Three-dimensional edge plasma and neutral gas modeling with the EMC3-EIRENE code on the example of RMP application in tokamaks - status and development plans

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Motivation: Quantification of a 3D plasma edge

One promising approach to control particle and heat loads onto divertor targets is the application of resonant magnetic perturbations (RMPs).

RMP application results in the formation of a non-axisymmetric configuration. → 3D modeling

Intrinsic error fields are non-axisymmetric as well!

What we ultimately want to address:

What is the impact of RMPs on detached divertor operation?

What do we need to do:

Provide a reliable simulation model, at least of the same maturity as state of the art 2D models (e.g. SOLPS).
1. Introduction to EMC3-EIRENE

2. Overview on simulation results for DIII-D

3. Numerical access to high $n_e$, low $T_e$ divertors
A 3D steady state fluid model for the edge plasma

Particle balance ($n$: plasma density)

$$\nabla \cdot \left[ nu || e || - D_\perp e_\perp e_\perp \cdot \nabla n \right] = S_p$$

$D_\perp$: anomalous cross-field diffusion, $S_p$: ionization of neutral particles
A 3D steady state fluid model for the edge plasma

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Momentum balance ($u_{||}$: fluid velocity parallel to magnetic field lines)

$$\nabla \cdot \left[ m_i n u_{||}^2 e_{||} - \eta_{||} e_{||} e_{||} \cdot \nabla u_{||} - D_\perp e_\perp e_\perp \cdot \nabla (m_i n u_{||}) \right] = -e_{||} \cdot \nabla n (T_e + T_i) + S_m$$

$\eta_{||} \propto T_i^{5/2}$: parallel viscosity, $\eta_\perp = m_i n D_\perp$: cross-field viscosity, $S_m$: interaction (CX) with neutral particles
A 3D steady state fluid model for the edge plasma

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Energy balance ($T_e$, $T_i$: electron and ion temperature)

$$\nabla \cdot \left[ \frac{5}{2} T_e (n u_\parallel e_\parallel - D_\perp e_\perp e_\perp \cdot \nabla n) - (\kappa_e e_\parallel e_\parallel + \chi_e n e_\perp e_\perp) \cdot \nabla T_e \right] = +k (T_i - T_e) + S_{ee}$$

$$\nabla \cdot \left[ \frac{5}{2} T_i (n u_\parallel e_\parallel - D_\perp e_\perp e_\perp \cdot \nabla n) - (\kappa_i e_\parallel e_\parallel + \chi_i n e_\perp e_\perp) \cdot \nabla T_i \right] = -k (T_i - T_e) + S_{ei}$$

$\kappa_{e,i} \propto T_{e,i}^{5/2}$: classical parallel heat conductivity, $\chi_{e,i}$: anomalous cross-field transport, $k \propto n^2 T_e^{-3/2}$: energy exchange between el. and ions, $S_{ee}, S_{ei}$: interaction with neutral particles and impurities (radiation)
A Monte Carlo method for fluid edge plasmas

- Balance equations can be cast in generic Fokker-Planck form:

\[
\frac{\partial}{\partial t} \mathcal{F} + \nabla \cdot \left[ \mathbf{V} \mathcal{F} - \nabla \cdot \mathbf{D} \mathcal{F} \right] = S
\]  

(1)

with corresponding drift (\(\mathbf{V}\)) and diffusion (\(\mathbf{D}\)) coefficients and sources/sinks (\(S\)).

- (1) is related to a **stochastic process** → apply Monte Carlo method: follow “fluid particles” from source to sink.

- The motion of simulation particles is determined by the coefficients \(\mathbf{V}\) and \(\mathbf{D}\) and numerical time step \(\tau\). Along field lines we have:

\[
\Delta l_{||} = \mathbf{V}_{||} \tau + \sqrt{2 \mathbf{D}_{||} \tau} \xi, \quad \langle \xi \rangle = 0, \quad \langle \xi^2 \rangle = 1
\]  

(2)
A Monte Carlo method for fluid edge plasmas

- Balance equations can be cast in generic Fokker-Planck form:

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\frac{\partial}{\partial t} F + \nabla \cdot [\mathbf{v} F - \nabla \cdot \mathbf{D} F] = S
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(2)

- Classical parallel heat conduction (\(q_{||} = -\kappa_{||} \nabla_{||} T\), \(\kappa_{||} \sim T^{5/2}\)):

\[
q_{||} = -\nabla_{||} \frac{2 \kappa_{||}}{7} T
\]  

(3)

H. Frerichs (hfrerichs@wisc.edu)  
3D edge plasma and neutral gas modeling with EMC3-EIRENE
Self-consistent solution by iterative application

- **Input for EMC3-EIRENE:**
  - User-defined boundary conditions: $n_{\text{ISB}}$ or $\Gamma_{\text{rec}}$ or $(\Gamma_{\text{in}}, \varepsilon_{\text{pump}})$, $P_{\text{in}}$.
  - User-defined model parameters: $D_\perp, \chi_e \perp, \chi_i \perp$.

- **Built-in boundary conditions:** $c_s$ at target, sheath heat transmission coefficients $\gamma_e, \gamma_i$.

- **A relaxation factor** $\alpha_{\text{rlx}}$ needs to be introduced because of the strong non-linearity:
  \[
  F_{n,\text{rlx}} = \alpha_{\text{rlx}} F_{n-1} + (1 - \alpha_{\text{rlx}}) F_n
  \]

- **Approximate convergence:** small changes between iterations at intrinsic noise level.

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**Magnetic field structure reconstructed from 3D grid**

**Plasma Transport**
- EMC3: Fluid model
- Monte Carlo method

**Neutral Gas Transport**
- EIRENE: Kinetic Model
- Monte Carlo method

![Graph](image)

- $\Delta T_e$
- Number of iterations
- $\alpha_{\text{rel}} = 0, 0.1, 0.2, 0.4$

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H. Frerichs (hfrerichs@wisc.edu) 3D edge plasma and neutral gas modeling with EMC3-EIRENE
The field line reconstruction module allows geometric flexibility

- Magnetic field lines are reconstructed from a 3D finite flux-tube grid (bilinear interpolation).

- The 3D grid is generated by field lines tracing starting from 2D base grids.
  → finite flux-tube length for good cross-section.
  - Discretization in the cross-field direction can be adapted to the magnetic configuration at hand.
  - Single null and disconnected double null configurations available.
  - Application: DIII-D, MAST, JET, ITER, …
  - Easy to setup advanced magnetic divertor configurations (Super-X or Snowflake).

H. Frerichs (hfrerichs@wisc.edu)
Introduction to EMC3-EIRENE

Overview on simulation results for DIII-D

Numerical access to high $n_e$, low $T_e$ divertors
An ITER similar shape plasma at DIII-D

Vacuum RMP configuration:

- Magnetic field structure at the plasma edge: island chains, chaotic regions, short flux tubes.
- The perturbed separatrix introduces a helical deformation of the regular SOL, and guides field lines to a non-axisymmetric divertor footprint.

DIII-D discharge 132741: $I_c = 4 \text{kA}(n = 3)$
$B_t = 1.8 \text{T, } I_p = 1.5 \text{ MA, } q_{95} = 3.5$
Discrepancy between simulations and experiments

DIII-D: ITER similar shape H-mode plasma at low collisionality

- **Experiment**: Striation pattern in particle loads, but **not** in heat loads. Moderate temperature reduction by RMPs.
- **Simulation**: Striation pattern in both particle and heat loads. Significant temperature reduction by RMPs.

Possible reasons for this discrepancy:
1. “Kinetic corrections” to fluid model necessary at low collisionalities?
2. Partial screening of RMPs by plasma response?
3. Recycling conditions?
1. Adjust el. heat conduction at low collisionalities

- An upper limit is given by free streaming particles (with thermal velocity):
  \[ q_{\text{lim}} = \alpha_e n_e \nu_{th,e} T_e, \quad \alpha_e \approx 0.03 \ldots 0.15. \]

- This can be related to a correction factor \( \beta \) for the heat conductivity:
  \[ \kappa^*_e = \beta \kappa_e, \quad \beta = \left( 1 + \frac{\kappa_e |\nabla T_e|}{q_{\text{lim}}} \right)^{-1} \leq 1. \]

- Explore the impact of a reduced \( \kappa_e \), set fixed value for \( \beta \):

![Graph showing the impact of RMPs on the electron temperature](image-url)

A correction of \( \beta \approx 10^{-3} \) is required to be consistent with an experimentally observed temperature reduction of \( \sim 20\% \).
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2. Approximation of screening of RMPs

- The plasma may screen external magnetic perturbations, which would result in a modification of the magnetic field structure.

- A helical current sheet model has been used to explore the impact of RMP screening by plasma response. Here: $m = 7 - 11$ resonances are screened:

  $\therefore$ The open chaotic layer is limited to the very edge ($\sim 0.96$).
Screening of RMPs cannot be too strong!


- The striation patterns of particle and heat loads follow the magnetic field structure. → Secondary peaks are reduced with "plasma response".
- While this gives better agreement for the heat loads, it is against experimental observations regarding the particle load!

- The plasma response is consistent with a core temperature drop of 20% in the experiment.
- A plateau remains in the (reduced) open field line region.
  → combination of moderate screening and heat flux limit?
3. Recycling conditions can explain the qualitative difference between particle and heat flux pattern

- The pumping parameter $\varepsilon_{\text{pump}}$ allows to control recycling conditions (although it is determined by the present pump setup).
- Reducing $\varepsilon_{\text{pump}}$ to small values significantly increases the total recycling flux, but the splitting into primary and secondary peaks remains.

The secondary heat flux peaks “detach” under (artificial?) high-recycling conditions. But peak level is still too high (“radiation shortfall”)!
Introduction to EMC3-EIRENE

Overview on simulation results for DIII-D

Numerical access to high $n_e$, low $T_e$ divertors
Numerical access to detachment: generalize coupling between EMC3 and EIRENE

- Include neutral **gas-puffing** and **volume recombination**.

  → Particle balance from plasma (EMC3) and neutral gas (EIRENE) point of view:

  \[
  \Gamma_{\text{fuel},P} + \Gamma_{\text{ion}} = \Gamma_{\text{target}} + \Gamma_{\text{vol. rec.}} \\
  \Gamma_{\text{rec}} + \Gamma_{\text{fuel},N} + \Gamma_{\text{vol. rec.}} = \Gamma_{\text{pump}} + \Gamma_{\text{ion}}
  \]

- Different operation modes available: set control parameter $\Gamma_{\text{tot}}$, $n_{\text{ISB}}$ or $c_{\text{rec}}$ allows explicit ($\Gamma_{\text{pump}}$) and implicit ($c_{\text{rec}} < 1$) treatment of particle sinks.

- Stable access to high density, low temperature divertor conditions remains an issue: oscillations occur even before volume recombination is switched on.
Numerical instability related to simulation procedure?

- The transport solver (EMC3-EIRENE) is a non-linear operator
  \[ \Phi_{\text{EMC3-EIRENE}} : \mathcal{P} \rightarrow \mathcal{P}', \quad \mathcal{P} = \{ n(x), M(x), T_e(x), T_i(x) \} \]
  which maps the plasma state \( \mathcal{P} \) to \( \mathcal{P}' \) (because transport coefficients and sources depend on \( \mathcal{P} \)).

- For a self consistent plasma solution we need to find a fixed-point
  \[ \mathcal{P}^* = \Phi_{\text{EMC3-EIRENE}}(\mathcal{P}^*) \]

- The simulation procedure resembles an iterative approximation
  \[ \mathcal{P}_{n+1} = \Phi_{\text{EMC3-EIRENE}}(\mathcal{P}_n) \quad \text{until} \quad \| \mathcal{P}_{n+1} - \mathcal{P}_n \| \leq C \]

- However, “complicated” dynamics is a well known feature of non-linear maps.
Two-point model analysis of the simulation procedure

- Oscillations of the plasma state occur when the divertor temperature drops below a few eV.
- This behavior can be captured within a two-point model (2PM) analysis of the simulation procedure ($P_{n+1} = \Phi_{\text{EMC3-EIRENE}}(P_n)$):

\[
2 n_t T_t = f_{\text{mom}} n_u T_u \quad (4)
\]

\[
T_u^{7/2} = T_t^{7/2} + \frac{7 f_{\text{cond}} q_{\parallel} L}{2 \kappa_0 e} \quad (5)
\]

\[
(1 - f_{\text{power}}) q_{\parallel} = \gamma e n_t T_t c_{st} \quad (6)
\]

- Account for $T_t$ and $n_t$ dependence in $f_{\text{power}}, f_{\text{mom}}$ and $f_{\text{cond}}$
- A relaxation factor $\alpha$ is applied in the simulations with the intention to stabilize the iterative procedure:

\[
Q_{n+1}' \mapsto \alpha Q_n + (1 - \alpha) Q_{n+1}
\]
Oscillations of the plasma state occur when the divertor temperature drops below a few eV.

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\[
T_{t,(n+1)} = \frac{(1 - f_{\text{power}}) q_{\parallel}}{\gamma e n_t c_{si}(T_{t,(n)})}
\]

\[
T_{u,(n+1)} = \frac{1}{T_{u,(n)}^{5/2}} \left[ T_{t,(n)}^{5/2} T_{t,(n+1)} + \frac{7 f_{\text{cond}} q_{\parallel} L}{2 \kappa_{0e}} \right]
\]

\[
n_{t,(n+1)} = \frac{f_{\text{mom}} n_u T_u}{2 T_t}.
\]

Account for \( T_t \) and \( n_t \) dependence in \( f_{\text{power}}, f_{\text{mom}} \) and \( f_{\text{cond}} \)

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Convergence control by adaptive relaxation

- The orbits in $n_t-T_t$ space are rather robust with respect to the relaxation factor, however, the frequency of the cycle $\Omega \to 0$ for $\alpha \to 1$.

- An **adaptive relaxation** method is motivated by the character of the cycle in $n_t-T_t$ space:
  1. weak relaxation for $T_t$ in quad. 1 and 3
  2. strong relaxation for $T_t$ in quad. 2 and 4

- Analyze history of $n_t$ and $T_t$ to approximate the phase $\varphi_n$. Then apply adaptive relaxation:

\[
\alpha_n = \alpha_{\text{weak}} + (\alpha_{\text{strong}} - \alpha_{\text{weak}}) A_n, \quad A_n = \frac{1}{2} \left(1 \pm \sin(2\varphi_n)\right)
\]

An adaptive relaxation scheme is straightforward to implement into the EMC3-EIRENE code as a post-processing subroutine, although robustness is still an issue for complex 3D simulations.
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- Such an adaptive relaxation scheme is straightforward to implement into the EMC3-EIRENE code as a post-processing subroutine, although robustness is still an issue for complex 3D simulations.

The experimentally observed pattern of divertor particle and heat fluxes can be reconstructed by adjusting the recycling conditions.

Some discrepancies remain regarding the global power balance and pumping efficiency (boundary condition).

Model extensions require (at least) a formulation of a “heat flux limit” suitable for Monte Carlo methods, and coupling to realistic modeling of MHD effects (plasma response from M3D-C1, NIMROD, VMEC).

An adaptive relaxation method has been proposed to stabilize simulations at high divertor density and very low temperatures, with promising results for application in EMC3-EIRENE.
Extended operation mode of EMC3-EIRENE

EMC3
3D fluid edge plasma transport code

\[ n, M, T_e, T_i \]

EIRENE
kinetic neutral particle transport code (3D)

\[ n_H, n_{H_2} \]

\[ \Gamma_{rec} = \Sigma_{vol} + \Gamma_{ISB} \]

\[ \Sigma_{vol} = \int_{V_{sim}} dV S_p \]

\[ \Gamma_{ISB} = \Gamma_{fuel} + \Gamma_{core} \]

\[ = \Gamma_{pump} \text{ in steady state} \]

Pumping by partially absorbing surface
new free model parameter:

\[ \epsilon_{pump} \]
The overestimation of the peak heat flux is related to missing/underestimated other power losses.

- The experimental **steady state** power balance at DIII-D (ISS H-mode plasmas, ELM suppression by RMPs): $P_{in} = 6 - 8 \text{ MW}$ edge input power.
- **Very weak striation** pattern from RMPs: (shot 132741: Schmitz, JNM 415 (2011) S886)

![Graph showing heat flux vs. distance along wall]

- Power deposition profile can be fitted to generic formula:
  
  $q(\bar{s}) = \frac{q_0}{2} \exp \left( - \frac{S}{2 \lambda q f_x} \right) - \frac{\bar{s}}{\lambda q f_x} \text{erfc} \left( \frac{S}{2 \lambda q f_x} - \frac{\bar{s}}{S} \right) + q_{BG}$

- Integral: $Q \approx 2\pi R_0 \lambda q f_x q_0$

- Some power losses unaccounted for? (Radiation, fast particles?)
- “Radiation shortfall” is a known issue in 2D simulations.
Implementation of heat flux limit in Monte Carlo scheme

- Adapted parallel heat flux: \( q_\parallel = -\beta \kappa_\parallel \nabla_\parallel T_e \)

\[
q_\parallel = -\nabla_\parallel \left( \frac{2 \beta \kappa_\parallel}{7} T_e \right) + T_e \left( \frac{-2 \beta \kappa_\parallel}{7} \nabla_\parallel \ln \beta \right)
\] (4)

- Direct implementation (explicit):

\[
\Delta l_\parallel = \mathbf{V}_\parallel \tau + \sqrt{2 \mathcal{D}_\parallel \tau \xi}
\] (5)

- Two-step method (implicit, predictor-corrector): \( \Delta l_\parallel = l_1 + l_2 \)

\[
l_2 = l_1 \left( \sqrt{1 - \Delta} - 1 \right), \quad \Delta = \ln \beta(l_1) - \ln \beta(0)
\] (6)

\[
n \approx \mathbf{V}_\parallel \tau \xi^2
\] (7)
Magnetic field lines are reconstructed from a field aligned grid, which allows a significant speedup of the parallel motion of particles.

Bilinear interpolation between 4 pre-defined field lines $\mathbf{F}_i(\varphi)$ at the position $(\xi, \eta, \varphi)$ of a simulation particle:

$$\mathbf{F}^*_{\xi,\eta}(\varphi) = \sum_{i=1}^{4} \mathbf{F}_i(\varphi) \, N_i(\xi, \eta)$$

where

$$N_i = \frac{1}{4} (1 + \xi_i \xi)(1 + \eta_i \eta)$$

are shape functions (known from Finite Element Methods) and $\xi, \eta$ are field line labels.

Grid cells must be convex for a unique relation $(R, Z) \leftrightarrow (\xi, \eta)$, therefore toroidal sub-domains are necessary.
Even the 2PM exhibits bifurcations and oscillations

\begin{align*}
\alpha = 0.2 & \quad 0.4 \\
0.6 & \quad 0.8
\end{align*}

\begin{align*}
T_1 [eV] & \\
\text{Iteration number}
\end{align*}

a) \hspace{1cm} b)
2PM analysis

\[ T_u \approx \left( \frac{7 q_{\parallel} L}{2 \kappa_0 e} \right)^{2/7} f_{\text{cond}}^{2/7} = T_{u0} \]

\[ T_t = \frac{m}{2 e} \frac{4 q_{\parallel}^2}{\gamma^2 e^2 n_u T_u^2} \frac{(1 - f_{\text{power}})^2}{f_{\text{mom}}^2 f_{\text{cond}}^{4/7}} = F_u \]

\[ n_t = \frac{f_{\text{mom}} n_u T_u}{2 T_t} = \frac{n_u T_{u0}}{2 F_u} \frac{f_{\text{mom}}^3 f_{\text{cond}}^{6/7}}{(1 - f_{\text{power}})^2} \]

\[ f_{\text{power}} = \varepsilon(n_t, T_t) \Gamma_t q_{\parallel} \]

\[ f_{\text{mom}} = 1 - \exp(-\Delta X_{\perp} / \lambda), \quad \lambda = \frac{v_{th}}{n_t \langle \sigma_{iz} v \rangle} \]

\[ f_{\text{cond}} = 1 - \left( \frac{T_t - T_c}{T_c} \right)^2 \text{ for } T_t < T_c = 4 \text{ eV} \]