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Gyrokinetic simulations with GYSELA: Main current issues in physics & numerics

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- Fusion plasmas weakly collisional (ITER:  $v^* \sim n/T^2 \sim 10^{-3} \sim qR/\lambda_{lpm}$ )
  - F can depart from a Maxwellian  $\Rightarrow$  kinetic description mandatory
- Gyro-freq.  $d\phi_c/dt \sim 10^8 >>$  Turb. freq.  $\sim 10^5 \rightarrow \phi_c$  can be safely "averaged out"
  - $\Rightarrow$  phase-space reduction: 6D F(**x**,v<sub>//</sub>,µ, $\phi_c$ ,t)  $\rightarrow$



4D+1D 
$$F_G(\mathbf{x}_G, \mathbf{v}_{//}, \mu, t)$$
  
Adiabatic invariant  
 $\mu = m v_{\perp}^2 / 2B$ 

[Frieman-Chen, 1982, Littlejohn, 1983; Brizard-Hahm, 2007]

Maxwell's eqs. on F  $\Rightarrow$  requires relation F $\leftrightarrow$ F<sub>G</sub>  $\Rightarrow$  polarization density: n = n<sub>G</sub> + n<sub>pol</sub>



IRfm

[Grandgirard, CPC 2016]

#### Self-consistently coupled Gyrokinetic & Quasi-Neutral eqs:

$$dF_{Gs}/dt = S + C(F_{Gs}) + D_{BC}$$
  
4D advection Source Collisions Boundary Conditions  
$$L(\phi) = \sum_{s} \int d\mathbf{v} J_{s} \cdot F_{Gs}$$

 $\begin{array}{|c|c|c|} \hline \mbox{Peculiarities:} & \mbox{global} & \rightarrow \mbox{ boundary conditions} \\ \hline \mbox{full-F} & \rightarrow \mbox{ multi-scale physics} \\ \hline \mbox{flux-driven} & \rightarrow \mbox{ steady-state on } \tau_{\rm E} \end{array}$ 



Backward semi-Lagrangian scheme: Trajectories (F<sub>G</sub>=Cst) followed backwards on fixed grid (weak noise, moderate dissip.)







Physics upgrades  $\rightarrow$  numerical challenges  $\rightarrow$  present solutions & issues

- Boundary conditions: core (r=0) & scrape-off layer
- Kinetic electrons: Field aligned method & open issues
- Small scale physics: gyro-average operator & boundary issue
- Neoclassical transport: collision operator & parallelization issue

#### **Removing Inner Boundary Condition:** r = 0



#### Issue at r=0: divergence of metric (1/r) + too many $\theta$ points

Previously:  $r_{min} > 0 \rightarrow |$  Dirichlet for  $\phi_{mn}$ Neumann for  $\phi_{00}$ 

Upgrade:

Poisson (trick):  $r_{min} = \Delta r/2 \Rightarrow$  no BC required in r

Vlasov: bilinear interpolation in 0<r<r<sub>min</sub>





0.8

n

-0.2

0.2

Zoon on poloidal cut (f - f\_init) [ at nu=0.05, vpar=3.1 vth, phi=0

0

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0.2

0

0.0001

-0.0001

-0.0002 -0.0003 -0.0004

Я

#### Towards Scrape-Off Layer physics r>a

# Coupling core (r/a<1) – SOL (r/a>1) is important: H-mode, impurities & neutrals

Critical challenges:

close/open magnetic surfaces (periodicity; plasmasurface interaction) relative fluctuation levels

particle sources/sinks



Possible alternatives: penalization and/or transition towards fluid description?

#### Kinetic electrons & spurious ω<sub>H</sub> modes

- Kinetic electrons mandatory: particle transport + trapped electron modes
- Electrostatic limit  $\rightarrow$  spurious " $\omega_{H}$ " modes:  $\omega_{H} / \omega_{ci} = (k_{//} / k_{\perp}) (m_{i} / m_{e})^{1/2}$ [Lee 1987]
  - Correspond to hydro-dynamical limit ( $\omega >> k_{//} v_{th}$ ) of ITG disp. rel.
  - Also: electrostatic limit ( $\beta=0$ ) of kinetic Alfvén wave

$$\omega_{KAW}^2 = k_{\parallel}^2 v_A^2 \; \frac{1 + k_{\perp}^2 \rho_i^2}{1 + k_{\perp}^2 d_e^2} = \frac{k_{\parallel}^2 \rho_i^2 \; \omega_{ci}^2}{k_{\perp}^2 \rho_i^2 (m_e/m_i) + \beta/2} \; (1 + k_{\perp}^2 \rho_i^2)$$
[Scott 1997]

 $\Rightarrow$  Should disappear in electromagnetics (for  $\beta > (k_{\perp}\rho_i)^2 m_e/m_i \sim 2.10^{-5})$ 

Trick: disappear when filtering out  $(m \neq 0, n=0)$  modes in QN eq.

[Idomura 2016]



IPL FRATRES, Strasbourg, November 16-18, 2016

[Ehrlacher 2016]

#### Kinetic electrons & Field-aligned method



- Kinetic electrons mandatory: particle transport + trapped electron modes
- Numerical issues  $v_{the} \sim (m_i/m_e)^{1/2} \times v_{thi} \sim 10^8 \text{m.s}^{-1} \Rightarrow \text{time step / } (m_i/m_e)^{1/2}$  $\rho_e \sim \rho_i/(m_i/m_e)^{1/2} \sim \rho_i/60 \sim 50 \mu \text{m} \Rightarrow \text{nb grid points} \times (m_i/m_e)^{3/2}$ 
  - Reducing numerical cost:
    - filtering passing electrons (adiabatic)  $\rightarrow$  artificially large (m<sub>e</sub>/m<sub>i</sub>) ~OK [Bottino 2016]
    - Using field-aligned method

<sup>[</sup>Ottaviani 2011; Hariri 2013]



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 $<sup>\</sup>rightarrow$  nb grid points  $\times (m_i/m_e)$  only



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 $\rightarrow$  nb grid points ×(m<sub>i</sub>/m<sub>e</sub>) only



[Ottaviani 2011; Hariri 2013]

- Optimized parallelization: memory OK, time+30%
- Less toroidal points:
   ~ Ν<sub>ω</sub> / 8

## Kinetic electrons & Field-aligned method



- Kinetic electrons mandatory: particle transport + trapped electron modes
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  - Reducing numerical cost:

Log  $|FT\{\phi(\theta,\phi)\}|$ 

- filtering passing electrons (adiabatic)  $\rightarrow$  artificially large (m<sub>e</sub>/m<sub>i</sub>) ~OK [Bottino 2016]
- Using field-aligned method



[Ottaviani 2011; Hariri 2013]

- t=6000 t=7000 -1.6 -2.4 -3.2 n n -4.0  $000.0/\omega_c$  $00.0/\omega_c$ -10 -10 0.09  $\bar{\mathsf{m}}^{100}$  $\overline{\mathsf{m}}^{100}$ 0.4 0.06 Aliasing Spurious 0.2 0.03  $\Rightarrow OK$ 0.00 0.0  $\rightarrow$  origin? -0.03 -0.2 -0.06 -0.4 -0.09 -0.6 IPL FRATRES, \$ 0.12
  - Optimized parallelization: memory OK, time+30%
  - Less toroidal points: ~ N<sub>\oppi</sub> / 8
  - Spurious modes: under investigation



- Kinetic electrons mandatory: particle transport + trapped electron modes
- Numerical issues  $v_{the} \sim (m_i/m_e)^{1/2} \times v_{thi} \sim 10^8 \text{m.s}^{-1} \Rightarrow \text{time step } / (m_i/m_e)^{1/2}$  $\rho_e \sim \rho_i / (m_i/m_e)^{1/2} \sim \rho_i / 60 \sim 50 \mu \text{m} \Rightarrow \text{nb grid points} \times (m_i/m_e)^{3/2}$ 
  - Reducing numerical cost:
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    - Using field-aligned method



- Optimized parallelization: memory OK, time+30%
- Less toroidal points: 0.12 ~ N<sub>0</sub> / 8 0.09 0.06

 $\rightarrow$  nb grid points  $\times (m_i/m_p)$  only

0.00

-0.06

-0.09

-0.12

- 0.03 Spurious modes: under investigation -0.03
  - $\Rightarrow$  OK when filtered out

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<sup>[</sup>Ottaviani 2011; Hariri 2013]

#### Small scales & gyro-average operator





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#### Collisions: physical & numerical issues

- Critical for: flow damping: friction on trapped particles, Zonal Flow damping impurity transport (synergy turbulent-neoclassical) [Estève 2016] momentum & energy exchanges between species
- Constraints: Boltzmann H-theorem (entropy production, equil.=Maxwellian)
   [Hirshman-Sigmar 1977; Helander-Sigmar 2005]
   Neoclassical transport = collisions
  - Collisions break down  $\mu$ -invariance  $\rightarrow$  parallelization issue

$$C_{a}(F_{a}) = \sum_{b} \left[ \frac{T_{b} - T_{a}}{T_{a}} \frac{m_{a}v^{2}}{2T_{a}} \nu_{E,ab} - \nu_{s,ab}(v) \frac{m_{a}}{T_{a}} v_{\parallel} \left( U_{\parallel d,a} - U_{\parallel ba} \right) \right] F_{M0a} + C_{v,ab}(F_{a}) + C_{d,ab}(F_{a})$$
  
**v**-motion
  
(radial & deflection)

- Conservation properties OK (on  $\tau_{coll.}$ ):  $\frac{\Delta n}{n} \simeq 10^{-5} \quad \frac{\Delta p_{\parallel}}{p_{\parallel}} \simeq 10^{-5} \quad \frac{\Delta E}{E} \simeq 10^{-4}$
- Neoclassical results under investigation

[Donnel 2016] **Projection on Laguerre polynomials in**  $u = \frac{\mu B}{T}$   $F(\mathbf{r}, v_{\parallel}, u, t) = F_{M0a} \sum_{l} \alpha_{\ell}(\mathbf{r}, v_{\parallel}, t) P_{\ell}(u)$  $\Rightarrow$  replace differential operators by integrals

[Garbet 2009: Dif Predalier 2011:

Estève 20



# Collisions: physical & numerical issues

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[Garbet 2009: Dif Pradalier 2011:





#### Intricate upgrades of physics & numerical methods / parallelization

- **Boundary Conditions**": towards a model for the SOL  $\rightarrow$  gyro-fluid?
- Fully kinetic electrons (trapped & passing) still out of reach on present HPC Electromagnetics cure electrostatic artifacts Trapped kinetic + heavy electrons
- Multi-scale physics requires accurate gyro-average operator
- Collisions mandatory BUT: complex (linearized) operator + parallelization issue!





# **Back-up slides**

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[Donnel 2016]

$$\begin{split} C_{a}\left(F_{a}\right) &= \sum_{b} \left[ \frac{T_{b} - T_{a}}{T_{a}} \frac{m_{a}v^{2}}{2T_{a}} \nu_{E,ab} - \nu_{s,ab}(v) \frac{m_{a}}{T_{a}} v_{\parallel} \left(U_{\parallel d,a} - U_{\parallel ba}\right) \right] F_{M0a} + C_{v,ab}(F_{a}) + C_{d,ab}(F_{a}) \\ & \text{Energy exchange} & \text{Momentum exchange} \\ \hline C_{v,ab}\left(F_{a}\right) &= \frac{1}{2B_{\parallel}^{*}v_{\perp}} \frac{\partial}{\partial v_{\perp}} \left[ B_{\parallel}^{*}F_{M0a}\nu_{v,ab}v_{\perp}^{2} \left( v_{\perp} \frac{\partial g_{a}}{\partial v_{\perp}} + v_{\parallel} \frac{\partial g_{a}}{\partial v_{\parallel}} \right) \right] \\ & + \frac{1}{2B_{\parallel}^{*}} \frac{\partial}{\partial v_{\parallel}} \left[ B_{\parallel}^{*}F_{M0a}\nu_{v,ab}v_{\parallel} \left( v_{\perp} \frac{\partial g_{a}}{\partial v_{\perp}} + v_{\parallel} \frac{\partial g_{a}}{\partial v_{\parallel}} \right) \right] \\ & C_{d,ab}\left(F_{a}\right) &= \frac{1}{2B_{\parallel}^{*}v_{\perp}} \frac{\partial}{\partial v_{\perp}} \left[ B_{\parallel}^{*}F_{M0a}\nu_{d,ab}v_{\perp}v_{\parallel} \left( v_{\parallel} \frac{\partial g_{a}}{\partial v_{\perp}} - v_{\perp} \frac{\partial g_{a}}{\partial v_{\parallel}} \right) \right] \\ & + \frac{1}{2B_{\parallel}^{*}} \frac{\partial}{\partial v_{\parallel}} \left[ B_{\parallel}^{*}F_{M0a}\nu_{d,ab}v_{\perp}v_{\parallel} \left( - v_{\parallel} \frac{\partial g_{a}}{\partial v_{\perp}} + v_{\perp} \frac{\partial g_{a}}{\partial v_{\parallel}} \right) \right] \\ & + \frac{1}{2B_{\parallel}^{*}} \frac{\partial}{\partial v_{\parallel}} \left[ B_{\parallel}^{*}F_{M0a}\nu_{d,ab}v_{\perp}v_{\parallel} \left( - v_{\parallel} \frac{\partial g_{a}}{\partial v_{\perp}} + v_{\perp} \frac{\partial g_{a}}{\partial v_{\parallel}} \right) \right] \\ & \left\langle \dots \right\rangle_{a} = \int d^{3}v \frac{F_{M0a}}{n_{a}} \dots \\ \end{split}$$

- These terms are treated by projection on Laguerre polynomials, using a Crank-Nicolson scheme
- All the other terms are treated via finite differences with an explicit scheme