle_r$
- Momentum & Energy transfers $\rightarrow \langle\sigma v\rangle_{CX}$, $\langle\sigma v\rangle_i$ & $\langle\sigma v\rangle_r$

Neutrals modelled as a fluid → coupling to kinetic plasma species

- **Neutral-plasma coupling via source terms**
  - So far, source/sink restricted to particles (ioniz. + recomb.)
  - Constraint: ensure proper balance "1 neutral ↔ 1 ion + 1 electron"

- **General method: projection on Hermite (& Laguerre) polynomials** [Sarazin 2011]
  - $\mathcal{S}_{\mathrm{v}}(v_a) = \sum_{h=0}^{+\infty} c_h\, H_h\left(\frac{v_a}{\sqrt{2T_{\mathrm{sc}}}}\right) \mathrm{e}^{-\frac{v_a^2}{2T_{\mathrm{sc}}}}$ → Fluid moments related to c_h coefficients
  - Pure Sce of particles: $\mathcal{S}_{\mathrm{n}}(v_a) = c_0 \left(\frac{3}{2} - \frac{v_a^2}{2T_{\mathrm{sc}}}\right) e^{-\frac{v_a^2}{2T_{\mathrm{sc}}}}$ with $c_0 = \frac{S_{n,N}}{\sqrt{2\pi T_{\mathrm{sc}}}}$, $S_{n,N} = n_N n_e \langle\sigma v\rangle_{\mathrm{i}} - n_i n_e \langle\sigma v\rangle_{\mathrm{r}}$

$$\left(\int_{-\infty}^{+\infty} dv_a\, \mathcal{S}_{\mathrm{n}}(v_a) = \sqrt{2T_{\mathrm{sc}}} \sum_h \langle H_0, c_h H_h \rangle = \sqrt{2\pi T_{\mathrm{sc}}}\, c_0 = S_{n,N} \qquad \langle f, g \rangle = \int_{-\infty}^{+\infty} f(y) g(y) \mathrm{e}^{-y^2} dy \right)$$

- **Conservation equations:**

$$\left[\begin{array}{l} \frac{\mathrm{d}f_a}{\mathrm{d}t} = \mathcal{C}(f_a) + \mathcal{S}_{\mathrm{n}}(v_a) \\ \partial_t n_N + \nabla.\Gamma_N = -S_{n,N} \end{array} \right.$$

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Plasma-wall interaction in the GK framework: main issues

Debye sheath physics — GK physics

- Non-neutral plasma → violates usual GK assumption
- Strong parallel electric field on a few λ_D → subgrid w.r.t. typical scales $L_{//} \approx L_s/k_\theta \rho_s$

Main objectives / challenges

- Keep the plasma quasi-neutral ($k\lambda_D$<<1)
- Recover linear dependency of ϕ with T_e

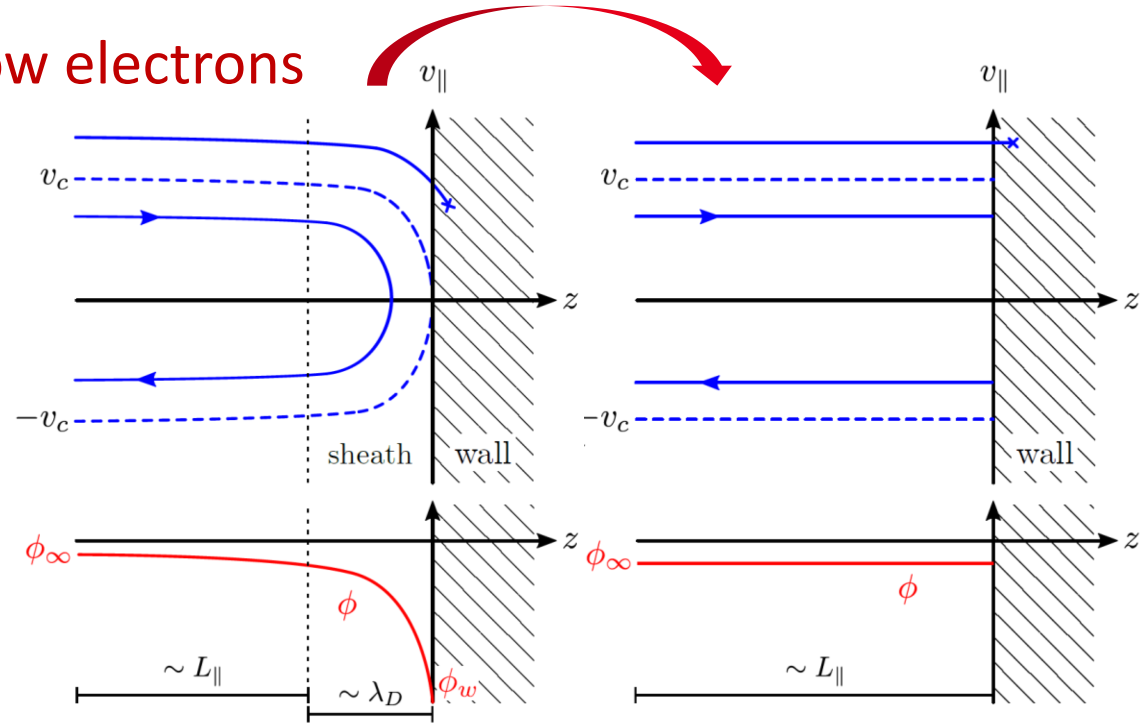
} OK with adiabatic electrons [Caschera 2018, Dif-Pradalier 2022]

- Ensure absorption of all ions & reflection of slow electrons

State-of-the-art

- *Logical* sheath
- *Conducting* sheath
- New model: *"flux-averaged sheath"*

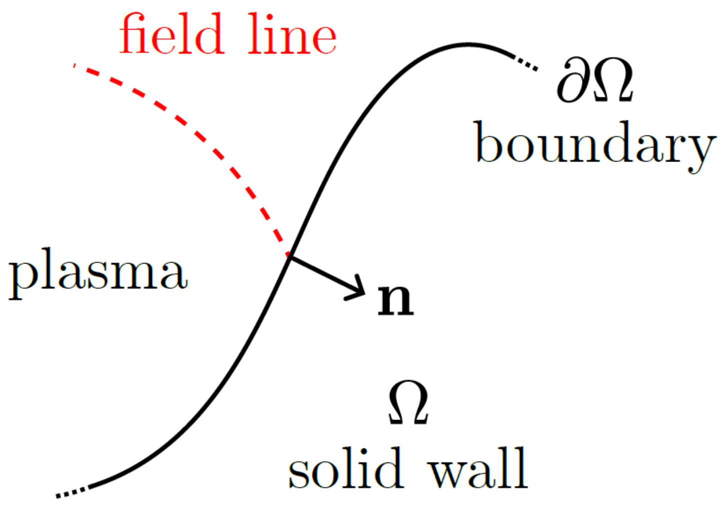
adapted to semi-Lagrangian full-f



Constraining the cut-off velocity $v_c = \sqrt{(2e\,\Delta\phi/m_e)}$ (I)

Electrons with $|v_{//}| \leq v_c$ are reflected back

$\rightarrow$ different strategies to estimate $v_c(\Delta\phi)$



- **Logical sheath** (initially developed for PIC codes): [Parker 1993]

  enforces **j=0 at each time/position on $\partial\Omega$**

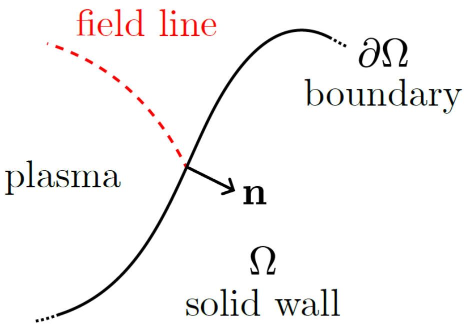
  - At each time, count the N_i ions crossing $\partial\Omega$
  - Remove the N_i fastest electrons $\rightarrow$ v_c is the velocity of the fastest reflected electron

- **Conducting sheath**: allows for **finite local currents on $\partial\Omega$** [Shi 2015]
  - GK quasi-neutrality $\nabla_\perp^2\phi = \rho$ $\rightarrow$ ϕ at any position on $\partial\Omega$
  - $v_c = \sqrt{(2e\,\Delta\phi/m_e)}$ defines the velocity of the slowest absorbed electron

Constraining the cut-off velocity $v_c = \sqrt{(2e\,\Delta\phi/m_e)}$ (II)

Electrons with $|v_{//}| \leq v_c$ are reflected back

$\rightarrow$ different strategies to estimate $v_c(\Delta\phi)$



- **"Flux-averaged sheath"**: [Munschy 2024 c]
  - Enforces *vanishing current* ***on average*** *over ∂Ω* → allows for **finite local currents**
  - v_c implicitly defined by $\left\langle \Gamma_i^{\partial\Omega}(\mathbf{x},t)\right\rangle_{\partial\Omega} = \left\langle \bar{\Gamma}_e^{\partial\Omega}(\mathbf{x},v_c,t)\right\rangle_{\partial\Omega}$

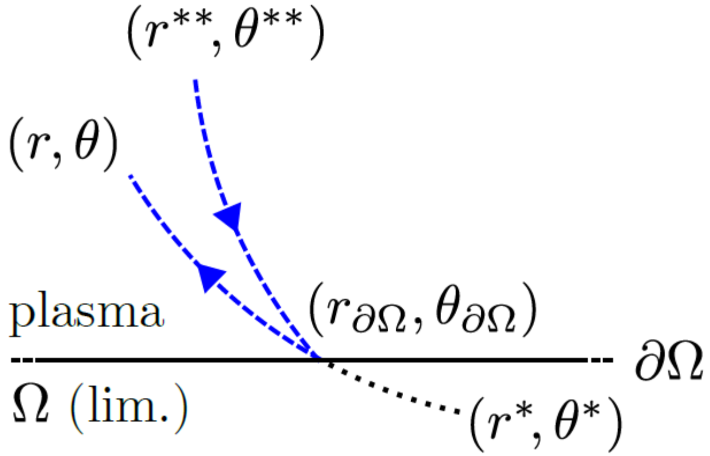
$\Updownarrow$

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

with $\mathbf{b}^*_\parallel \approx \mathbf{B}/B$, $\quad \mathbf{v}_E \approx \dfrac{\mathbf{E}\times\mathbf{B}}{B^2}$, $\quad \mathbf{v}_D \approx \dfrac{m_s v_\parallel^2 + \mu B}{e_s B}\dfrac{\mathbf{B}\times\nabla B}{B^2}$

  - All crossing ions are absorbed (penalization)
  - Slow electrons are reflected back into the plasma

    N.B.: additional complexity arising from backward semi-Lagrangian scheme

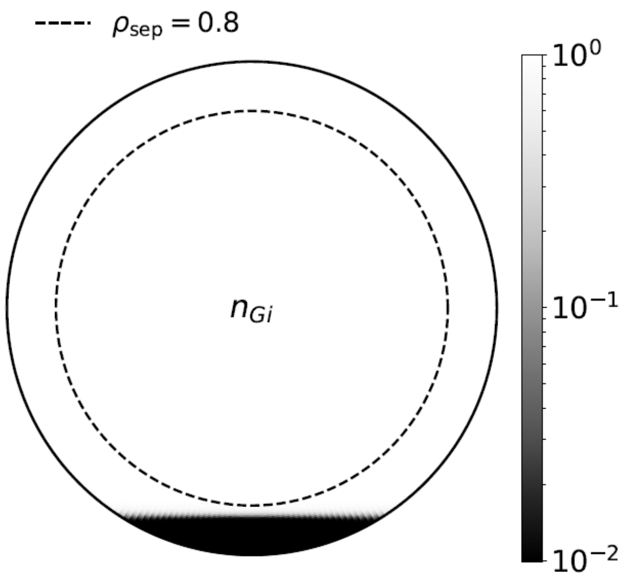


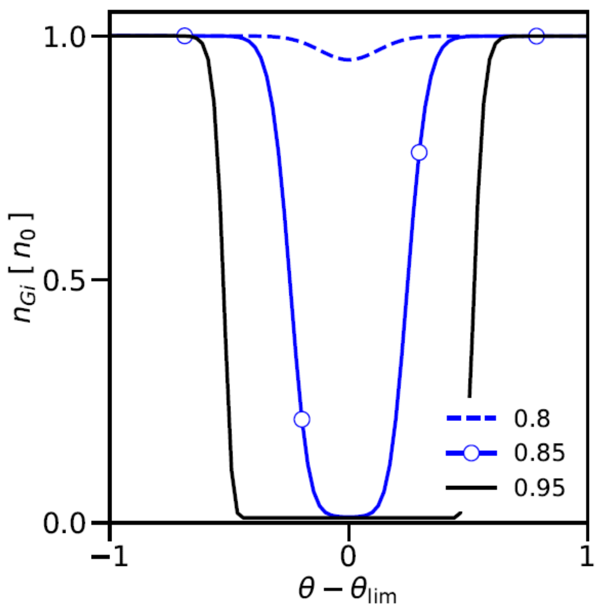
Plasma-wall boundary: ions absorbed & electrons reflected

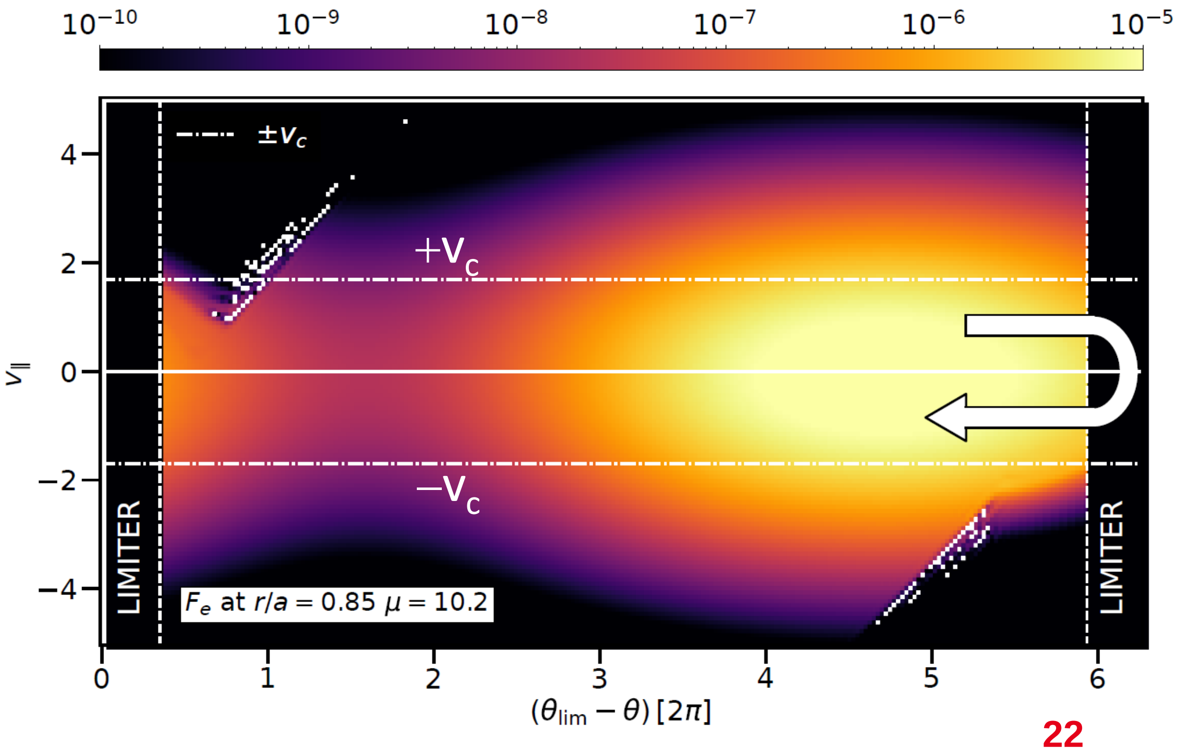
Simulations w/o quasi-neutrality → successful check of ion & electron dynamics

- **Ions absorbed within the limiter**
  via penalization → **mask M_{lim}**
  $dF_i/dt = \ldots - \nu\,(F_i - F_{lim})\,M_{lim}$

- **Electrons reflected back at the cut-off velocity v_c**
  Depletion front propagates along θ away from limiter / into the plasma







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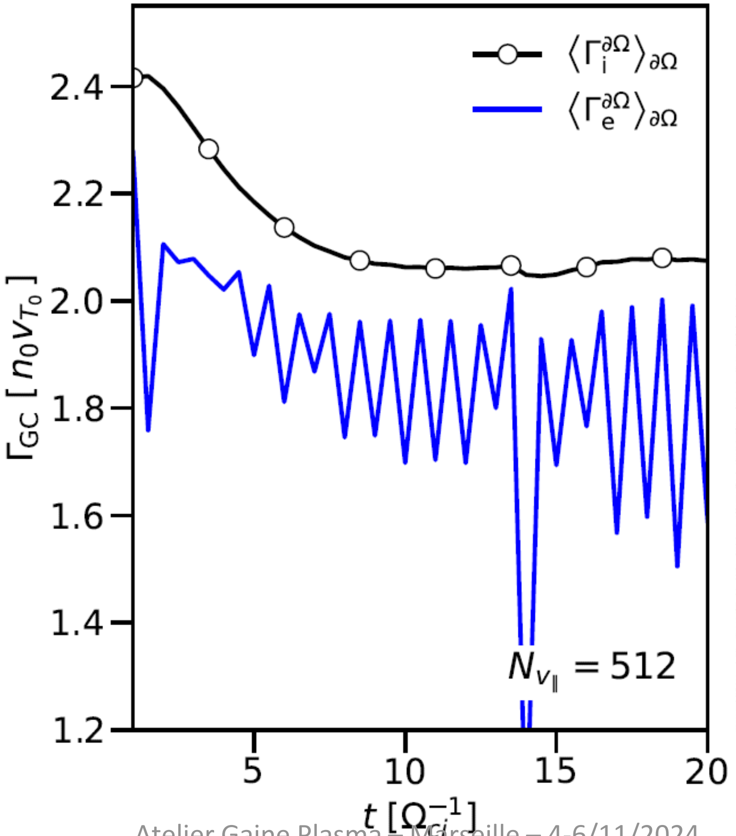
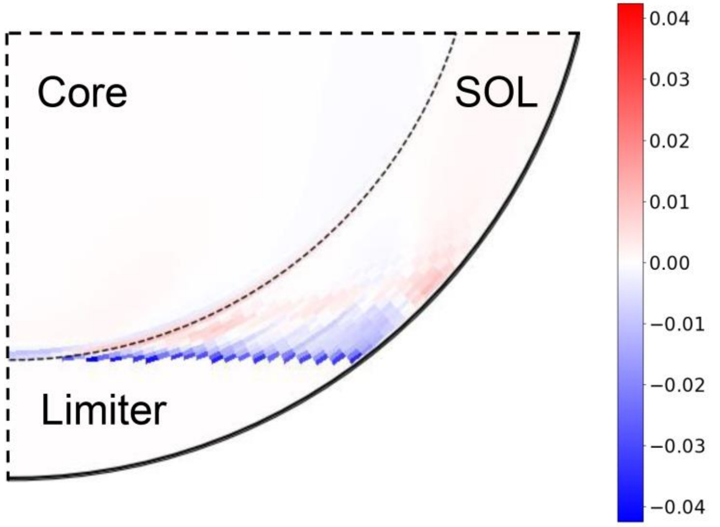


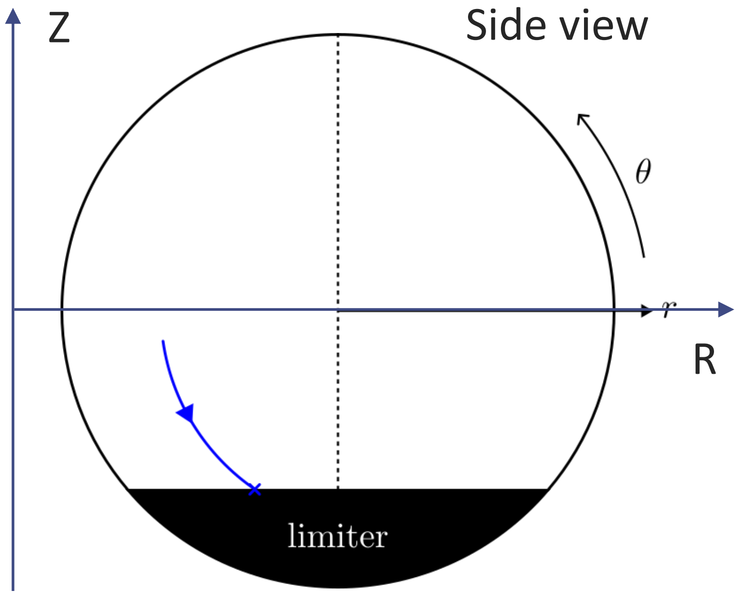


- **Electrons reflected back at the cut-off velocity v_c**
  Depletion front propagates along θ away from limiter / into the plasma

- **Current issue with QN:**
  Charge density build-up close to limiter due to imbalance between ion & electron particle fluxes

Thin toroidal limiter = "simple" alternative Boundary Condition

Axisymmetric limiter



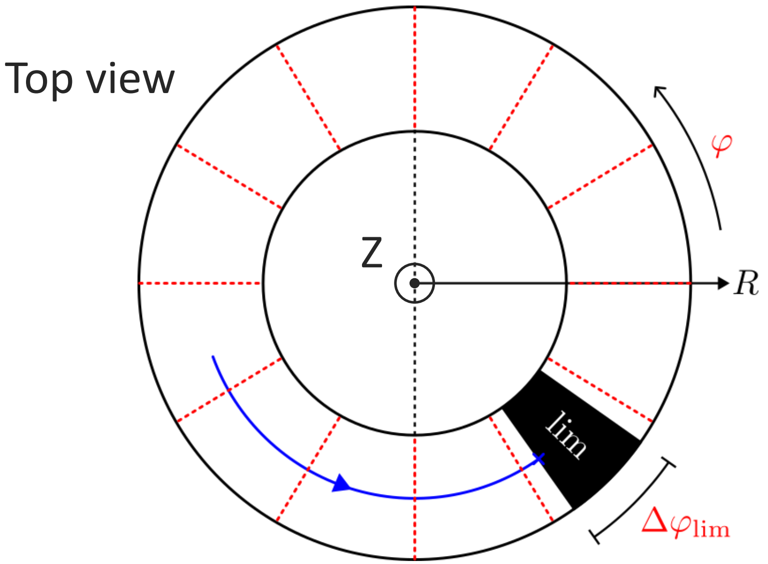
Particles intercept **axisymmetric** limiter during (r,θ) advection

$\Rightarrow$ immersed in Vlasov **and** Quasi-Neutrality

Strang splitting
$\rightarrow$ separate advections in (r,θ) and φ

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

Thin limiter located in between two toroidal mesh points

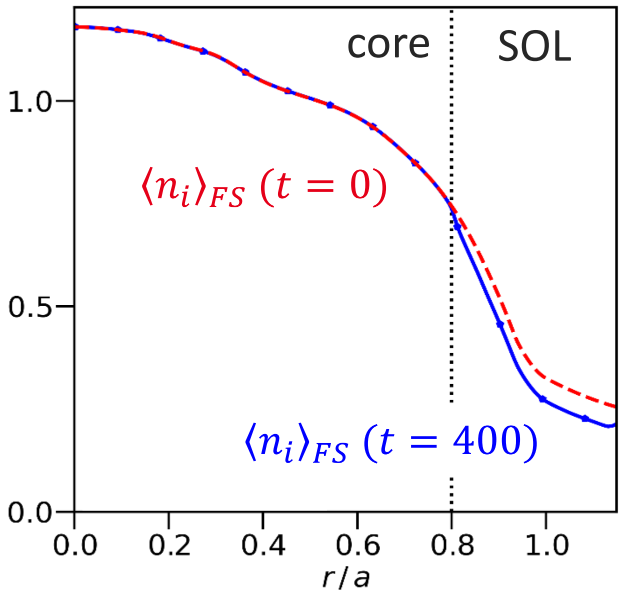


Particles intercept **thin** limiter during φ advection

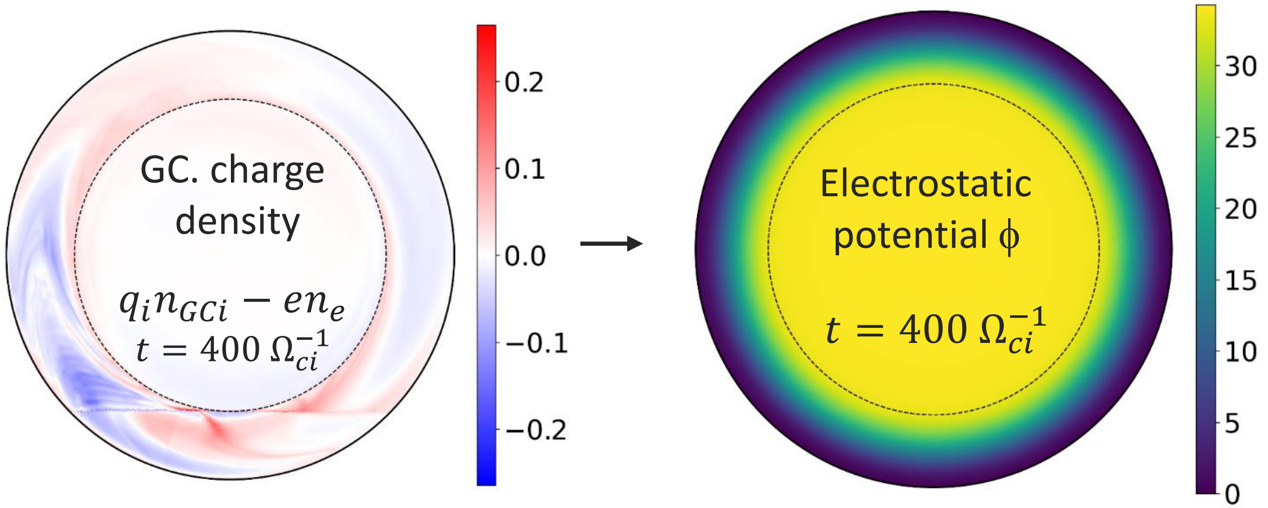
$\Rightarrow$ immersed in **Vlasov only** (not in Quasi-Neutrality)

Thin toroidal limiter → depletion of SOL density at early times

- Thin limiter → longer (~ ×10) simulations w.r.t. axi-symmetric limiter



- Large charge density at early times: $\phi \approx \langle \phi \rangle_{FS} \gg 1$ in simulation
  $\Rightarrow$ Necessity to modify quasi-neutrality & radial Boundary Condition



Dirichlet radial Boundary Condition:

$\phi(r=r_{max}) = 0$

↓

Translates into $v_c = 0$

$\Rightarrow$ no electron reflected

Conclusions

- **Kinetic Debye sheath (VOICE)**
  - Immersed boundaries (penalization) OK to recover main physics
  - Collisions mandatory $\rightarrow$ allow for steady-state – non "ideal" distribution functions
  - C_s loosely defined $\Rightarrow$ Bohm criterion not operational ($\rightarrow$ Debye sheath where ρ shoots-up)
  - Kinetic self-organization $\rightarrow$ finite ion & electron heat fluxes $\Rightarrow$ large sheath heat transmission factors

- **Neutrals as a fluid (VOICE $\rightarrow$ Gysela-X)**
  - Fluid model successfully coupled to kinetic plasma
  - Next steps: Add momentum & energy exchanges
    Account for recycling coefficients (> 99% for particles in W environment) $\rightarrow S_{n,N} \propto \Gamma_i^{\partial\Omega}$
    From 1D to 3D $\rightarrow$ implement in Gysela-X

- **Consistent plasma-wall interplay within Gyro-Kinetic description (GYSELA)**
  - Subgrid modelling of Debye sheath is challenging
  - Absorption of ions & reflection of slow electrons OK in GYSELA
  - New "Flux-averaged sheath" model – current issue (flux imbalance) under investigation
  - Promising alternative: toroidally localized limiter $\rightarrow$ requires adjustments

Associated publications

VOICE results

E. Bourne et al., *Non-uniform splines for semi-Lagrangian kinetic simulations of the plasma sheath*
J. Comput. Phys. 488 (2023) 112229

Y. Munschy (a) et al., *Kinetic plasma-wall interaction using immersed boundary conditions*
Nucl. Fusion 64 (2024) 056027

Y. Munschy (b) et al., *Kinetic plasma-sheath self-organization*
Nucl. Fusion 64 (2024) 046013

GYSELA results

E. Caschera et al., *Immersed boundary conditions in global, flux-driven, gyrokinetic simulations*
J. Phys. Conf. Series 1125 (2018) 012006

G. Dif-Pradalier et al., *Transport barrier onset and edge turbulence shortfall in fusion plasmas*
Commun. Phys. 5 (2022) 259

Y. Munschy (c), *Kinetic and Gyrokinetic physics of plasma-wall interaction in tokamaks*
PhD thesis, Aix-Marseille Univ. (2024)