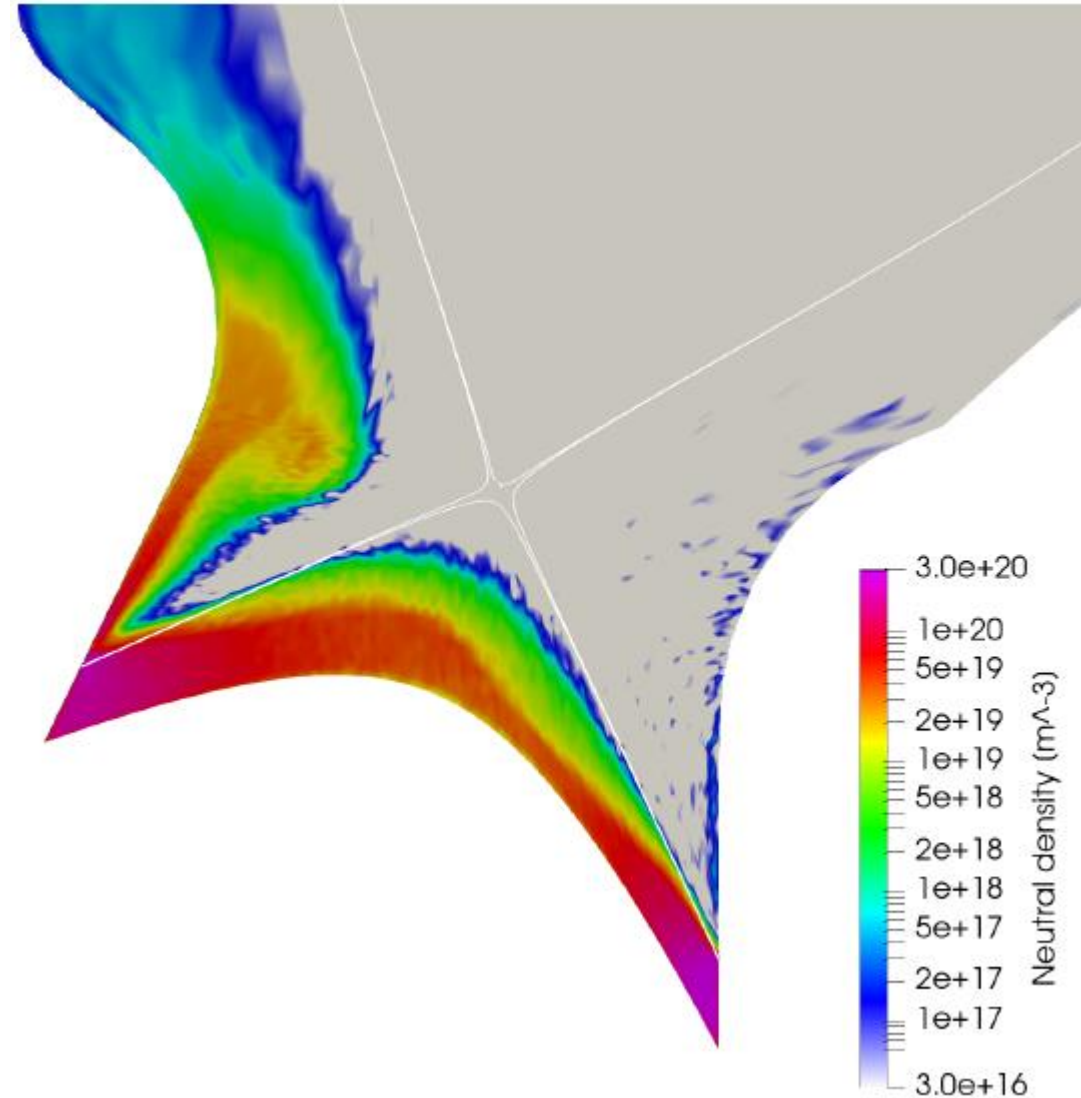


# The Neutral Model in JOREK

Guido Huijsmans

Sven Korving, Daan van Vugt,  
Stijn Franssen, Andres Cathey, Daniel Maris  
& JOREK Team

*Development of the neutral model in the nonlinear MHD code JOREK...*  
Sven Korving et al.,  
*Phys. Plasmas* 30, 042509 (2023)  
<https://doi.org/10.1063/5.0135318>



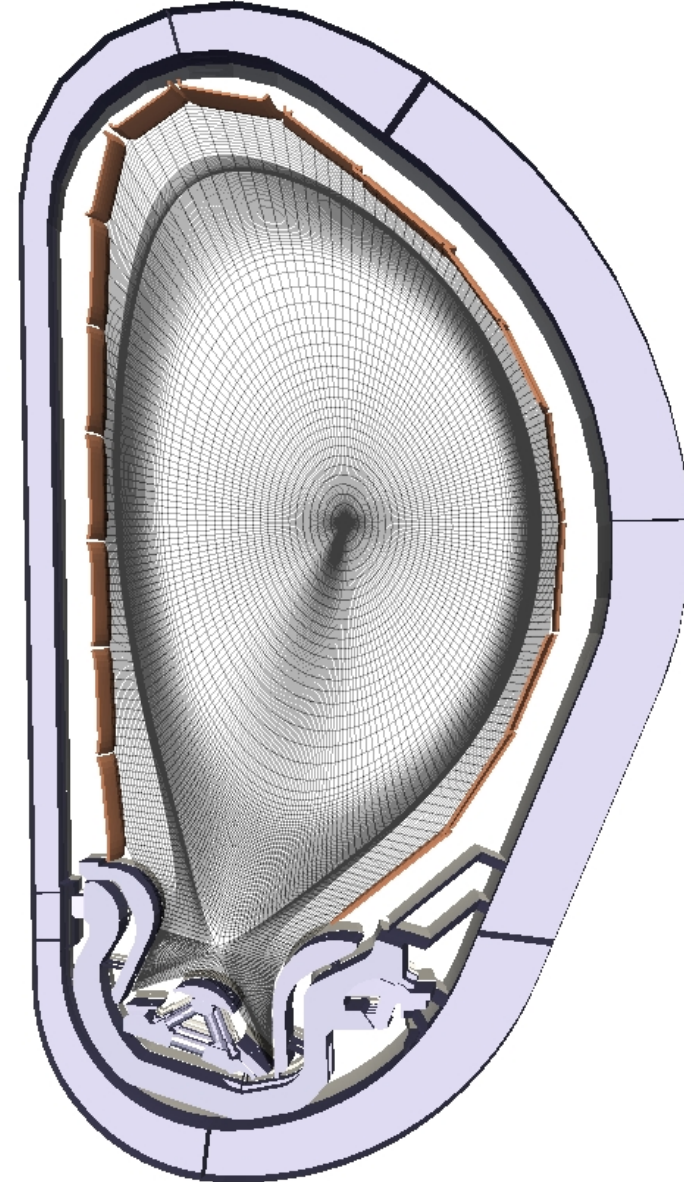
# Outline

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- Introduction JOEREK
- JOEREK particle model
  - applications
- JOEREK neutral model
  - applications
- Summary

# Nonlinear MHD code JOREK

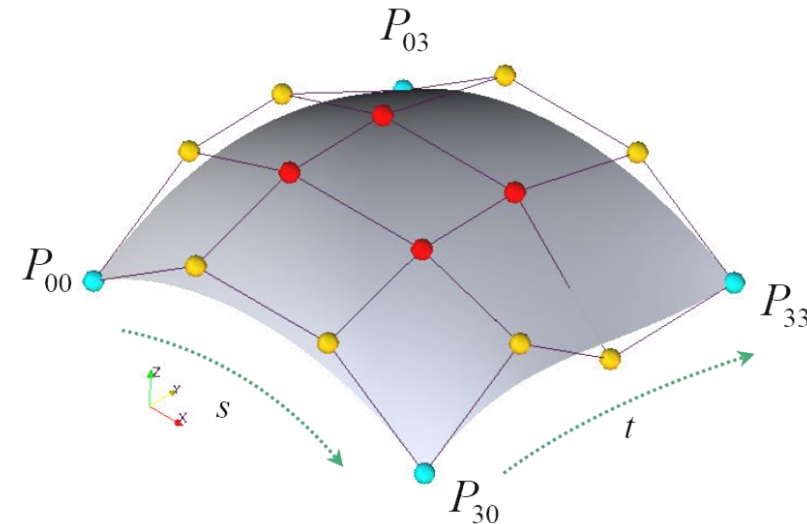
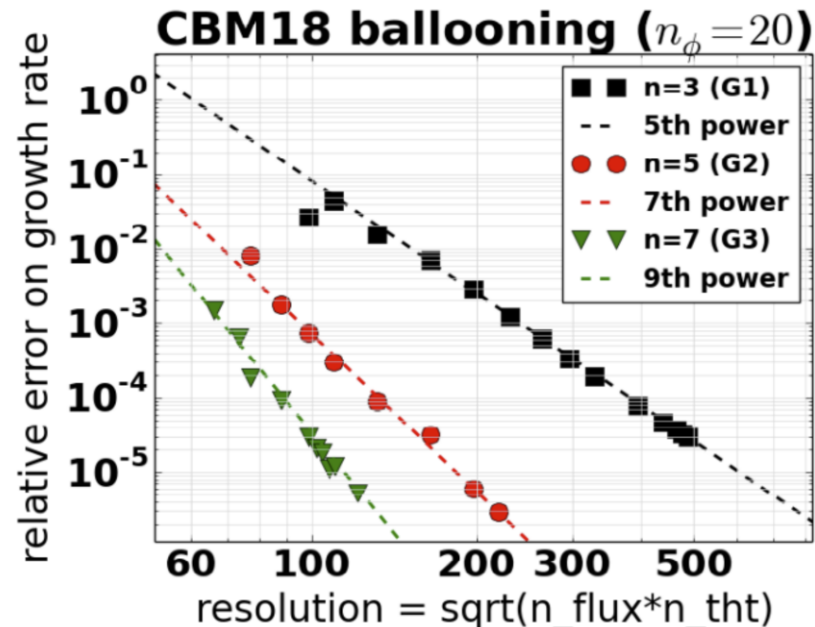
- (extended) MHD fluid model
  - full or reduced MHD, single or  $(T_e, T_i)$
  - impurities
  - neutrals
  - runaway electrons
- Flexible geometry
  - open, closed field lines, x-point(s)
  - divertor boundary conditions
  - tokamak and stellarator
- Free boundary: coupled to resistive wall/vacuum/coils codes
  - STARWALL (thin walls)
  - CARIDDI (3D volumetric walls)



# JOREK Numerics

- The basis of JOREK is formed by the isoparametric representation of the space (R,Z) and the physics variables.
  - using Bezier finite elements, initially G<sup>1</sup> cubic, now extended to higher order
    - Cubic Hermite elements extended to Bezier patches to allow element refinement

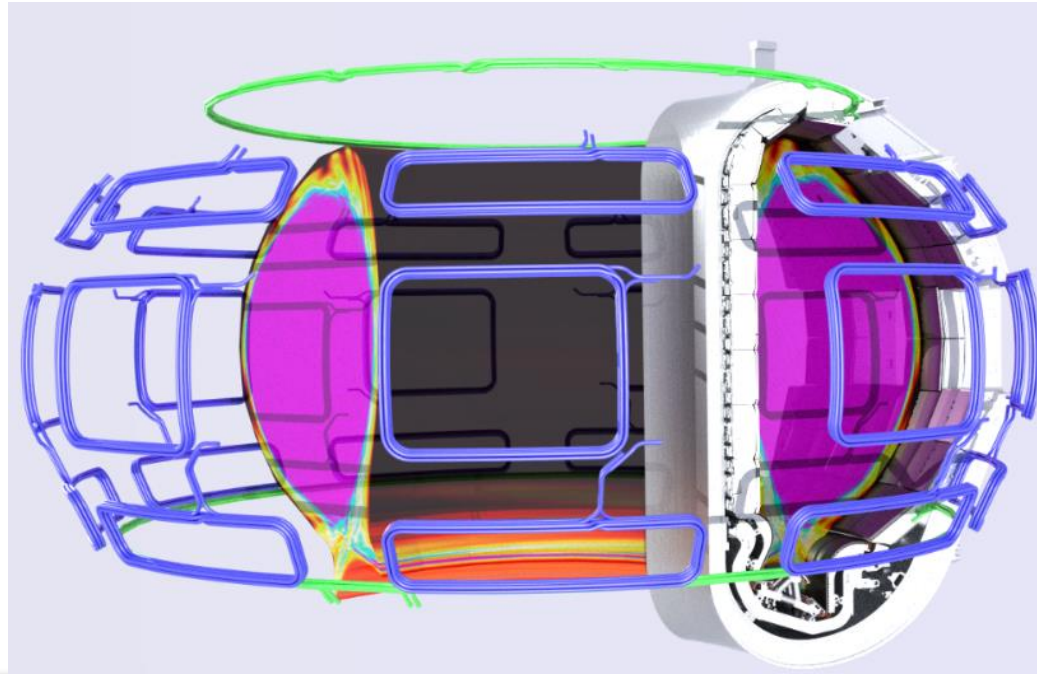
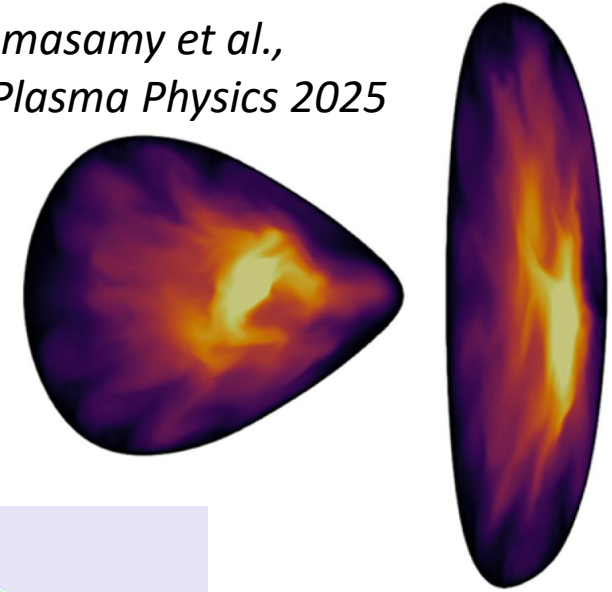
$$R(s, t) = \sum_{k=1}^n \sum_{l=1}^n R_{kl} B_k(s) B_l(t) \quad Z(s, t) = \sum_{k=1}^n \sum_{l=1}^n Z_{kl} B_k(s) B_l(t) \quad \psi(s, t, \phi) = \sum_{m=1}^{n_\phi} \sum_{k=1}^n \sum_{l=1}^n \psi_{kl} B_k(s) B_l(t) e^{im\phi}$$



# MHD Fluid Applications

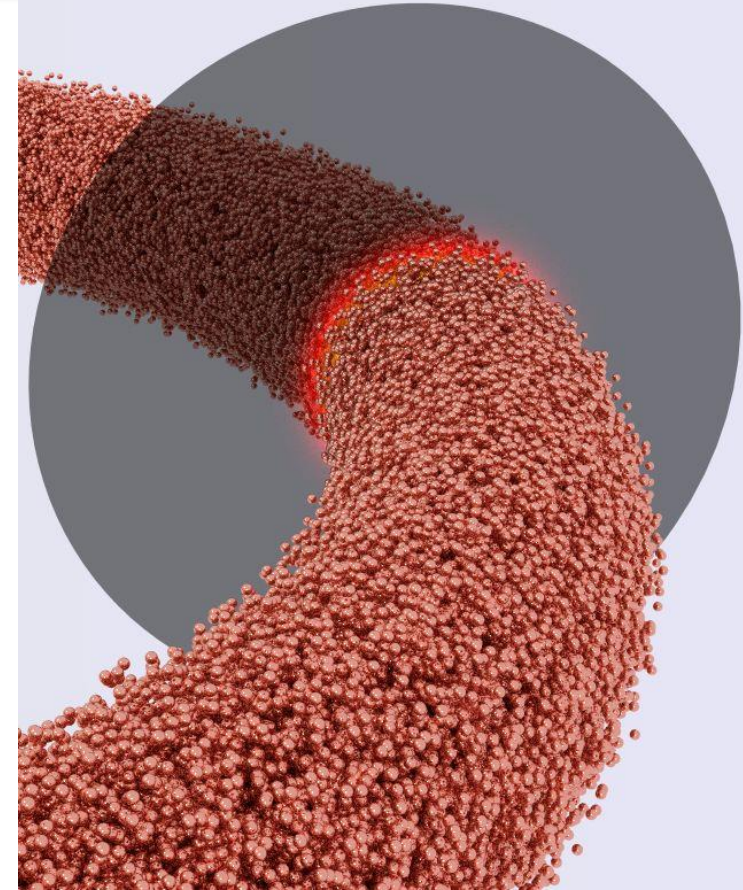
- Disruptions
  - Shattered pellet injection (D, impurities)
  - Vertical displacement events (VDE)
    - Eddy, halo currents, wall loads
- Runaway electrons
  - benign terminations
- Small ELM regimes
  - QCE regime, QH-mode
  - RMP ELM stabilisation
- flux pumping
- Stellarator stability

*Ramasamy et al.,  
J. Plasma Physics 2025*



# JOREK Kinetic Particle Model

- **Particles:** kinetic (i.e. full orbit) or gyro-centre
  - neutrals, impurities, runaway electrons, fast ions, marker particles
- **Pushers:**
  - particles move in  $(R, Z, \varphi)$  and  $(s, t, \varphi)$  space
  - Boris, RK4, RK4\_relativistic, variational, ...
- **Collisions with Maxwellian background**
  - Homma collision model
  - Donnel conservative collision model
  - Coulomb collisions relativistic electrons
- **Projections**
  - projection of particle properties onto JOREK finite elements
    - yields a  $G^1$  continuous representation of particle properties (density, pressure, energy, ...)
  - including filters (perpendicular and parallel)



# JOREK Particle Applications

- Neutrals
  - XPR (+impurities), detachment, small ELM regimes, ...
- Runaway electrons
  - avalanche, hot tail sources
- Impurity transport (neoclassical, MHD driven)
  - Tungsten transport in RMP plasmas, driven by ELMs
- Marker particle representation of shattered pellets (SPI)
  - simultaneous fluid and particle representation of impurities
  - representing a non-coronal charge distribution
- Fast particle driven MHD
- Gyro-kinetics
  - negative triangularity

# JOREK Neutral Model

- Why a neutral model in an MHD code?

- to (better) evaluate the consequences of MHD instabilities on energy deposition on the divertor and first wall
  - ELMs, disruptions, VDEs
- for an improved divertor model
  - Detachment, 3D divertor solutions, RMP, ELM burn through, sputtering yields
- to model interactions between divertor and MHD activity
  - XPR stability

- Why a **kinetic** neutral model?

- fluid behaviour only at high neutral density
  - Non-diffusive transport, non-Maxwellian, ...
- numerically more stable
- faster compared to fluid neutral model

# Particle Time Evolution

- MHD fluid uses fully implicit time evolution scheme (Crank-Nicholson, Gears)
- PIC approach for particles
  - particles live on the same FE grid as fluid
  - particles evolve self-consistently with fluid for the whole duration of a simulation
    - until they are lost (ionised, absorbed)
- Particle contributions to fluid system are (mostly) explicit

## MHD fluid loop

```
for 1:n_step do
```

```
  Recycling, sputtering, puffing (t_step_fluid)
```

## particle loop

```
  for 1:n_substep_particles do
```

```
    - ionisation, charge-exchange, radiation
```

```
    - collisions
```

```
    - collect RHS projection of sources/sinks
```

```
    - advance particles (t_step_particles)
```

```
  - recombination
```

```
  - projection neutrals/fluid exchange terms to  
    FE space
```

```
  Construct (matrix, RHS) MHD fluid
```

```
  Solve system
```

```
  Update state
```

# Kinetic Neutrals - Fluid coupling

- Coupling of JOREK MHD fluid and particles
  - Particle contributions become sources in MHD equations

- Conservative form:

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

$$\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) + \nabla \cdot \bar{\bar{P}} - \vec{J} \times \vec{B} = \vec{S}_v$$

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

- JOREK form

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

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

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

# Kinetic Neutral Model

- Neutrals are born from reflection of the incoming fluid particle flux
  - incoming ion flux from parallel velocity, diffusion and diamagnetic flow
  - with a finite reflection coefficient
    - Using SDTRIM database for probability of fast reflection or thermal desorption
      - Depends on wall material and electron temperature
      - Energy is either a fraction of incoming flux (sampled) or a fixed value for thermal desorption
    - Neutrals reaching the wall are reflected (independent of fluid ion flux)
  - neutrals are super particles with a (time-varying) weight

# Ionisation

- Ionisation using the OPENADAS ionisation rate
  - neutrals are not ionised in one step but **evaporating (losing weight)** along their path
    - Until their weight falls below a given minimum
    - **Sources/sinks collected at every kinetic particle time step** (typically 100x smaller than fluid step)

$$\mathcal{P}_{ion} = \left( 1 - e^{-S_{ion}(n_e, T_e)n_e \Delta t_{kinetic}} \right)$$

if  $\mathcal{U}_{rng}[0, 1] \leq \mathcal{P}_{ion}$ , then

$$w_n^{t+\Delta t_{kinetic}} = w_n^t \mathcal{P}_{ion}.$$

$$S_{\rho}^{ion} = m_i w_n (1 - \mathcal{P}_{ion}),$$

$$S_{\mathbf{v}}^{ion} = S_{\rho}^{ion} \mathbf{v} \quad \text{or} \quad S_{\mathbf{v}_{\parallel}}^{ion} = S_{\rho}^{ion} \mathbf{B} \cdot \mathbf{v},$$

$$S_E^{ion} = S_{\rho}^{ion} \left( \frac{1}{2} v_n^2 - \phi_{ion}/m_i \right),$$

# Charge Exchange, Line Radiation

- Sample an ion from fluid Maxwellian distribution, exchange charge:
  - no radiation losses, no neutral source

$$\mathcal{P}_{CX} = (1 - e^{-S_{CX}(n_e, T_e)n_e \Delta t_{kinetic}})$$

if  $\mathcal{U}_{rng}[0, 1] \leq \mathcal{P}_{CX}$ , then

$$\mathbf{v}_n = \mathcal{N}_{rng} \sqrt{\frac{T_e}{m_i}} + \mathbf{v}_{drift},$$

$$S_{\rho}^{CX} = 0,$$

$$S_{\mathbf{v}}^{CX} = w_n \left( \mathbf{v}_n^{old} - \left( \mathcal{N}_{rng} \sqrt{\frac{T_e}{m_i}} + \mathbf{v}_{drift} \right) \right)$$

$$S_E^{CX} = \frac{1}{2} w_n \left( (v_n^{old})^2 - (v_n^{new})^2 \right).$$

- Line radiation:

– effective radiated power

$$P_{rad,line} = n_e w_n S_{PLT}(n_e, T_e) \Delta t_{kinetic}$$

# Recombination

- The number of ions to be recombined is calculated in each element
  - $S_{rec}$  from fluid density and temperature
  - also lost energy and momentum
- Density, momentum and energy conservation imposed per element
  - at least one neutral super particle is created per element
    - those in the core are rapidly ionised

$$w_n = \frac{1}{m_i} \int_{elm} \rho_{rec} dV = \int_{elm} S_{rec} n_e n_i \Delta t_{fluid} dV,$$
$$\mathbf{v} = \frac{\int_{rec} \rho_{rec} \mathbf{v}_{drift} dV}{m_i w_n}.$$

# Sources, Moments

- The sources are given by:
$$S_\rho(\vec{x}) = \int mf(\vec{x}, \vec{v}) d\vec{v}$$
$$S_v(\vec{x}) = \int m\vec{v}f(\vec{x}, \vec{v}) d\vec{v}$$
$$S_E(\vec{x}) = \int \frac{1}{2}mv^2 f(\vec{x}, \vec{v}) d\vec{v}$$

- Express sources in JOEREK finite element 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 (system of equations to be solved):

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

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

$$\int H(s,t) \sum_{ijk} p_{\rho,ijk} H_{ij}(s,t) H_{\varphi,k}(\varphi) d\vec{x} = \sum_n H(s,t) mw_n \delta(\vec{x} - \vec{x}_n)$$

# Moments: Filters

- Some smoothing is required
  - depending on number of particles
- Modified projection equation:

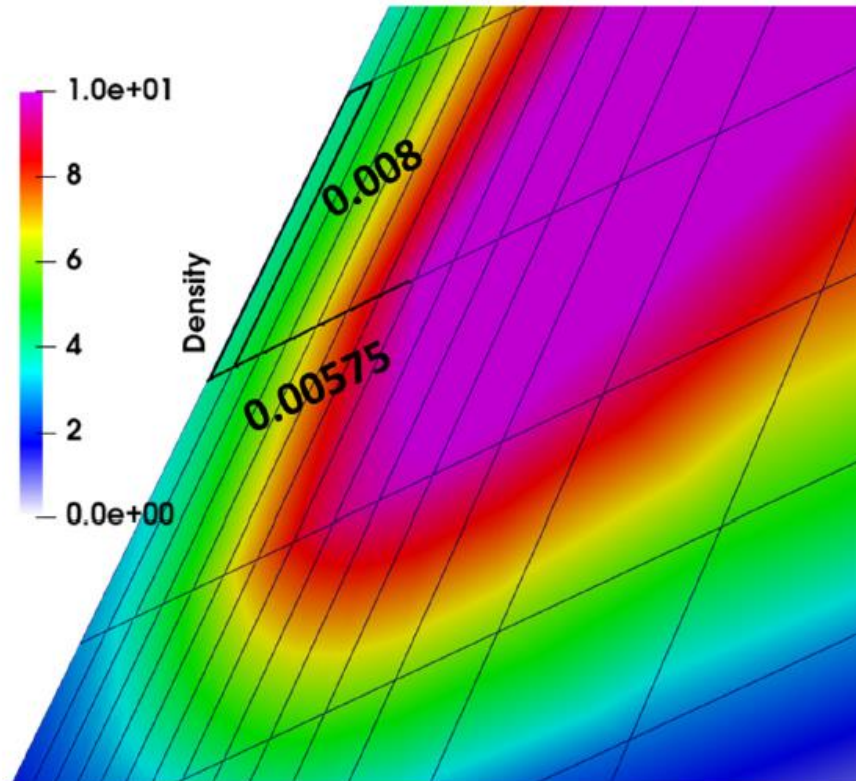
$$\int v^* (\vec{x}) (1 - \lambda \nabla^2 - \zeta \nabla^4) \tilde{S}_\rho (\vec{x}) d\vec{x} = \int v^* S_\rho (\vec{x}) d\vec{x}$$

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

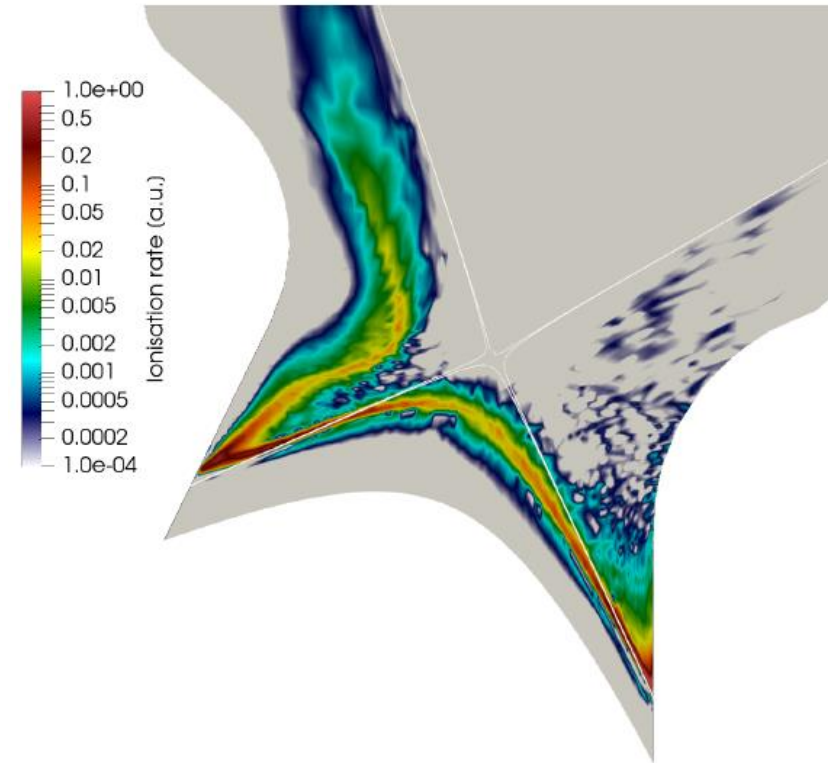
- LHS matrix is calculated and factorised only once
- **RHS is collected at every particle step**
  - Important for conservation properties
- Projection (solve step) at every JOEREK fluid time step
  - resulting sources available as  $G^1$  finite element discretisation

# Divertor Grid Resolution

- High grid resolution is required at the divertor targets
  - Accumulation of elements, grid aligned with equilibrium flux surfaces
  - ITER example: (cubic) element size (parallel) < 1mm, along divertor ~8mm



*Density at ITER inner divertor strikepoint*



*Ionisation pattern ITER case with ExB drifts*

# Example Energy Balance

- Energy balance (ITER high recycling, attached case)

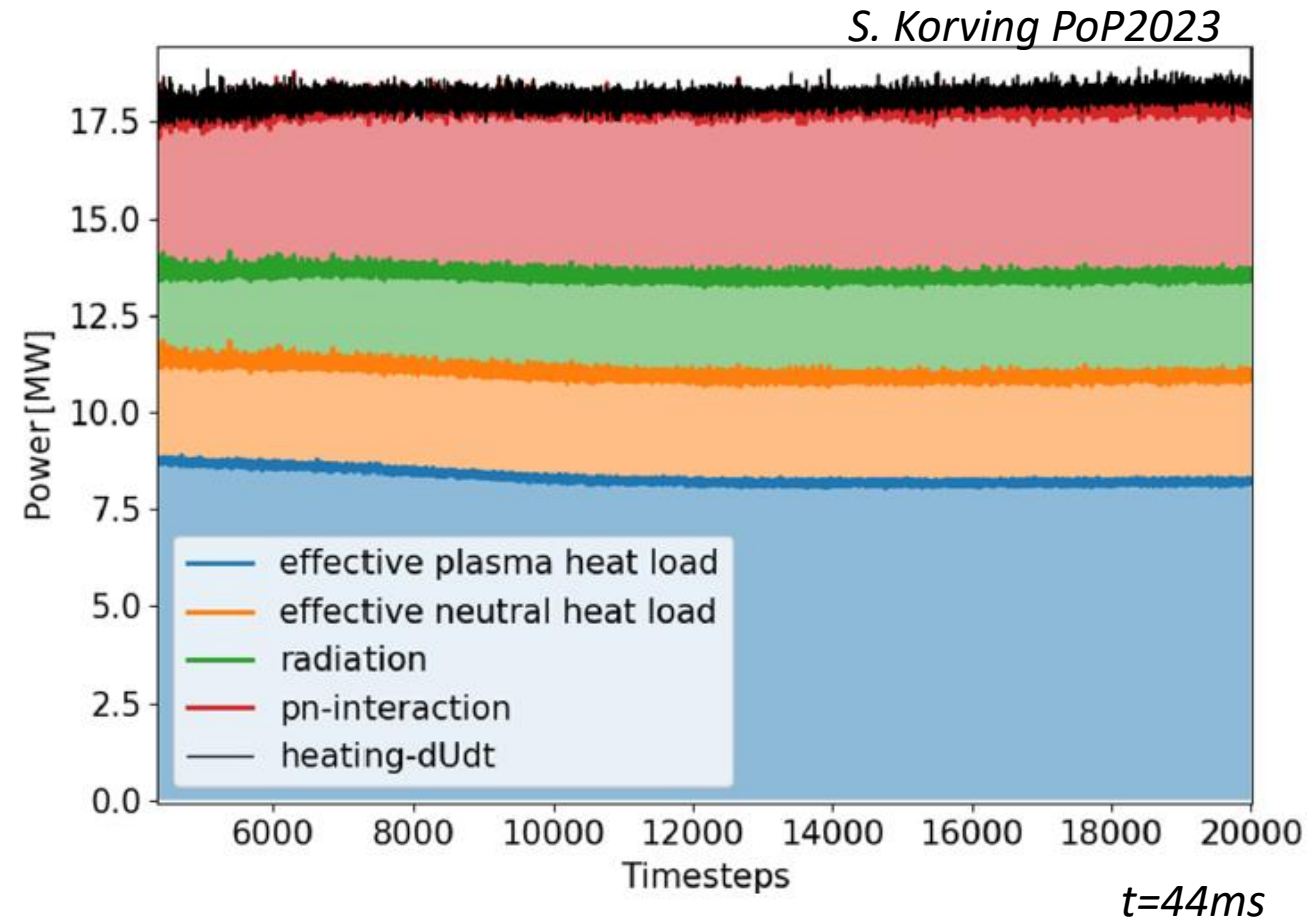
- $n_{\text{neutrals}} \sim 10^6\text{-}10^7$  super particles

- Time step =  $2.2 \times 10^{-6}$  s

- typical error  $\varepsilon \sim 10^{-2}\text{-}10^{-3}$

- depending on time step and # particles

- Particle conservation error is typically  $< 10^{-4}$



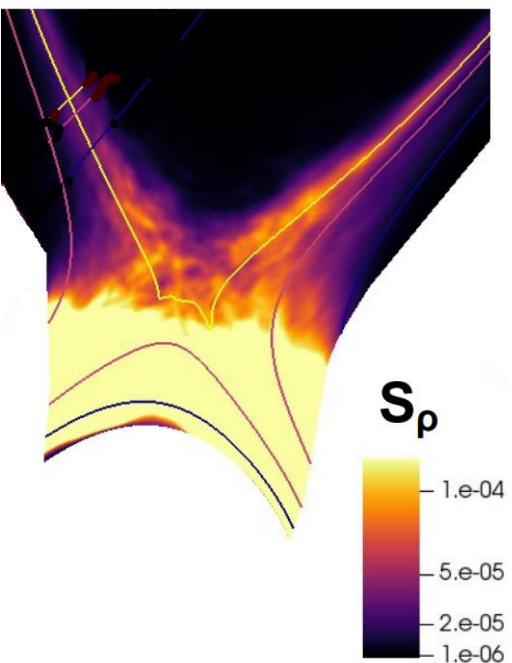
# Applications Kinetic Neutrals (and Impurities)

- Dynamic detachment for control (Daniël Maris)
- QCE regime (Andres Cathay)
- XPR regime (Máté Szűcs)
- ELM detachment burn through
- 3D Divertor with RMP
- ...

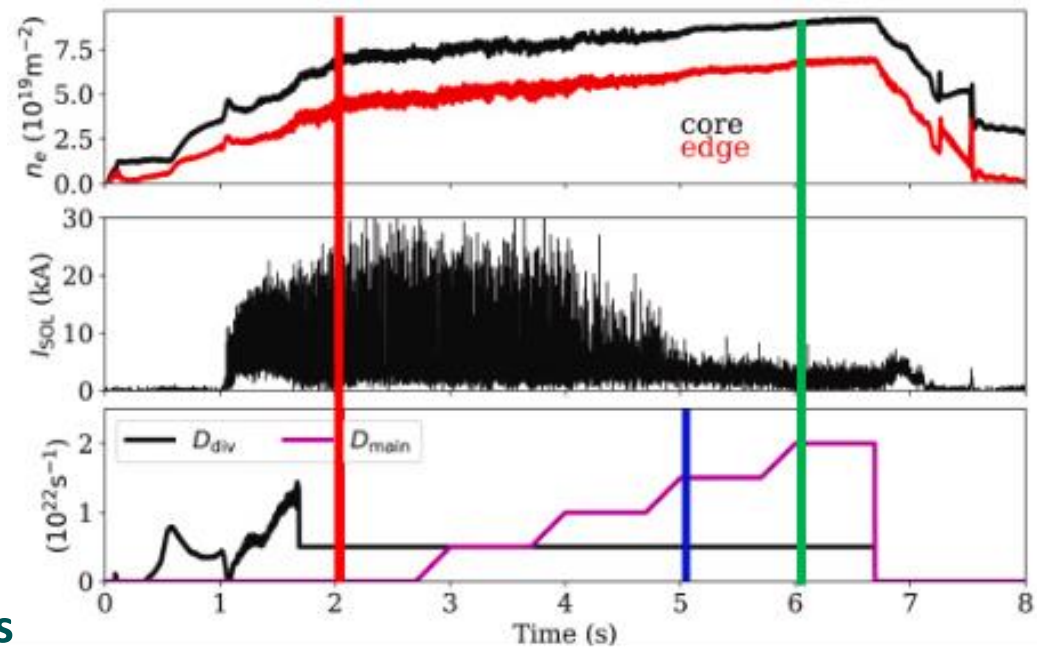
# JOREK modelling AUG #36165: kinetic neutrals and QCE (A. Cathey)

- 0.8 MA / 2.5 T,  $q_{95} = 5.3$  with constant shape:  $\delta_{up/lo} = 0.27 / 0.40$  and  $\kappa_{up/lo} = 1.58 / 1.85$
- Ramp  $\Gamma_D$  changes ELM behaviour (type I ELMy — QCE)
- JOREK input:  $t_0=6$  sec, reduced MHD with drifts, wall and recomb., CX, ionisation, line radiation, and  $\Gamma_D = 0, 1, 2.8, 3.2, 4, 6.0 \times 10^{22}$  e/sec

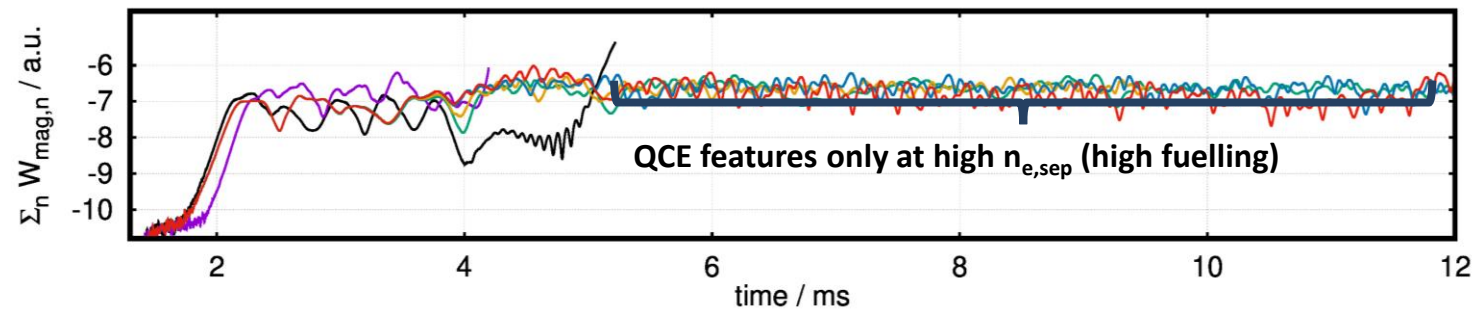
neutral density



- Ionisation peak moved out
- ELM onset at lowest puff rates
- High-n resistive peeling-ballooning modes regularly causing transport at higher puffing
- modes get stronger with more puffing — ballooning transport enhanced



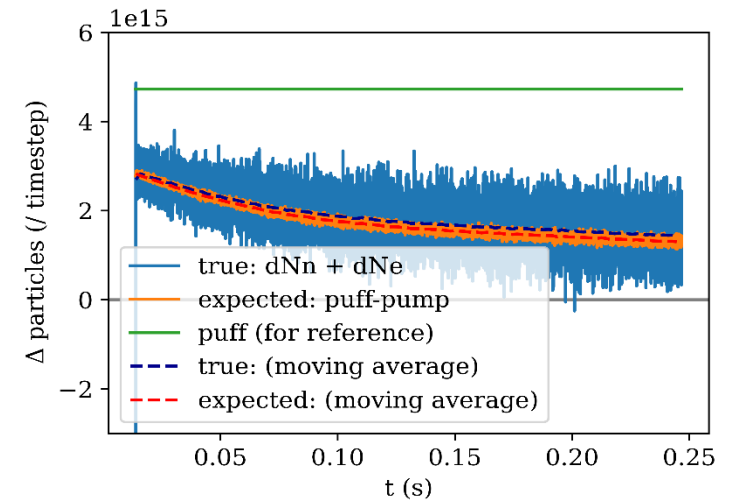
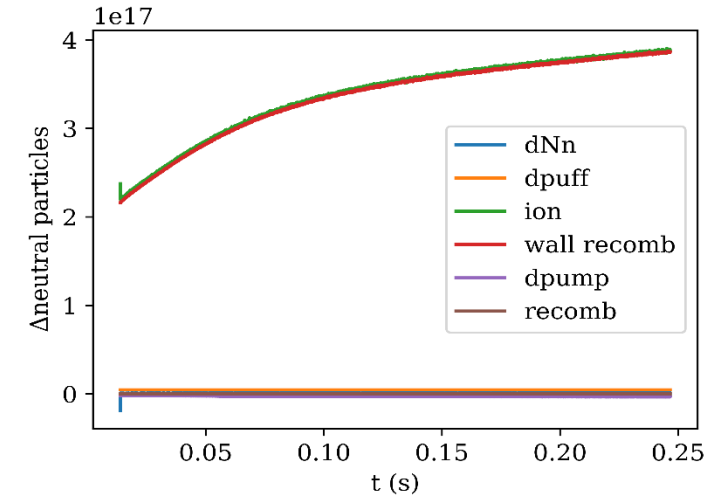
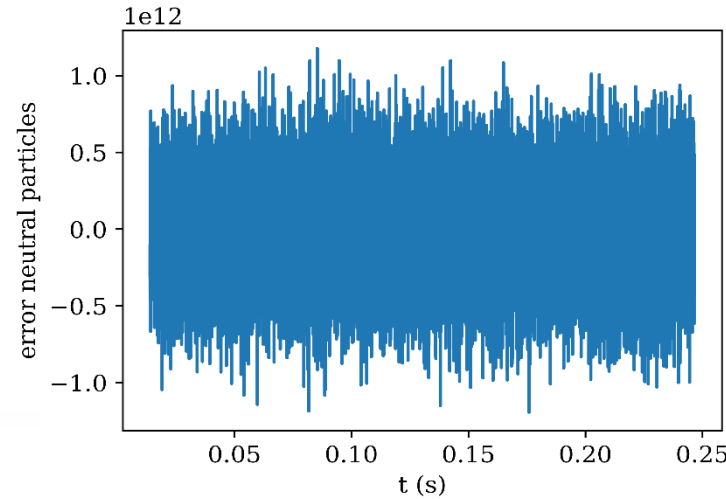
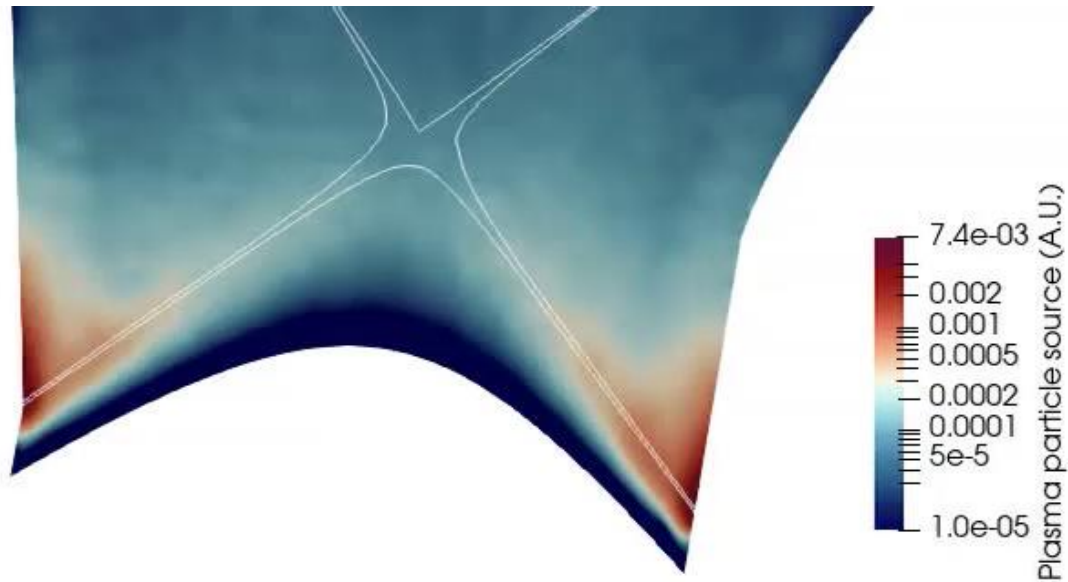
ELMs		QCE		QCE	
puff = 0.0e22 e/s	—	2.8e22 e/s	—	4.0e22 e/s	—
1.0e22 e/s	—	3.2e22 e/s	—	6.0e22 e/s	—



# Dynamics of Detachment (for control purposes, D. Maries)

- Long timescale 2D simulations of fluid+kinetic neutrals model (in AUG)
  - particle conservation:

Ionisation source



# Summary

- The JOREK kinetic neutral model is implemented as a PIC model:
  - neutrals are evaporating along their path
  - with self-consistent time evolution (no re-initialisation at fluid time steps)
  - on the same grid as the fluid model
  - appears to be robust, excellent parallelisation
  - no large slowdown of fluid simulations with kinetic neutrals
  
- Work in progress:
  - neutral-neutral collisions (DM)
  - molecules (DM)
  - neutrals in GK model (GH)