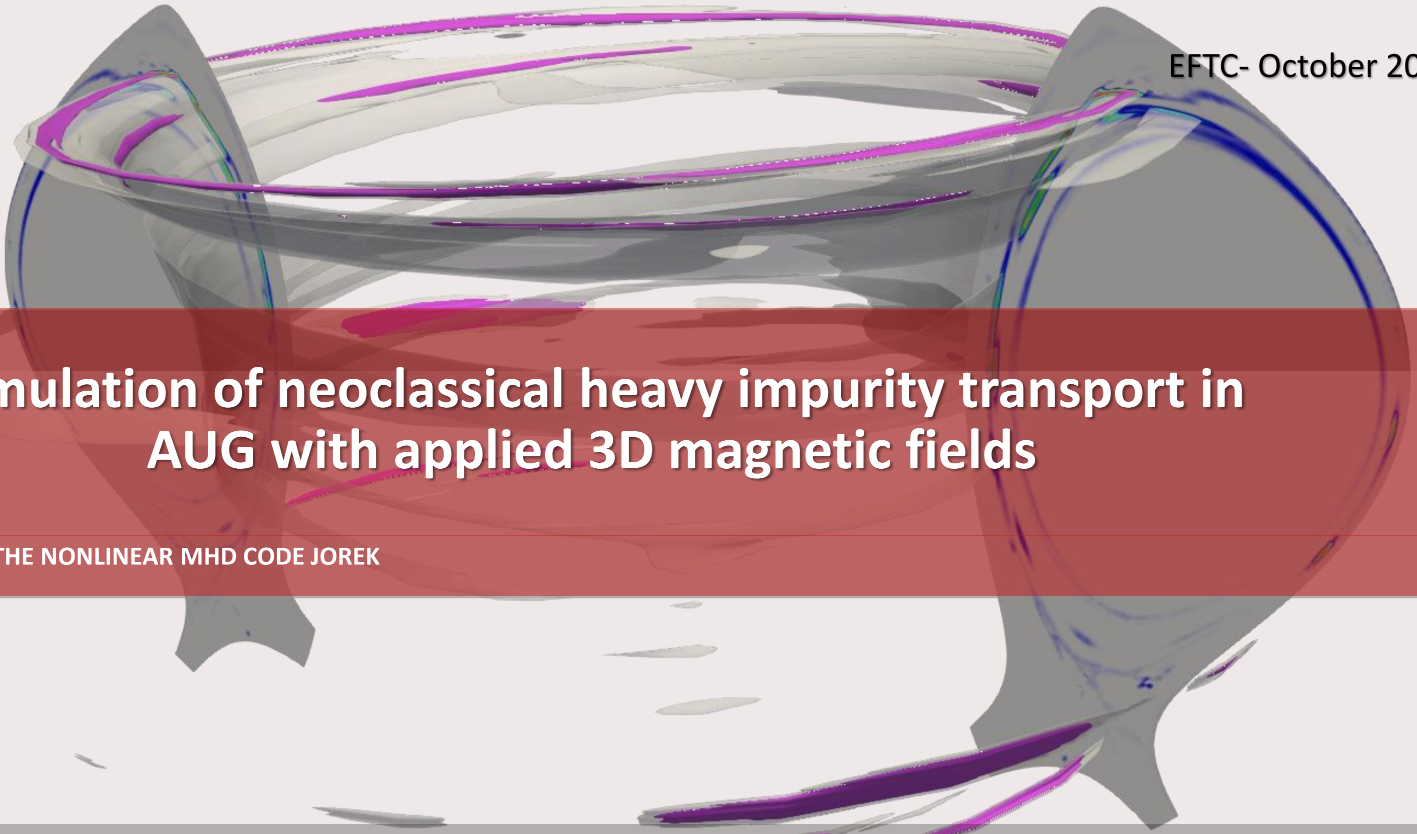

Simulation of neoclassical heavy impurity transport in AUG with applied 3D magnetic fields

WITH THE NONLINEAR MHD CODE JOREK

S.Q. Korving, G.T.A. Huijsmans, V. Mitterauer, A. Loarte, M. Hoelzl,
The JOREK Team, the ASDEX UPGRADE Team

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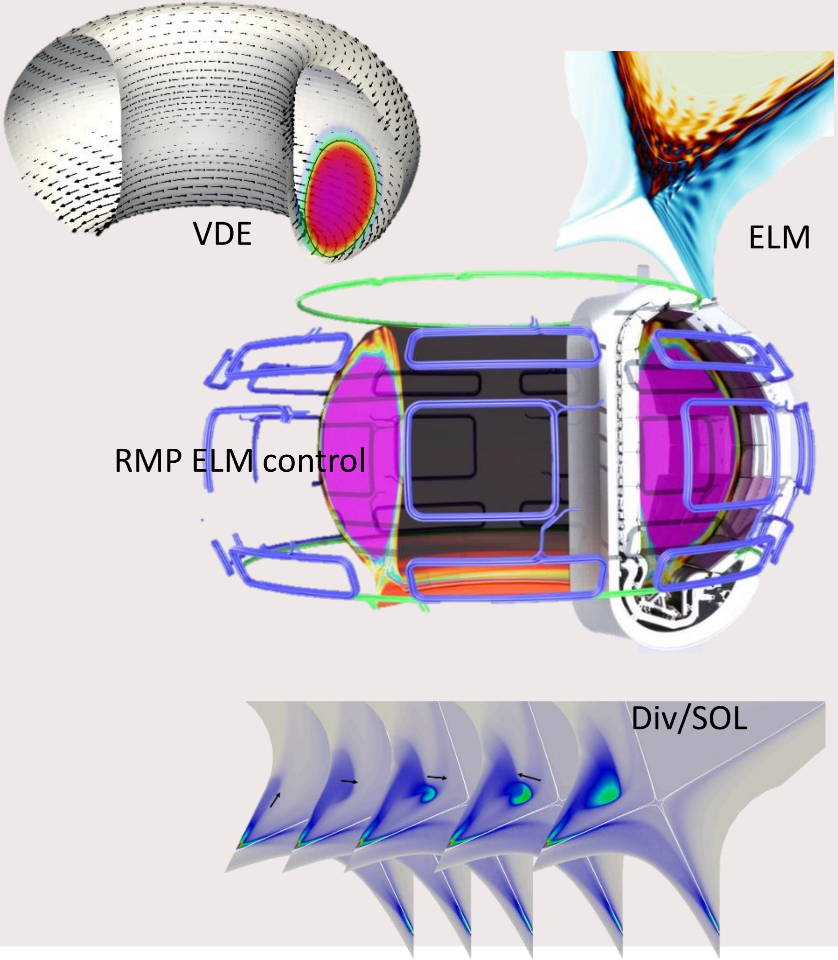
Motivation

- ELM-control in large tokamaks with Resonant Magnetic Perturbation
  - Prevent unacceptable heat loads on wall
  - Prevent W accumulation
- Transport in pedestal with ergodized magnetic field not fully known
  - Enhanced flushing out of impurities in AUG
- What modeling is needed to understand and predict this transport?
  - Plasmas with applied 3D fields
    - Ergodized field lines
  - Time dependent particles physics
    - Atomic physics, Neoclassical collisions, (plasma-wall interaction)
  - From wall-to-core
  - Fast enough

An overview of JOREK

- Extended nonlinear-MHD code
  - Typically used to study transient MHD instabilities.
    - E.g. ELMs, VDE's, CQ's, but also RMP operation

- JOREK Particle framework



https://www.jorek.eu/gallery/

JOREK reduced MHD

Induction equation: $\frac{\partial\psi}{\partial t} = R[\psi, u] + \eta J \ - F\frac{\partial u}{\partial\phi}, u \equiv \frac{\Phi}{F0}$ — ψ, j

Mass continuity: $\frac{\partial\rho}{\partial t} = -\nabla\cdot(\rho\vec{v}) + \nabla\cdot\left(\underline{D}\nabla\rho\right) + S_\rho$ — ρ

Momentum $\frac{\rho\partial v}{\partial t} = -\rho\vec{v}\cdot\nabla\vec{v} + J\text{x}B - \nabla p + \nabla\cdot\underline{\tau} + \vec{S}_v,$ — u, w; $v_\parallel$

with $\vec{v} = \overrightarrow{v_\parallel} + \vec{v}_{ExB} + \vec{v}_{dia}$

Energy $\frac{\partial\rho T}{\partial t} = -v\cdot\nabla(\rho T) - \gamma\rho T\nabla\cdot\vec{v} + \nabla\cdot\left(\underline{\kappa}\nabla T\right) + (\gamma-1)\underline{\tau}:\nabla\vec{v} + \eta J^2 + S_p$ — T

Variables: $\psi, u, j, w, \rho, T, v_\parallel$, optional $(T_i, T_e, \rho_n, \rho_z)$

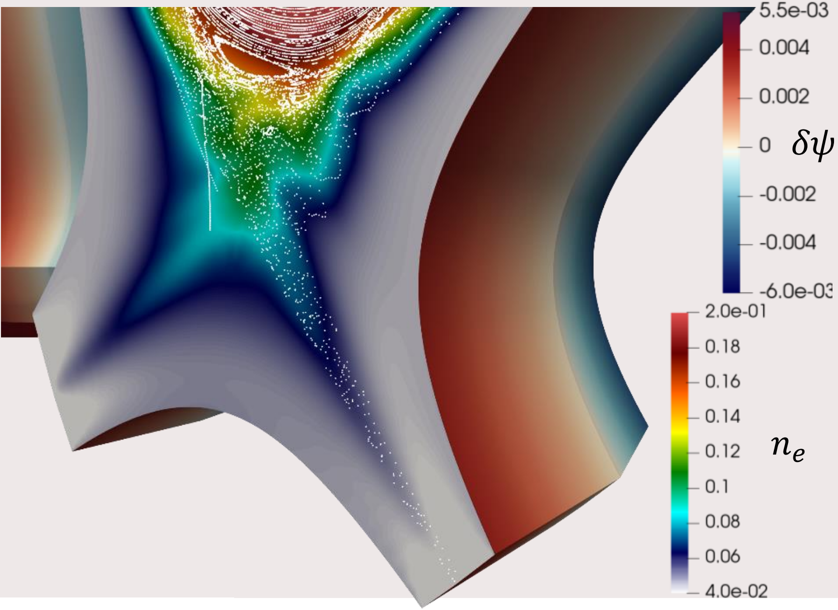
ψ, j BC's given by STARWALL

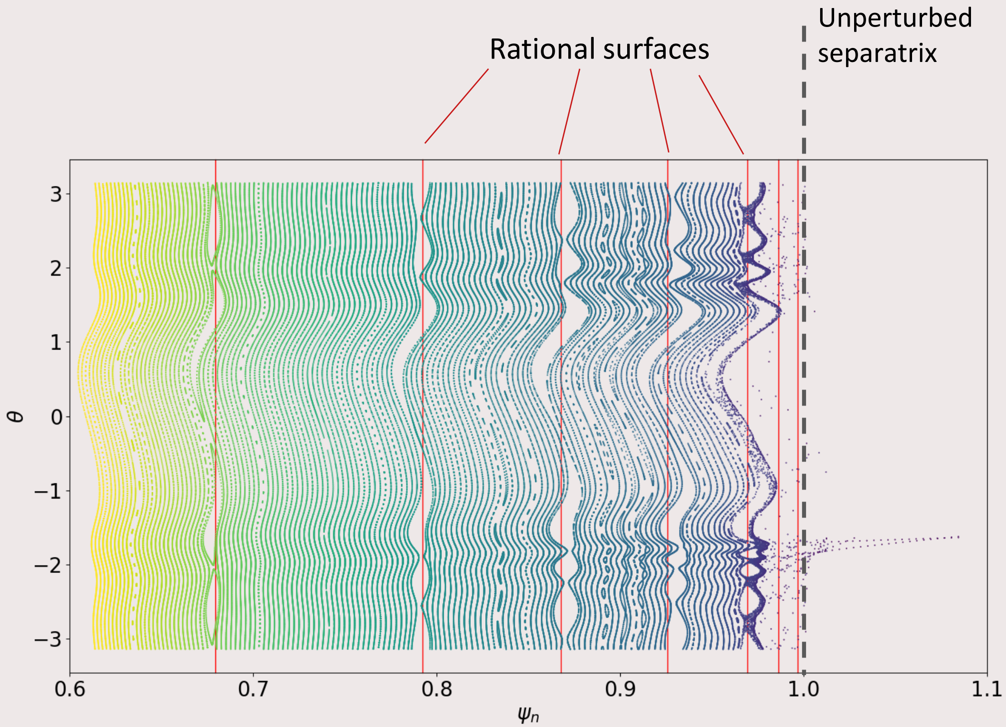
Dirichlet BC: u, w, Natural BC: ρ

Magnetized Bohm sheath BC: $v_\parallel, T$

JOREK +STARWALL

V. Mitterauer I.11 (previous talk)



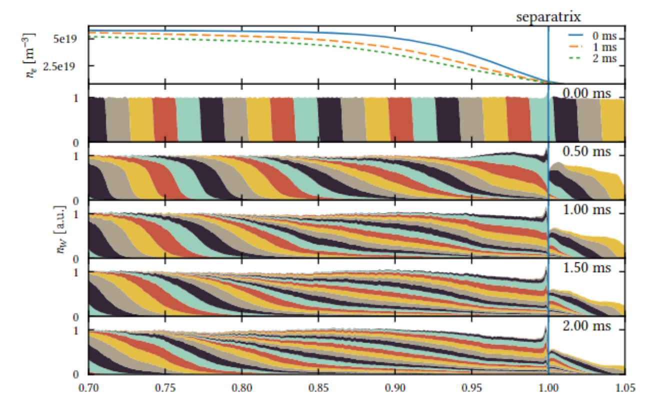


The particle extension

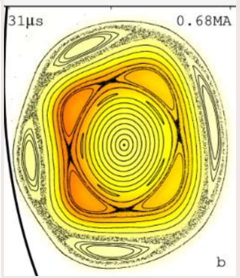
- Guiding Center, Full Orbit, Gyro-Kinetic
- Pushers: RK4, Boris, Qin

- (Two-way) coupled to JOREK MHD fields
  - Different coupling schemes

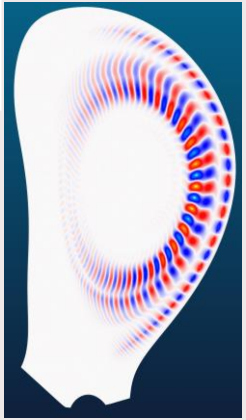
- Applications
  - Impurities (sputtering/transport/SPI)
  - Neutrals (recycling/puffing/MGI)
  - Runaway electrons
  - ITG turbulence
  - Fast ions



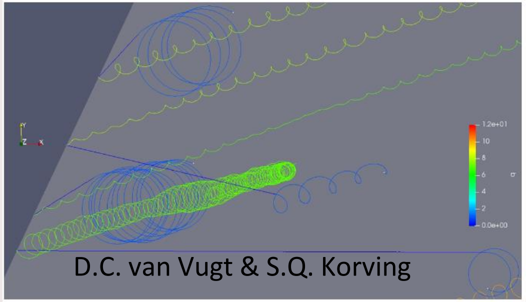
D.C. van Vugt PhD thesis



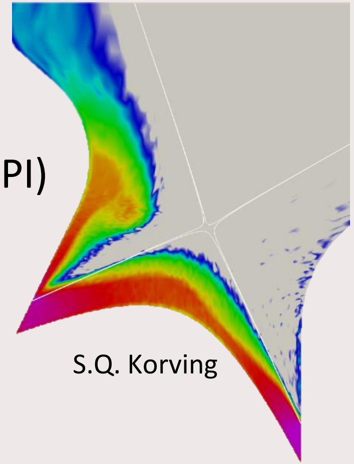
V. Bandaru



G.T.A Huijsmans



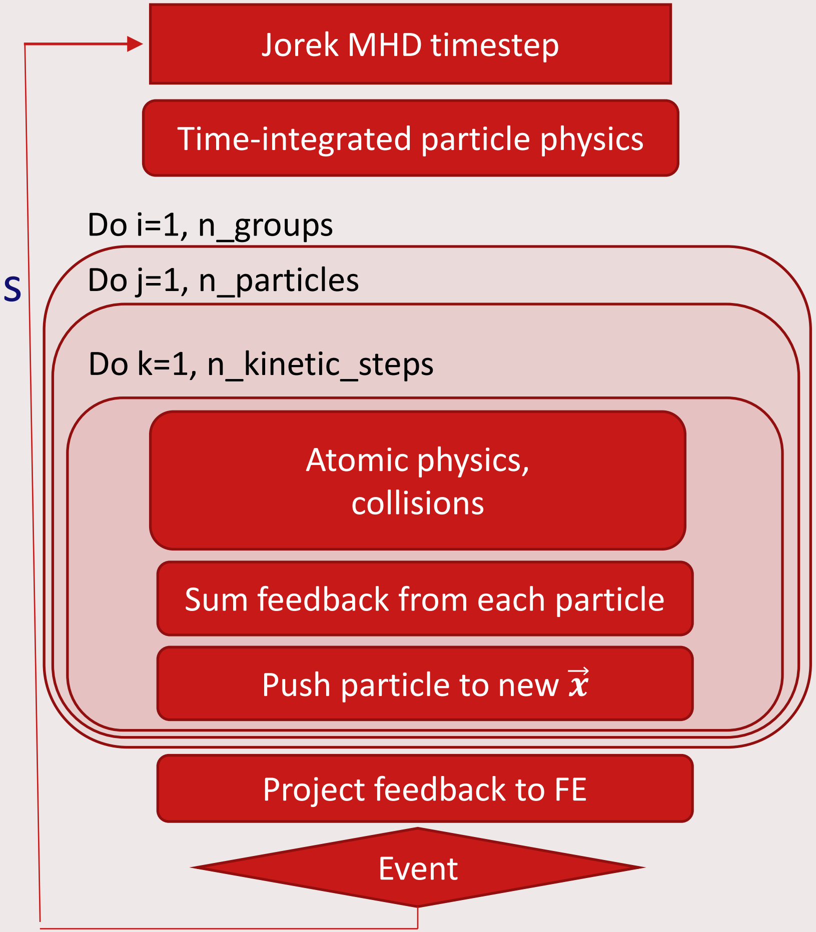
D.C. van Vugt & S.Q. Korving



S.Q. Korving

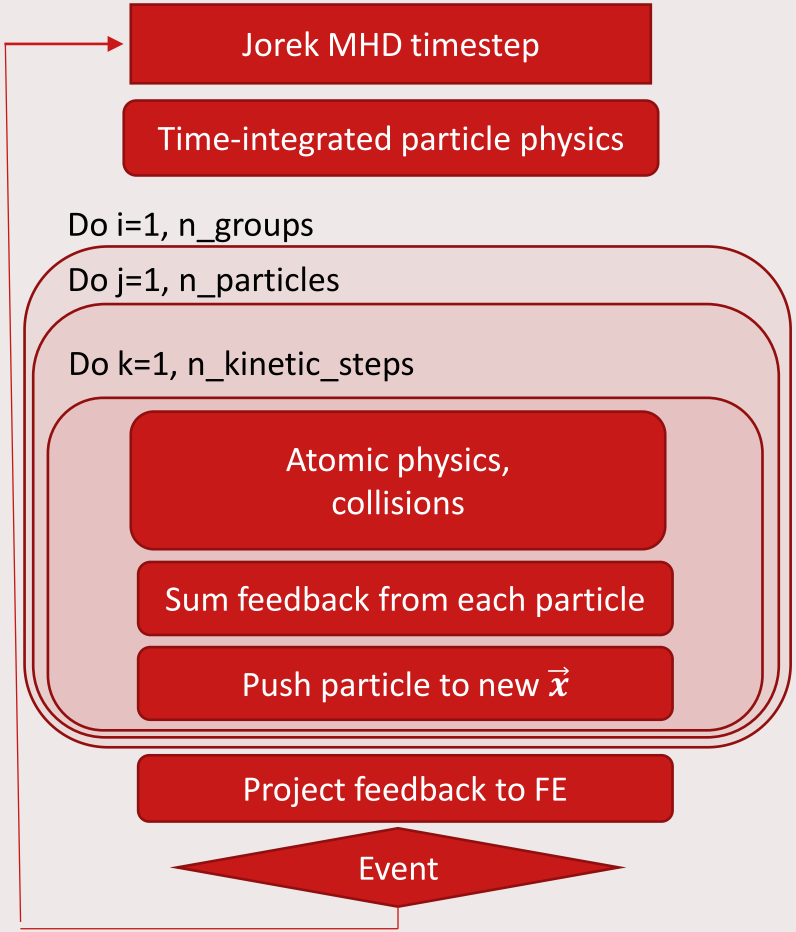
Kinetic Particle loop

- Different groups can have different properties
  - Coupled, trace
  - Neutrals, impurities
- Particle physics
  - Plasma-wall: effective coefficient from SDTrim
    - Based on time integrated values
  - Atomic: Effective rate coefficients from OpenADAS
- Events : puffing, LBO, SPI, diagnostics,etc..



Kinetic Particle loop

- Projecting arbitrary moments of particle distribution
  - Diagnostic and/or coupling
- Conservation of coupled variables
  - E.g. Mass, Momentum, Energy
- Particles stay alive between timesteps!



Collisional Neoclassical transport (1)

Enhanced diffusion: $D \approx D_{CL} + D_{PS} = \left(1 + 2q_{safe}^2\right) D_{CL}$

Cross-field transport:

CL, ExB, NC

$$\langle \boldsymbol{\Gamma}_\alpha \cdot \nabla\psi \rangle = \underbrace{\langle R F_{\alpha\perp} / e_\alpha \rangle}_{CL} + \underbrace{\left\langle n_\alpha \frac{E \times B}{B^2} \cdot \nabla\psi \right\rangle}_{ExB} + \underbrace{R_0 B_0 \left\langle \frac{F_{\alpha\parallel} + n_\alpha e_\alpha E_\parallel}{e_\alpha B} \right\rangle}_{NC}$$

$$\langle \boldsymbol{v}_z \cdot \nabla r \rangle^{NC} \approx 2q_{safe}^2 D_i^{CL} Z \left(K \frac{1}{n_i} \frac{\partial n_i}{\partial r} + H \frac{1}{T_i} \frac{\partial T_i}{\partial r} \right)$$, PS-model→ $H = -\frac{1}{2}, K = 1$

$$\boldsymbol{v}_{i,dia} = \frac{B \times \nabla p_i}{n_i e_i B^2} \qquad \boldsymbol{q}_{i,dia}^{heat} = \frac{5 p_i}{2 e_i B^2} B \times \nabla_\perp T$$

$$\nabla \cdot \left(n_i \boldsymbol{v}_{i,\parallel}^{PS} \right) = -\nabla \cdot \left(n_i \boldsymbol{v}_{i,dia} \right) \qquad \nabla \cdot \left(\boldsymbol{q}_{i,\parallel}^{PS} \right) = -\nabla \cdot \left(\boldsymbol{q}_{i,dia}^{heat} \right)$$

NC Inward Pinch

NC Temperature Screening Effect

Collisional Neoclassical transport (2)

- Tungsten is typically in the PS-regime, $\nu^* \epsilon^{3/2} > 1$
  - $\nu_i^* \epsilon^{3/2} = \frac{qR}{\nu_{ii}\tau_{ii}} \propto qR \frac{n_e}{T_i^2}$, $\quad \nu_z^* \epsilon^{3/2} \approx 2\nu_i^* \epsilon^{3/2} \boxed{\frac{Z_z^2}{\sqrt{A_z}}}$
    - Example: $Z_W = (10, 20) \rightarrow \frac{\nu_z^*}{\nu_i^*} \approx (15, 60)$
- Extended heat flux model for sampling from shifted-distorted-Maxwellian [Y.Homma 2013 JCP,2016 NF]
  - $f_b(v_b) = n_b \left(\frac{m_b}{2\pi k T_b}\right)^{3/2} e^{-\frac{m_b w^2}{2kT_b}} \left[1 - \frac{m_b}{n_b} \frac{1}{(kT_b)^2} \left(1 - \frac{w^2}{5v_{th,b}^2}\right)(\vec{\boldsymbol{q}} \cdot \vec{\boldsymbol{w}})\right] + \bar{\boldsymbol{v}}_b\, , \vec{\boldsymbol{w}} = \vec{\boldsymbol{v}}_b - \bar{\boldsymbol{v}}_b$
  - $\vec{\boldsymbol{q}} = -\kappa_\parallel \nabla_\parallel k T_b + \kappa_\wedge \vec{e}_\parallel \times \nabla_\perp k T_b - \kappa_\perp \nabla_\perp k T_b$
- Binary Collision model for coulomb collisions [Takizuka and Abe 1977 JCP]
  - $\left(\frac{\partial f_\alpha}{\partial t}\right)_{coll} = -\sum_b \frac{\partial}{\partial v_j} \frac{e_\alpha^2 e_b^2}{8\pi\epsilon_0^2 m_\alpha} \int d\boldsymbol{v}' \left[\frac{\delta_{jk}}{u} - \frac{u_j u_k}{u^3}\right] \left[\frac{f_\alpha}{m_b} \frac{\partial f_b(v\prime)}{\partial v_{k'}} - \frac{f_b(v\prime)}{m_\alpha} \frac{\partial f_\alpha}{\partial v_k}\right]$
- Results in frictional + thermal force: $F = F^0 + F^{\nabla T}$

Benchmark: NC IWP, NC TSE, Flow cancellation

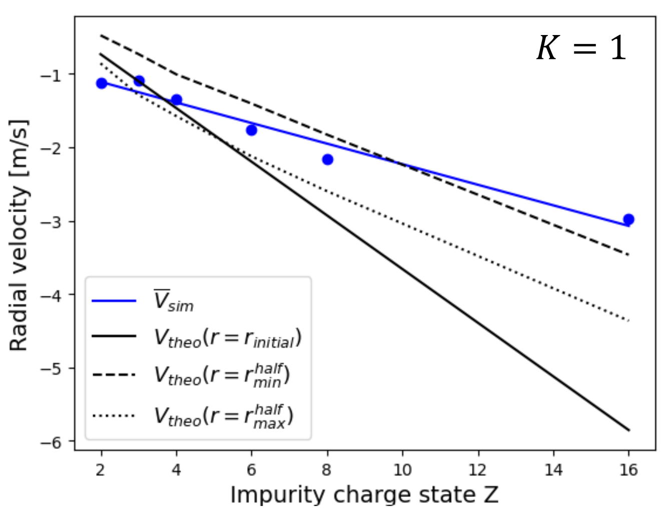
$R_{major} = 3\text{m}, B = 9\text{T}, r = 1\text{m}, \; n = 10^{20}\text{m}^{-3}, T = 250\text{eV}, t_{sim} = 70\text{ms}$

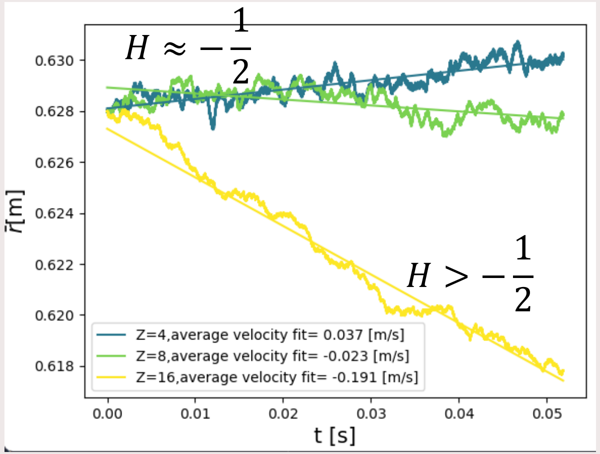
Although, plasma is axisymmetric, particle transport is always in 3D
Similar to [Homma et al 2016 NF], Transport corresponds with the lower q_{safe} in the distribution

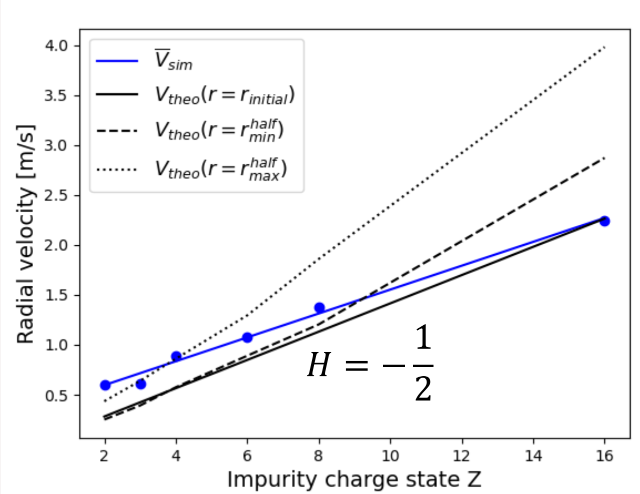
NC IWP $\frac{1}{n}\frac{\partial n}{\partial \psi_N} = -5$

Flow cancellation $\frac{1}{n}\frac{\partial n}{\partial \psi_N} = -5, \frac{1}{T}\frac{\partial T}{\partial \psi_N} = -10$

NC TSE $\frac{1}{T}\frac{\partial T}{\partial \psi_N} = -7.5$







Simulating W in AUG with RMPs

Particle model and physics included in this work

- Included physics:
  - Fully kinetic
  - Time-dependent
  - Test particle (no radiation feedback)
  - Atomic physics (ion/rec/rad)
  - Parallel friction (collisions with $H \approx -\frac{1}{2}$)
  - $E_{\|}$ and $E \times B$ transport
  - In 3D, stochastic fields.

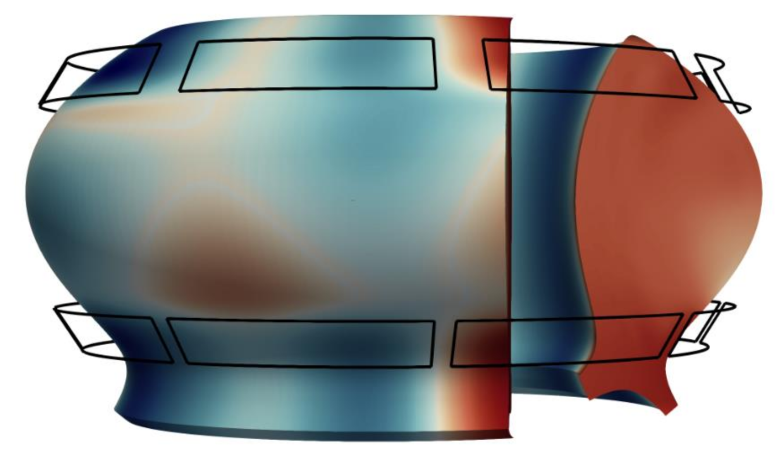
- Not used for this case:
  - Coupled particles, plasma-wall interaction

Computational cost:

Wall time: 29 hours
Simulated time: 72 ms
N particles: 10^6
N cpus: 9x36 = 324
CPU time ~10^4 cpuh

Setup AUG simulation with RMPs

$B_0 = -1.83\text{T},$
$I_p = 0.9\text{MA},$
$q_{95} = 3.6,$
$I_{rmp} = 0.9\sim 1.22\text{kA},$
$n_{rmp} = 2$



[V Mitterauer et al 2022 J. Phys.: Conf. Ser. 2397 012008]

- What is the effect of the 3D'ness on radial transport?
  - In 3D, with RMPs
  - In 2D, without RMPs

  (Ad hoc transport coefficient to force identical pedestal profile)

- Testing 2 effects:
  - Enhanced out flushing
  - Screening

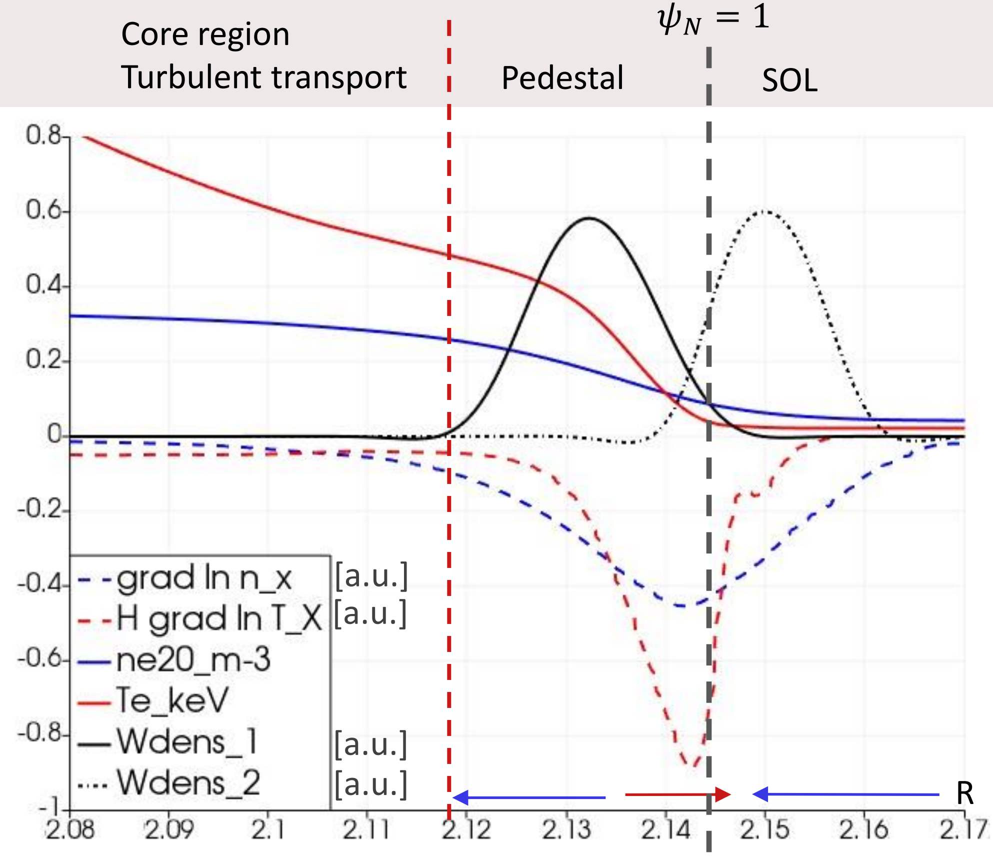
- Qualitive behavior of W transport

Initially with parallel friction only

Radial profiles

- Pedestal lowered due to RMPs
  - Low density pedestal due to pump-out
- OMP profiles of background plasma
- Initial W distribution
  - Axisymmetric, gaussian around a ψ_N
  - Coronal equilibrium, $T = T_b$

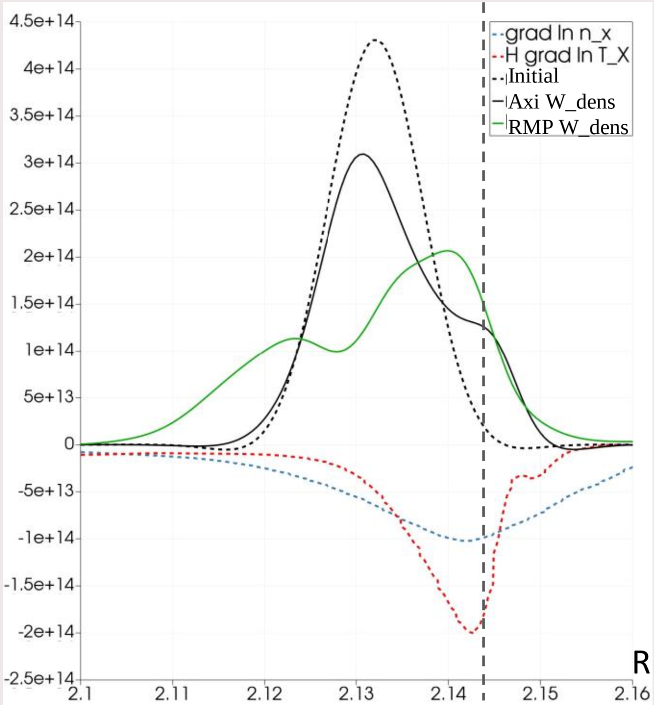
$$\langle v_z \cdot \nabla r \rangle^{NC} \propto \left(K \frac{1}{n_i} \frac{\partial n_i}{\partial r} - H \frac{1}{T_i} \frac{\partial T_i}{\partial r} \right)$$



Pedestal and edge results

Parallel smoothed W projection for flux surface average transport
Pedestal at OMP for indication

- After 10 ms
- RMP results in
  - Enhanced diffusion
  - Enhanced convection (outflushing)



$\psi_N = 1$

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Pedestal and edge results

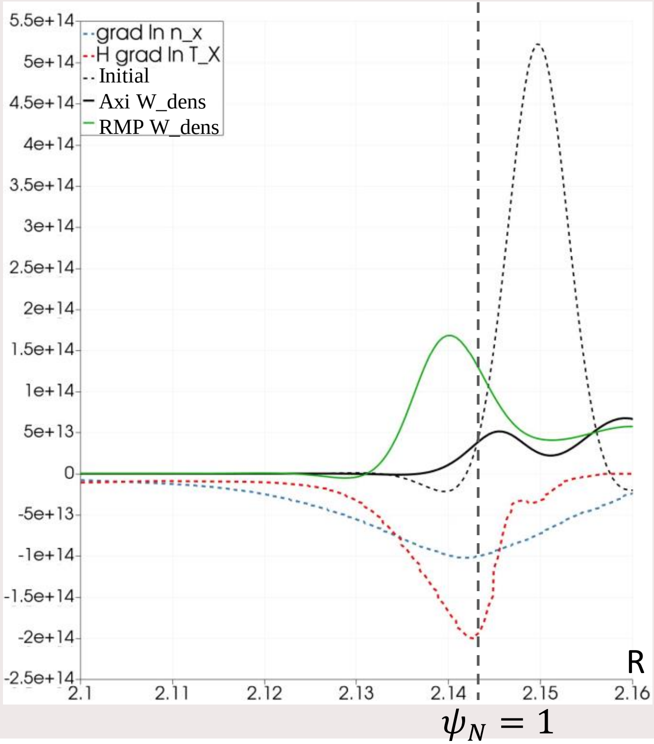
Parallel smoothed W projection for flux surface average transport
Pedestal at OMP for indication

- After 10 ms
- RMP results in
  - Enhanced diffusion
  - Enhanced convection (inwards)
- Axisymmetric case, W quickly decays in SOL
  - SOL is in convection-dominated regime
    low $\nabla_{\parallel} T$

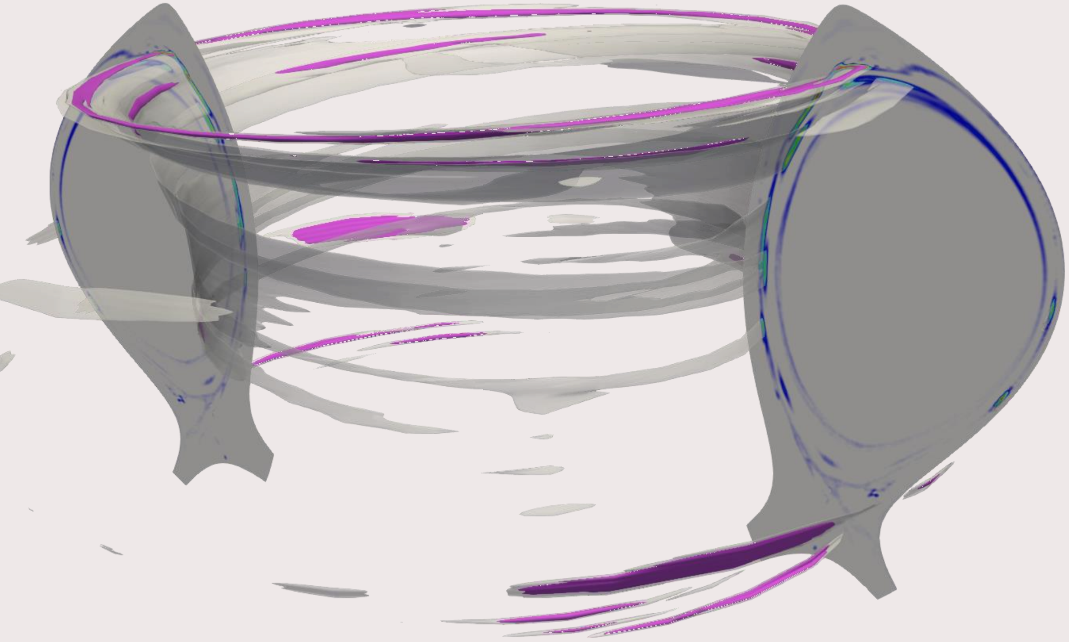
- W remains in the pedestal region and slowly diffuses

- However, transport and profiles are not axisymmetric

This is not the full picture!



Possibility of W trapping in potential wells



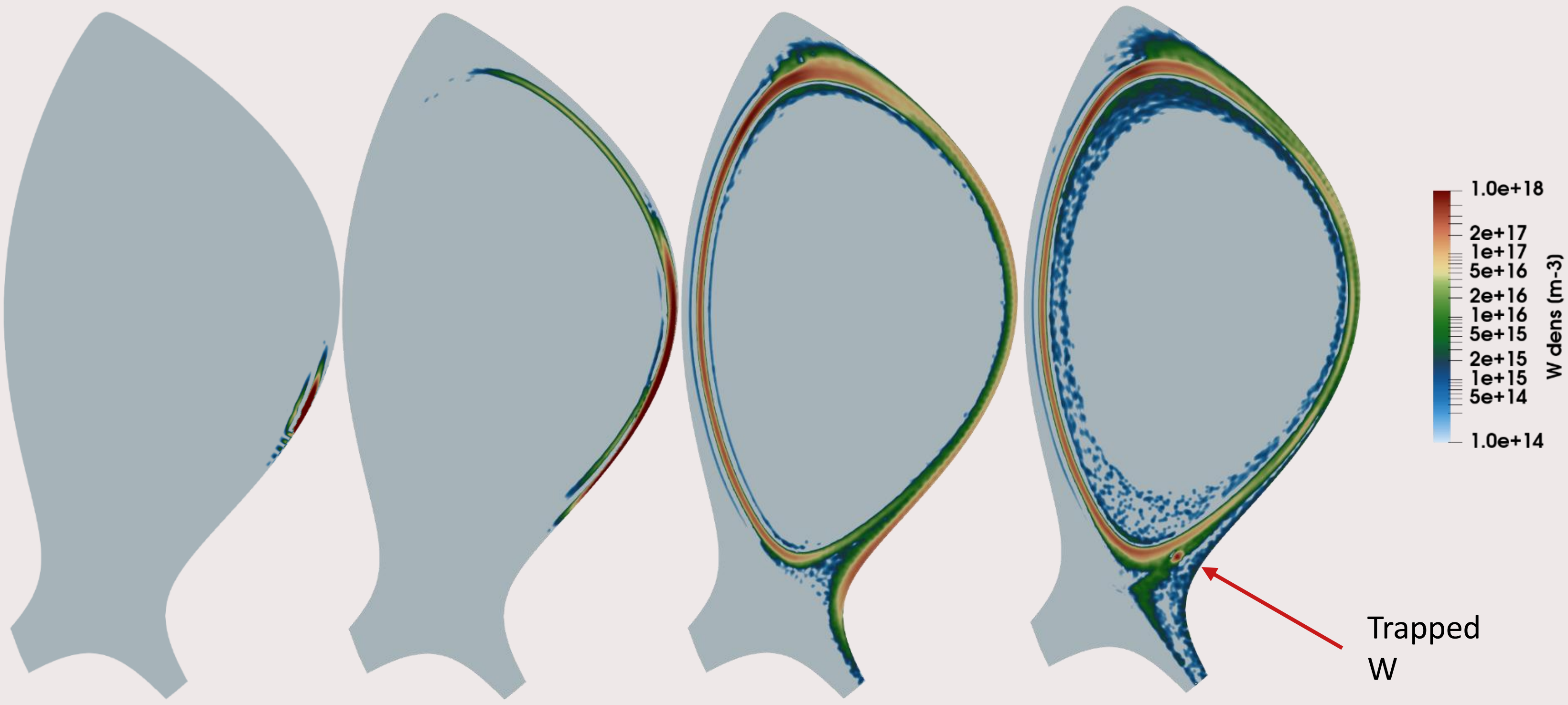
Contour: medium W density

Contour: high W density

- W density and transport strongest at HFS and Top,
- Localized trapping at the bottom of the pedestal and SOL due to electric potential wells.

W-LBO in AUG

$t - t_0 = 0.05$ ms   0.24 ms   1.5 ms   7 ms



N=0 component of the projected W density

Summary & Outlook

- JOREK + particles capabilities
  - Free-boundary visco-resistive-MHD with grid up to first wall
  - (trace and coupled) Kinetic particles with effects from:
    - E&M fields, stochastic field lines, ionization/recombination/radiation, NC collisions, sputtering
- JOREK particles reproduces neoclassical transport
  - NC Diffusion, NC Inward Pinch, NC Temperature screening, flow cancellation with $H \approx -\frac{1}{2}$
- First demonstration of time dependent W transport in AUG RMP
  - With Neoclassical collisions, E-field and stochastic field lines
- RMP enables more transport through the pedestal in both directions

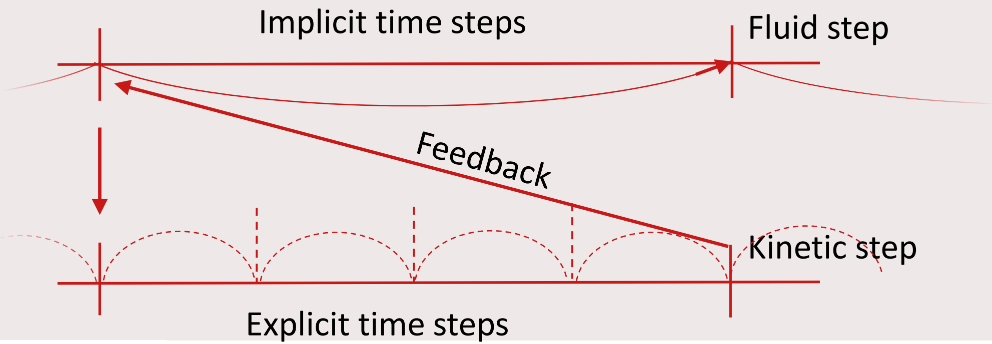
Outlook:

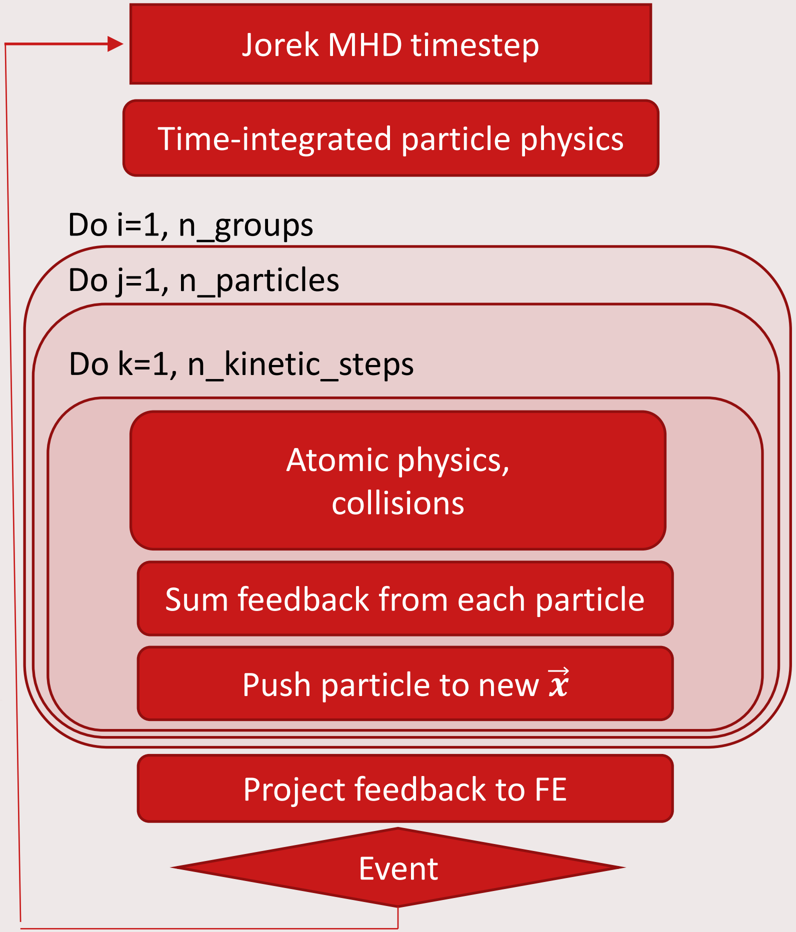
- More realistic scenario to replicate experiment
  - Fine-tuning physics models
- Neutral+impurities+sputtering+coupling
- Improved collision operator
- Synthetic spectrometer diagnostic

Backup slides

Kinetic Particle loop

- Particle physics
  - Atomic: Effective rate coefficients from OpenADAS
  - Plasma-wall: effective coefficient from SDTrim
    - Based on time integrated values
- Events : puffing, LBO, SPI, diagnostics,etc..
- Conservation of coupled variables
  - E.g. Mass, Momentum, Energy





Coupling and Projection to Finite Elements

Coupling in the JOREK form of the equations

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\vec{v}) = S_\rho$$

$$\rho\frac{\partial \vec{v}}{\partial t} + \rho(\nabla\cdot\vec{v})\vec{v} + \nabla\cdot\overline{\overline{P}} = \vec{S}_v - \vec{v}S_\rho$$

$$\frac{\partial\left(\frac{3}{2}\rho T\right)}{\partial t} + \vec{v}\cdot\nabla\left(\frac{3}{2}\rho T\right) + \frac{5}{2}\rho T(\nabla\cdot\vec{v}) = S_E - vS_v + \frac{1}{2}v^2 S_\rho$$

With :

$$S_\rho(\vec{x}) = \int mf(\vec{x},\vec{v})\,d\vec{v}$$

$$S_v(\vec{x}) = \int m\vec{v}f(\vec{x},\vec{v})\,d\vec{v}$$

$$S_E(\vec{x}) = \int \tfrac{1}{2}mv^2 f(\vec{x},\vec{v})\,d\vec{v}$$

Express source in JOREK FE representation to obtain a continuous function from a list of discrete particles

$$\tilde{S}_\rho(\vec{x}) = \sum_{ijk} p_{\rho,ijk} H_{ij}(s,t) H_{\varphi,k}(\varphi)$$

Projection using weak form:

$$\int v^*(\vec{x})\tilde{S}_\rho(\vec{x})\,d\vec{x} = \int v^* S_\rho(\vec{x})\,d\vec{x}$$

$$\int v^*(s,t,\varphi)\sum_{ijk} p_{\rho,ijk} H_{ij}(s,t) H_{\varphi,k}(\varphi)\,d\vec{x} = \int v^* mf(\vec{x},\vec{v})\,d\vec{v}\,d\vec{x}$$

$$\int v^*(s,t,\varphi)\sum_{ijk} p_{\rho,ijk} H_{ij}(s,t) H_{\varphi,k}(\varphi)\,d\vec{x} = \sum_n v^* m w_n \delta(\vec{x}-\vec{x}_n)$$

Smoothing:

$$\int v^*(\vec{x})\left(1-\lambda\nabla^2-\varsigma\nabla^4\right)\tilde{S}_\rho(\vec{x})\,d\vec{x} = \int v^* S_\rho(\vec{x})\,d\vec{x}$$

$$\int\left(v^*\tilde{S}_\rho + \lambda\nabla v\cdot\nabla\tilde{S}_\rho + \varsigma\nabla^2 v^*\nabla^2\tilde{S}_\rho\right)d\vec{x} = \int v^* S_\rho(\vec{x})\,d\vec{x}$$

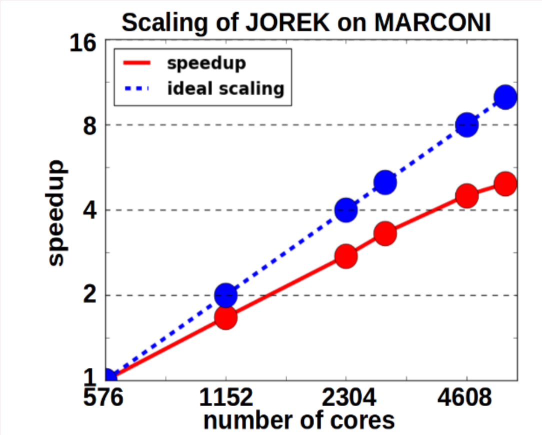
D.C. van Vugt, PhD thesis

JOREK Parallelization

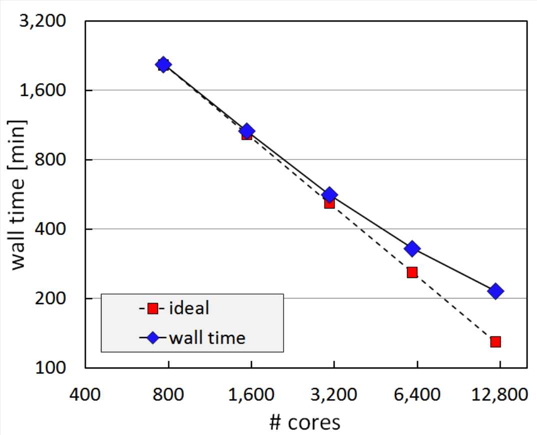
- MPI + openMP
- Main parts
  - Matrix construction, Preconditioner factorization, GMRES solve step

Scales very well
Scaling problematic

Fluid part



Kinetic particle part



G.T.A. Huijsmans, IRFM 2021

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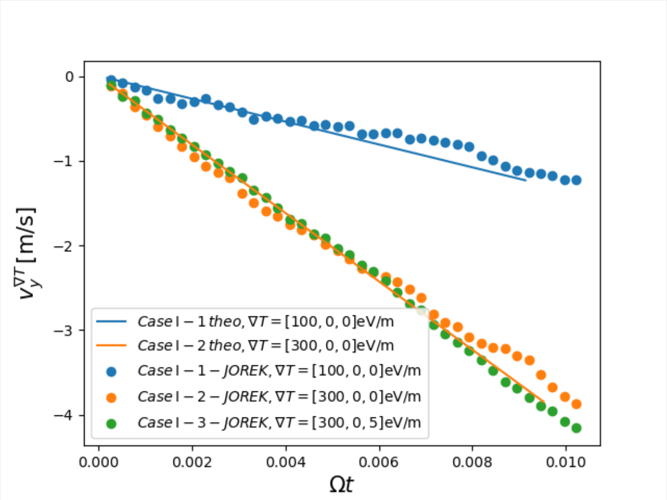
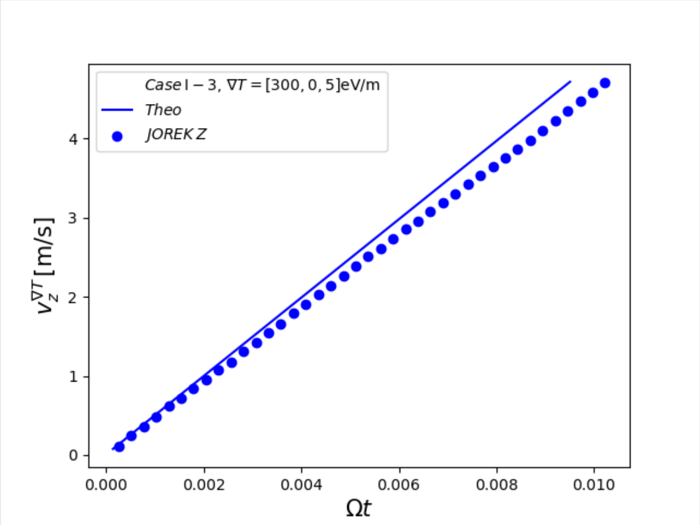
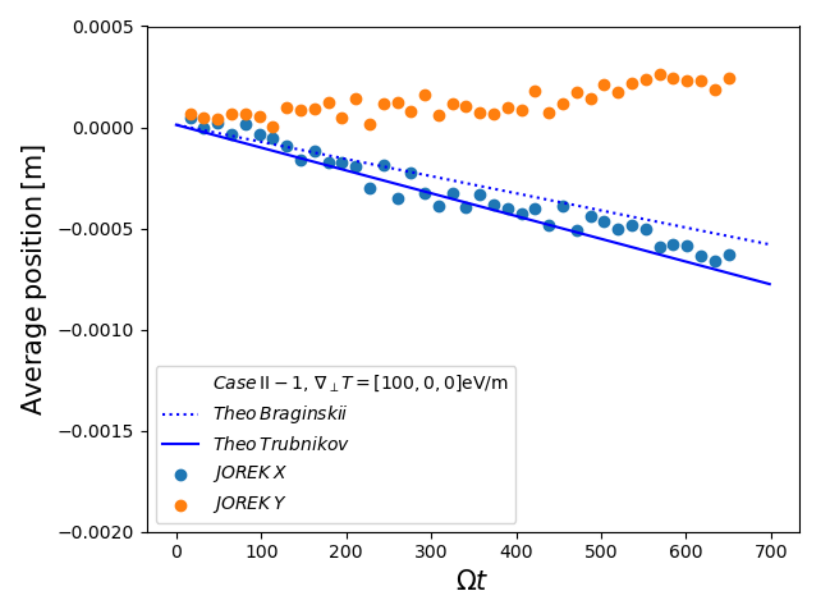
Collisions benchmarks

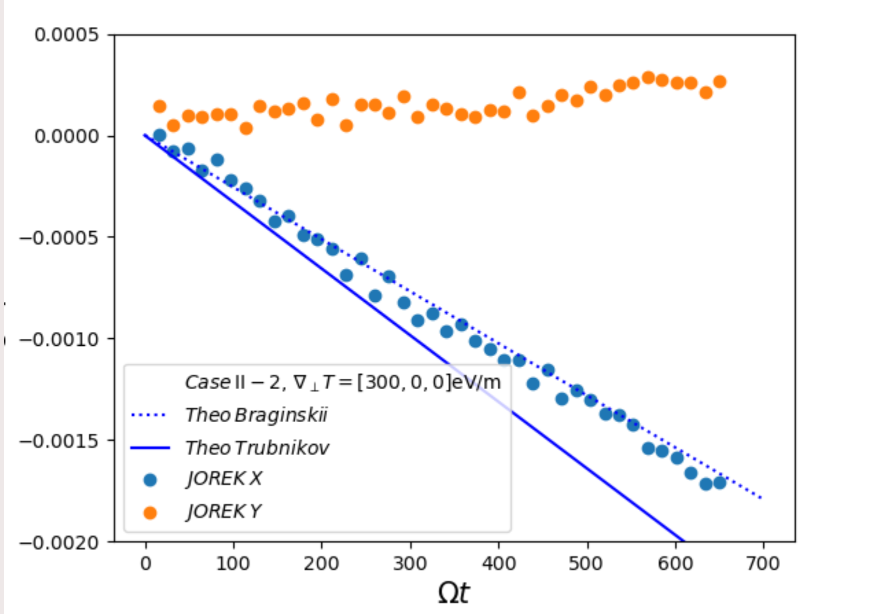
Homma tests (1)



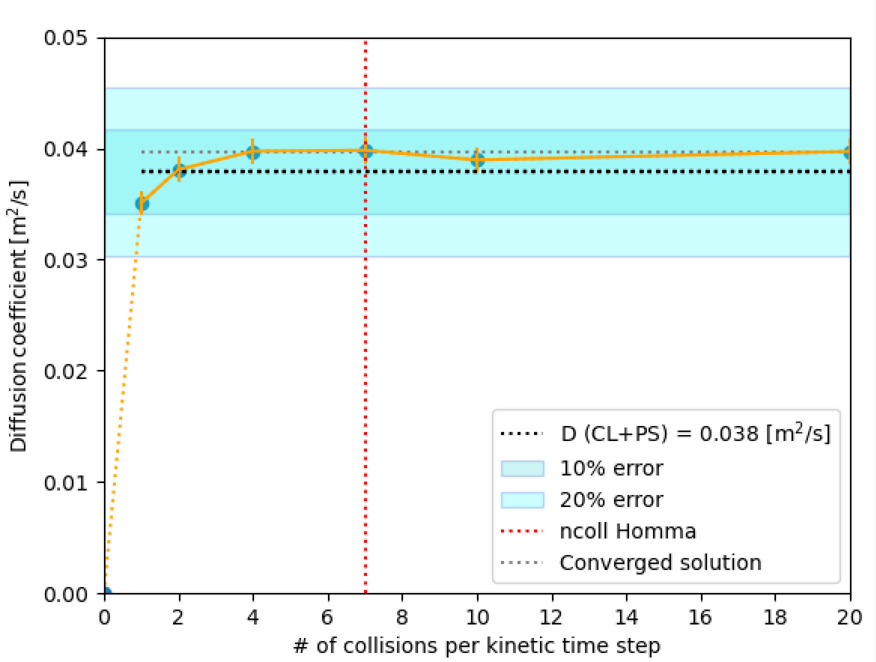


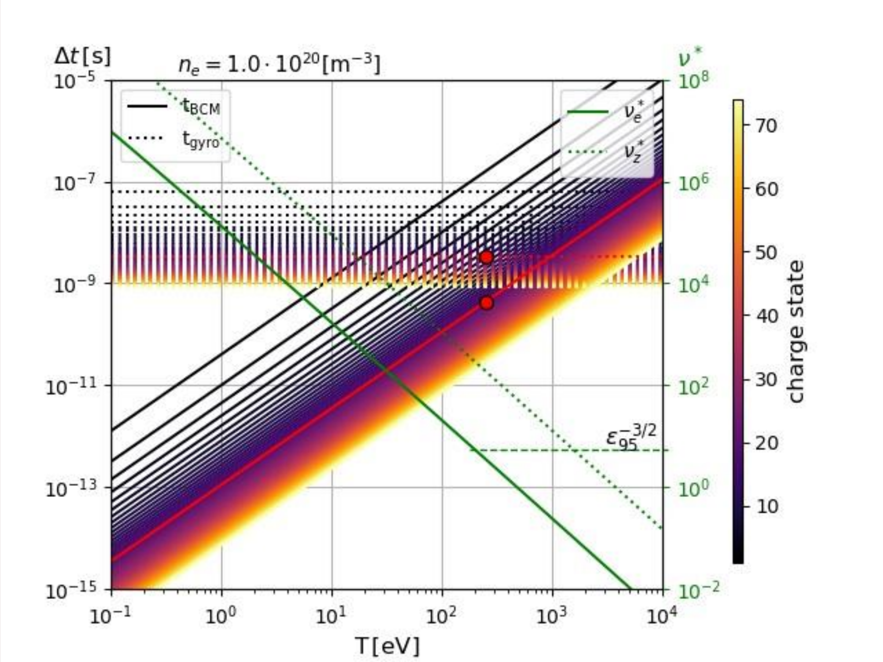
Homma tests(2)



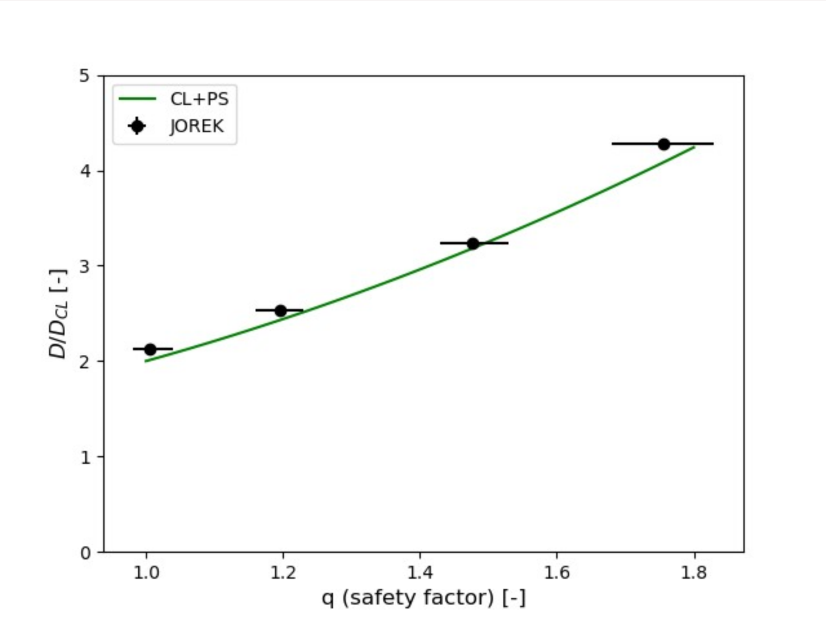


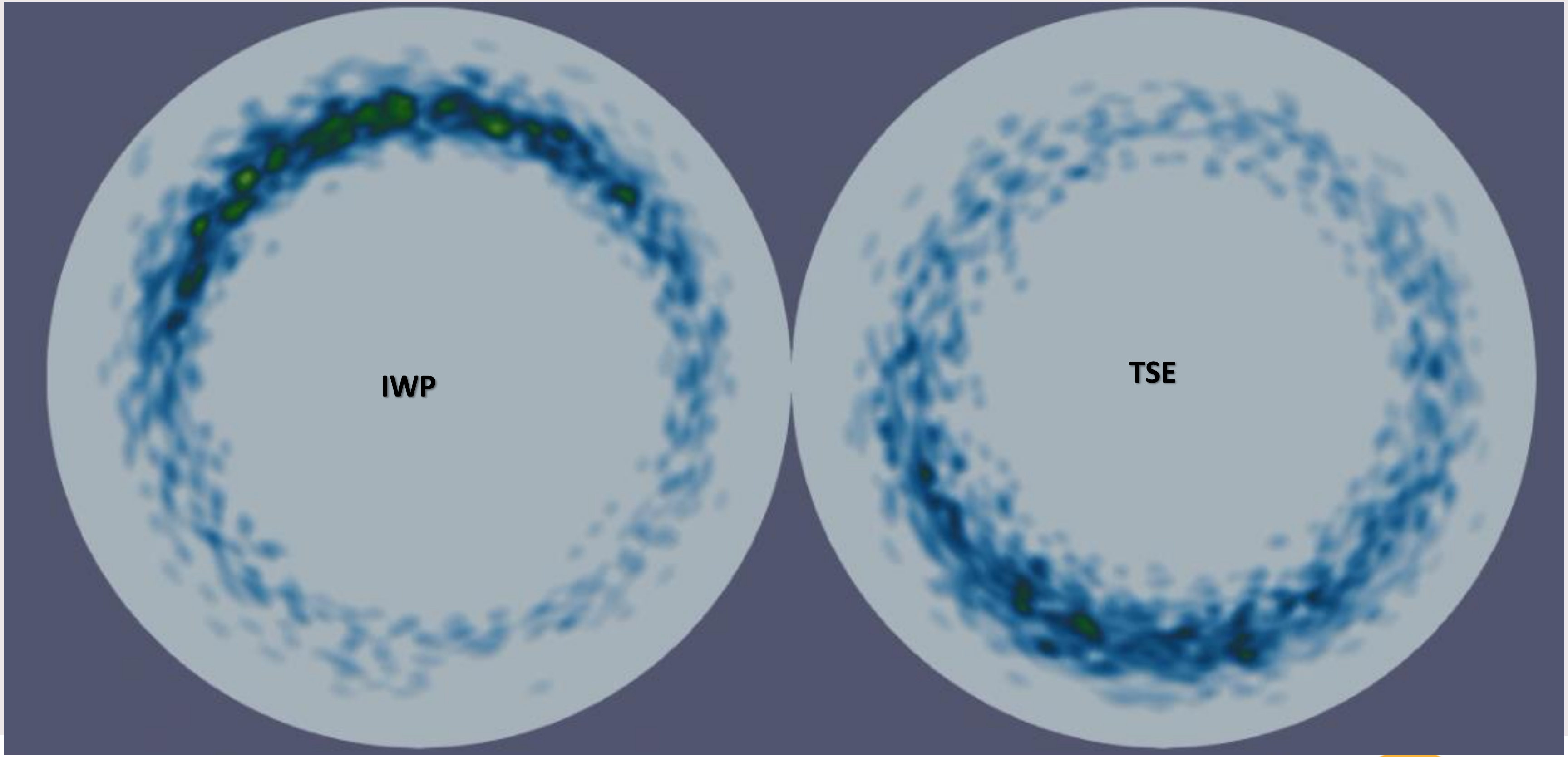
Convergence of gyro and Collision time steps





Diffusions as function of safety factor




IWP
TSE

Benchmark: NC IWP, NC TSE, Flow cancellation

$R_{major} = 3\text{m}, B = 9\text{T}, r = 1\text{m}, \ n = 10^{20}\text{m}^{-3}, T = 250\text{eV}, t_{sim} = 70\text{ms}$

Although, plasma is axisymmetric, particle transport is always in 3D
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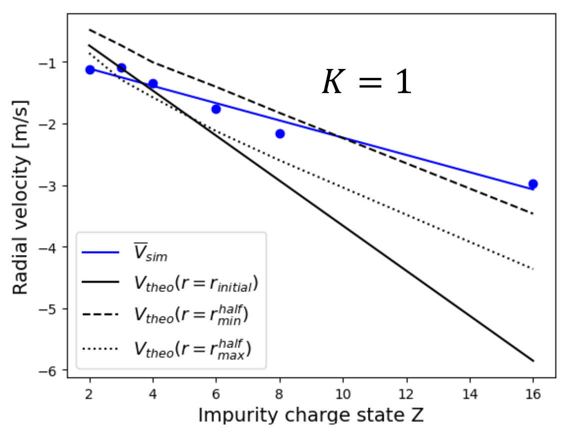
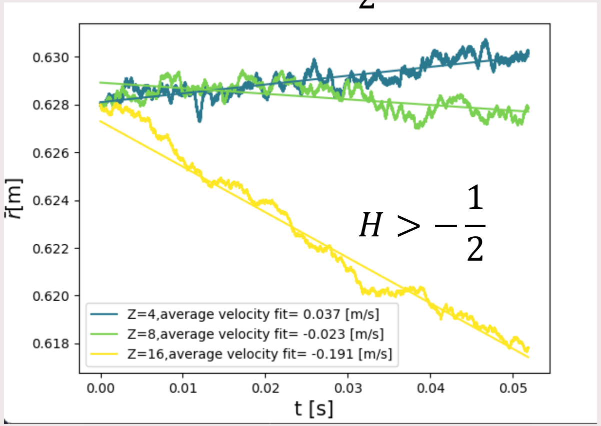
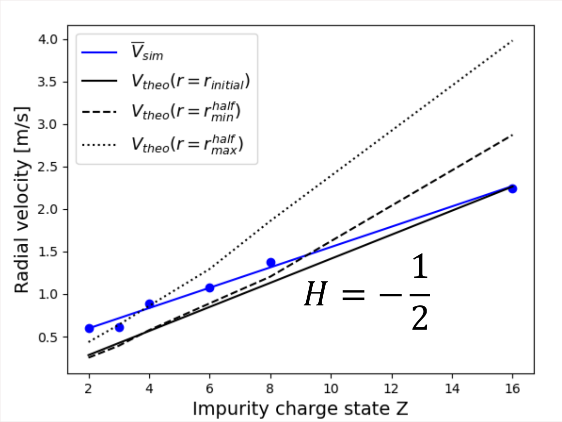
Flow cancellation $\frac{1}{n}\frac{\partial n}{\partial \psi_N} = -5, \frac{1}{T}\frac{\partial T}{\partial \psi_N} = -10$

NC TSE $\frac{1}{T}\frac{\partial T}{\partial \psi_N} = -7.5$

$H \approx -\frac{1}{2}$







W-LBO in AUG

W core relaxation 100~200 ms