Progress with practical implementation of neutrals models in SOLEDGE3X and perspectives

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Neutrals models in SOLEDGE3X

- 3 options: **none**, **fluid** and **kinetic** neutrals
- **Fluid neutrals** embedded in SOLEDGE3X:
  - Very crude diffusive model
  - Done in separate order 1 time-stepper compared (≠ plasma) - bad initial choice
  - Current work 3-fold:
    1. recast neutrals solver into main time-stepper
    2. Implement more advanced neutrals model from TSVV5
    3. Move towards 3D PFCs configuration (TSVV6)
- **Kinetic neutrals** implemented via coupling to EIRENE
  - First experienced in TOKAM3X
  - Current work 2-fold:
    1. Revive 3D axi-symmetric PFC version in SOLEDGE3X for turbulence studies
    2. Test and improve coupling strategy on 2D mean-field reactor relevant cases

Fluid neutrals in SOLEDGE3X

- Fluid neutrals implemented with extremely **crude model** until now:
    - **Purely diffusive** with constant and unique diffusion coefficient
    - for each element X in the plasma

$$\partial_t n_{X0} + \vec{\nabla} \cdot \vec{\Gamma}_{X0} = S_{X0} - \langle \sigma v \rangle_i^{nX0} n_e n_{X0} + \langle \sigma v \rangle_r^{nX+} n_e n_{X+}$$

$$\vec{\Gamma}_{X0} = -D_n \vec{\nabla} n_{X0}$$

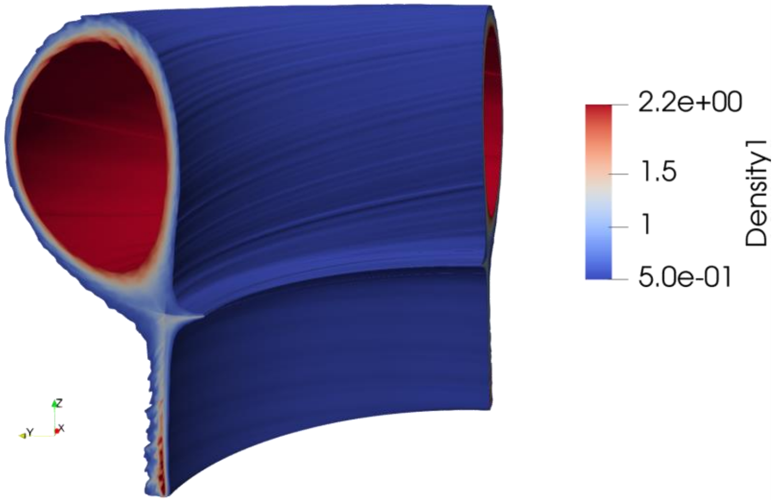
-
    - Boundary conditions: **recycling / sputtering** characterized by recycling matrix at wall + zero flux at center + possibly to add **puff** via S_{X0}

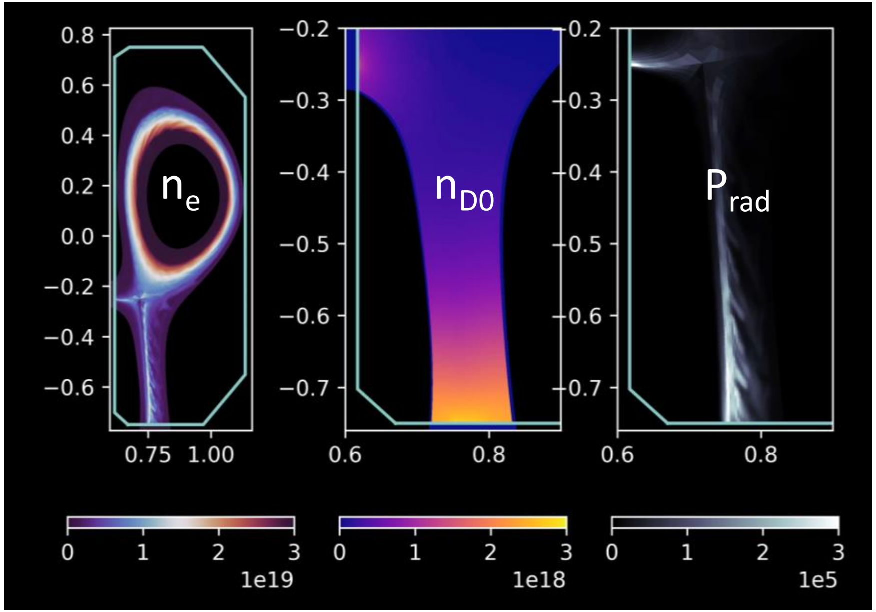
$$\vec{\Gamma}_{nX0} = -\sum_{X'} R_{X,X'} \sum_{i=1}^{Z_X} \left(\vec{\Gamma}_{X'i+} \cdot \vec{n} \right) \vec{n}$$

- $D_n \sim 1000\, m^2.s^{-1}$ => **3D implicit elliptic solver**
    - Much less costly than potential solver due to isotropy (AMG extremely effective)

Exemple of application: TCV case

- R = 0.8, high recycling case, puff feedback on separatrix density
- **Strong turbulence activity in divertor legs** in spite of particle source essentially in divertor (≠ first attempt with TOKAM3X + neutrals)

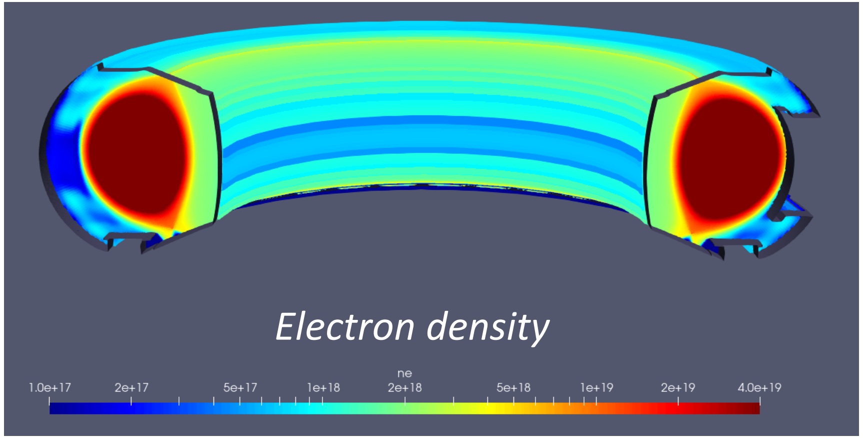




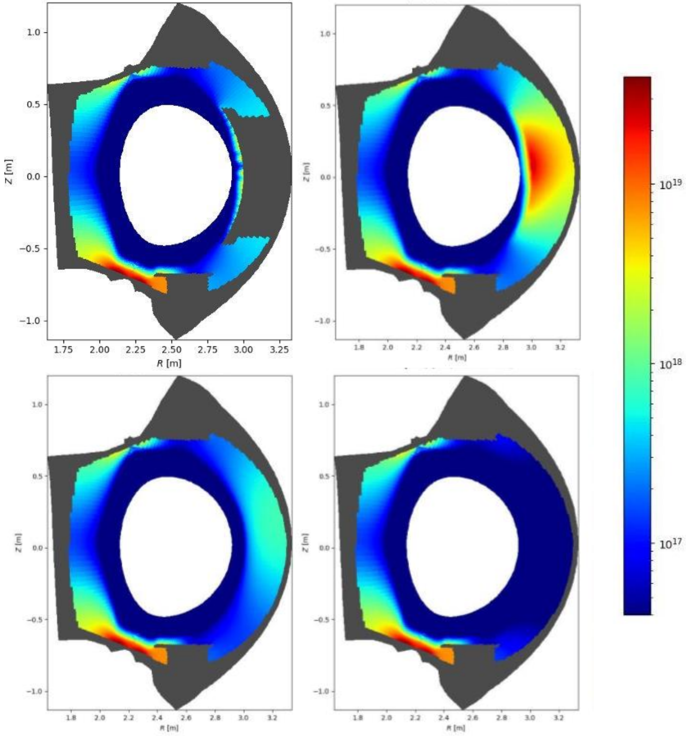
[H. Bufferand et al., CPP2021, submitted]

Fluid neutrals: extension to full 3D PFCs (TSVV6)

- ❖ SOLEDGE3X from start designed to handle not axisymmetric PFCs, but never tested until now
- ❖ After correction of a few issues, first successful tests at **running with 3D PFC (antenna) and fluid neutrals**



Electron density



Atoms density in 4 poloidal planes

Towards higher fidelity fluid neutrals model

- Simplistic diffusive model has **severe limitations**:
  - Neutrals transport independent on background plasma / recycling conditions
    - Exagerated neutrals penetration and radiative collapse at high densities
  - No track of momentum exchange which is key part of divertor dissipation

⇒ **Not suitable for high density cases**, especially up to detachment

- Currently working on implementing fluid neutrals models from *Horsten et al, 2017, Nucl Fusion 57, 116043*

The new model in a nutshell (for discussion)

- Currently working on implementing fluid neutrals models from Horsten et al, 2017, Nucl Fusion 57, 116043: model 2 (no energy balance, $T_n = T_i$)

Particle balance: $\vec{\nabla} \cdot \left(\boldsymbol{n_n} \left(\boldsymbol{u_{\parallel n}} \vec{b} + \vec{u}_{\perp n} \right) \right) = S_{n_n}$

Parallel momentum balance: $m_n \vec{\nabla} \cdot \left(\boldsymbol{n_n} \boldsymbol{u_{\parallel n}} \left(\boldsymbol{u_{\parallel n}} \vec{b} + \vec{u}_{\perp n} \right) - \eta^n \nabla_\parallel \boldsymbol{u_{\parallel n}} \vec{b} \right) = -\nabla_\parallel p_n + S_{mu_{n\parallel}}$

Perpendicular transport closure: $n_n \vec{u}_{\perp n} = -D_p^n \vec{\nabla}_\perp p_n$ $\quad D_p^n = \dfrac{1}{m_n \left(\langle \sigma v \rangle_{cx,m} n_i + \langle \sigma v \rangle_i n_e \right)}$

Sources: $S_{n_n} = \langle \sigma v \rangle_r n_i n_e - \langle \sigma v \rangle_i n_n n_e$

$$S_{mu_{n\parallel}} = m_n \left(\langle \sigma v \rangle_r n_i n_e + \langle \sigma v \rangle_{cx,m} n_n n_i \right) u_{\parallel i} - m_n \left(\langle \sigma v \rangle_i n_n n_e + \langle \sigma v \rangle_{cx,m} n_n n_i \right) u_{\parallel n}$$

Quid of multi-species case?
Quid of time dependent case?

Viscosity: $\eta^n = \dfrac{p_n}{\langle \sigma v \rangle_{cx,m} n_i}$

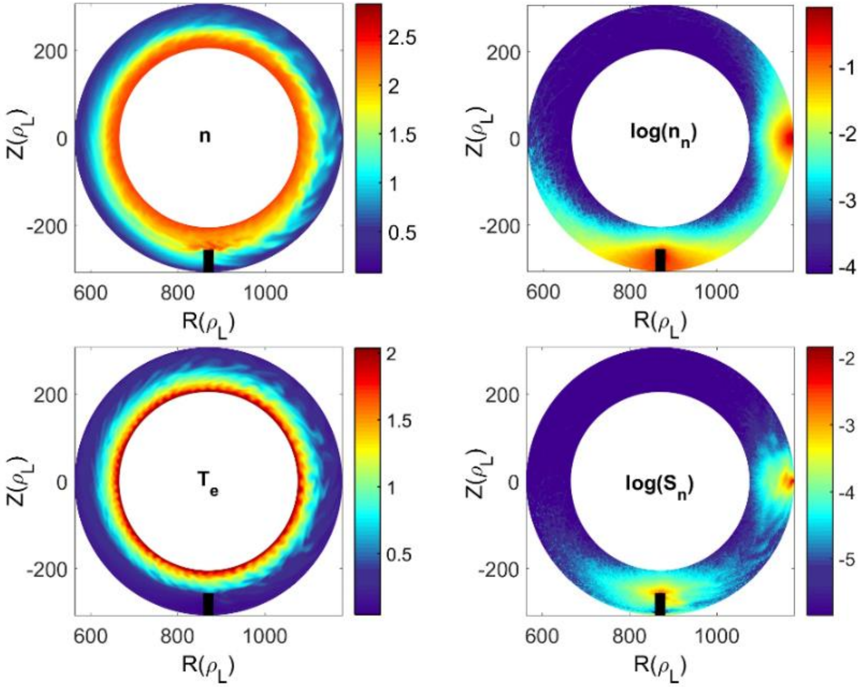
Kinetic neutrals: TOKAM3X as pathfinder

- Worked performed initially in TOKAM3X
  [P. Tamain, PSI conference 2018]
  [D.M. Fan et al., NME2019]

- **TOKAM3X coupled to EIRENE** via same architecture as SOLEDGE2D-EIRENE 2D transport package

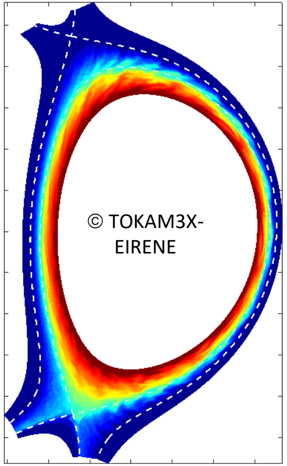
  *[H. Bufferand et al., Nucl. Fusion **55** (2015)]*

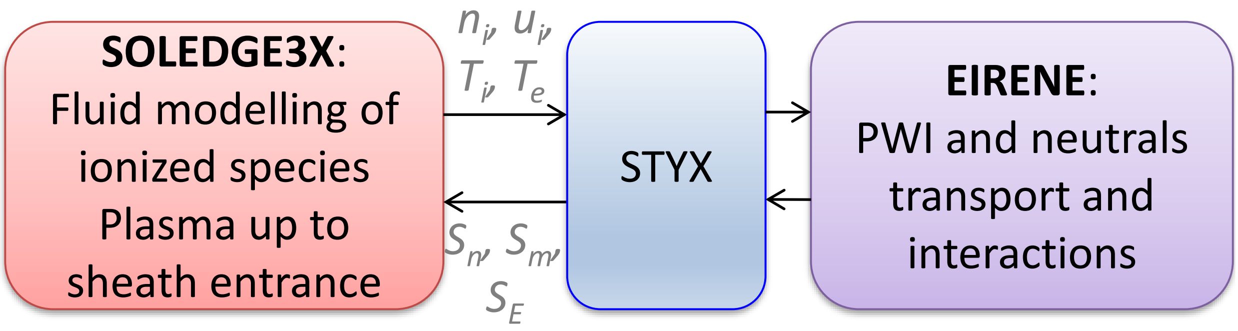
- 2 key assumptions, non design-locked
  - $\tau_{neut} \ll \tau_{turb}$ + tests in 2D turbulence simulations $\Rightarrow$ EIRENE used in **time-independent mode**
  - assumes **instantaneous recycling**



How does it work in practise?

- Coupling to EIRENE is not direct but done through **STYX interface**
  - Eases setup of EIRENE with **more user-friendly** input files
  - **Advanced sheath model** based in PIC simulations *[H. Bufferand et al, NF2015]*
  - Provides **additional diagnostics**, e.g particle / momentum / energy balances decomposed by A&M reaction (new!)
  - Allows to **reduce computational cost and improve stability** of coupling through “short-cycling” methods (new!)





SOLEDGE3X: Fluid modelling of ionized species Plasma up to sheath entrance

n_i, u_i, T_i, T_e

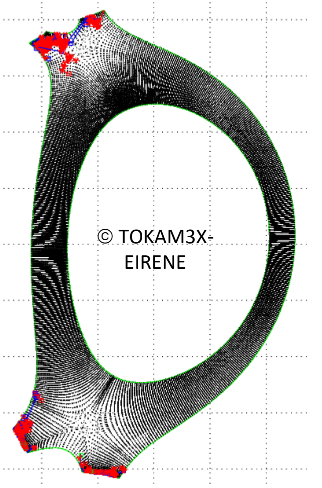
STYX

S_n, S_m, S_E

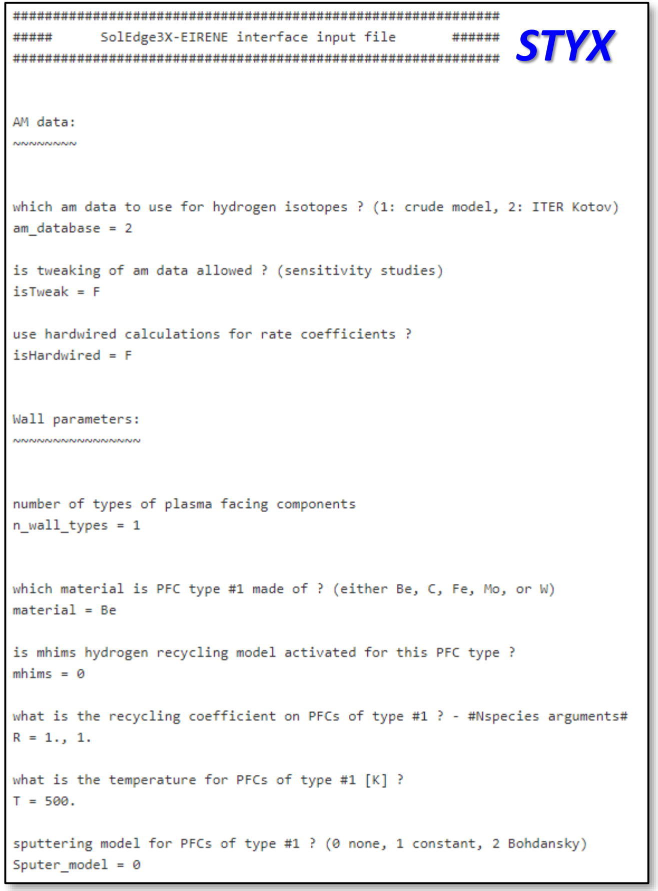
EIRENE: PWI and neutrals transport and interactions

Quasi-neutral plasma

Sheath, wall and neutrals



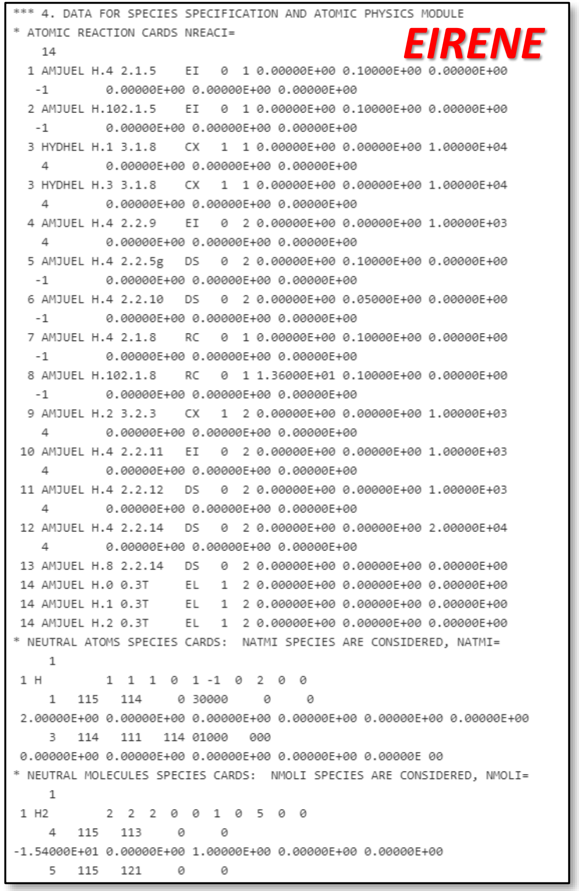
STYX: simplification of EIRENE ’s setup



STYX

```
#############################################################
#####      SolEdge3X-EIRENE interface input file       ######
#############################################################


AM data:
~~~~~~~~


which am data to use for hydrogen isotopes ? (1: crude model, 2: ITER Kotov)
am_database = 2

is tweaking of am data allowed ? (sensitivity studies)
isTweak = F

use hardwired calculations for rate coefficients ?
isHardwired = F


Wall parameters:
~~~~~~~~~~~~~~~~


number of types of plasma facing components
n_wall_types = 1


which material is PFC type #1 made of ? (either Be, C, Fe, Mo, or W)
material = Be

is mhims hydrogen recycling model activated for this PFC type ?
mhims = 0

what is the recycling coefficient on PFCs of type #1 ? - #Nspecies arguments#
R = 1., 1.

what is the temperature for PFCs of type #1 [K] ?
T = 500.

sputtering model for PFCs of type #1 ? (0 none, 1 constant, 2 Bohdansky)
Sputer_model = 0
```

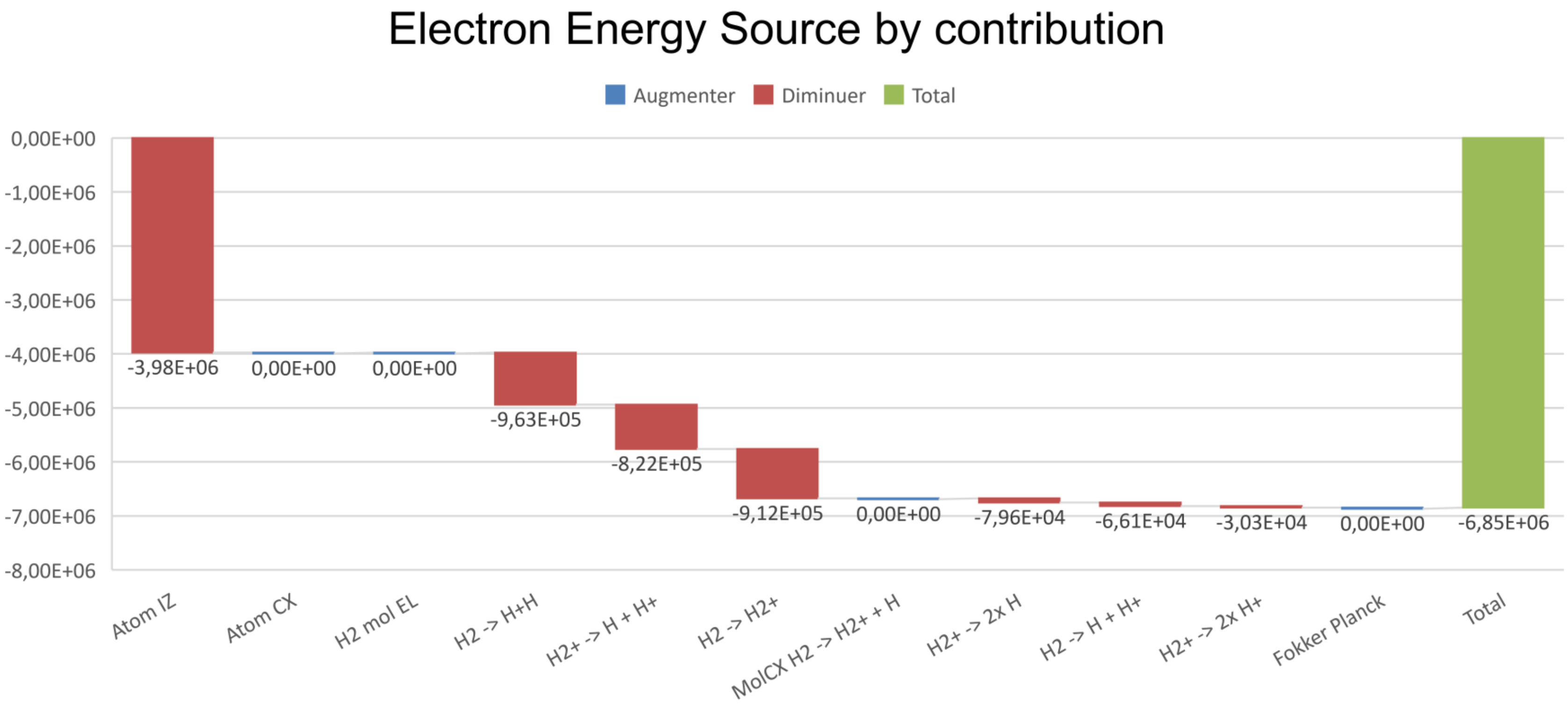
Automatically generated by STYX



EIRENE

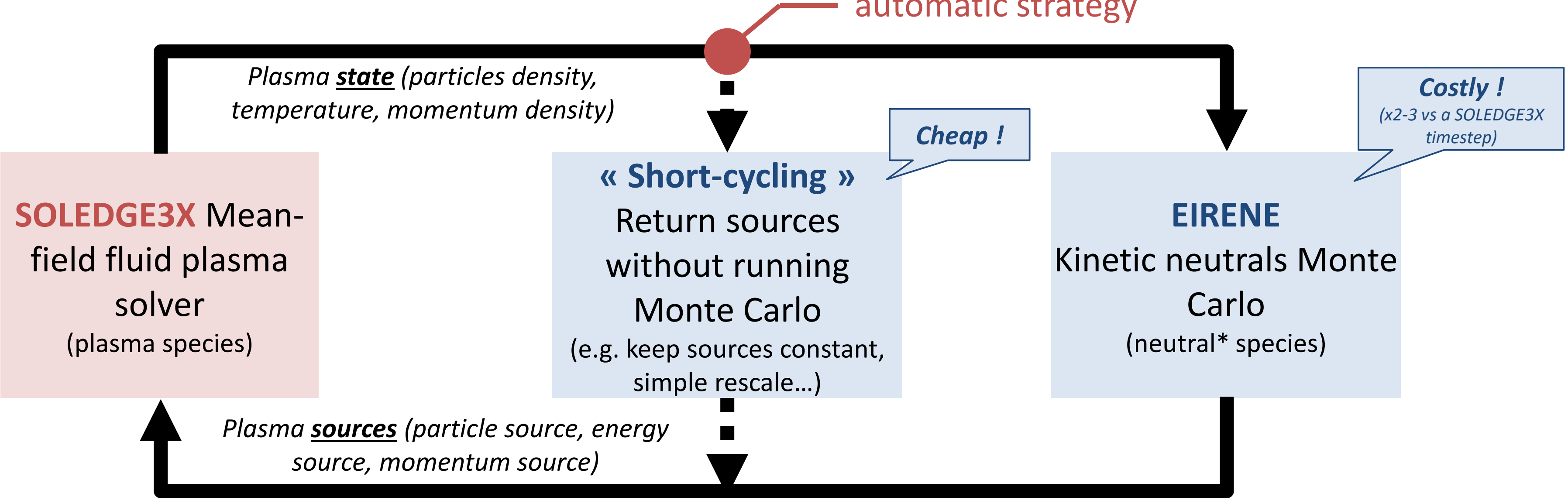
```
*** 4. DATA FOR SPECIES SPECIFICATION AND ATOMIC PHYSICS MODULE
* ATOMIC REACTION CARDS NREACI=
    14
  1 AMJUEL H.4 2.1.5    EI   0  1 0.00000E+00 0.10000E+00 0.00000E+00
   -1        0.00000E+00 0.00000E+00 0.00000E+00
  2 AMJUEL H.102.1.5    EI   0  1 0.00000E+00 0.10000E+00 0.00000E+00
   -1        0.00000E+00 0.00000E+00 0.00000E+00
  3 HYDHEL H.1 3.1.8    CX   1  1 0.00000E+00 0.00000E+00 1.00000E+04
    4        0.00000E+00 0.00000E+00 0.00000E+00
  3 HYDHEL H.3 3.1.8    CX   1  1 0.00000E+00 0.00000E+00 1.00000E+04
    4        0.00000E+00 0.00000E+00 0.00000E+00
  4 AMJUEL H.4 2.2.9    EI   0  2 0.00000E+00 0.00000E+00 1.00000E+03
    4        0.00000E+00 0.00000E+00 0.00000E+00
  5 AMJUEL H.4 2.2.5g   DS   0  2 0.00000E+00 0.10000E+00 0.00000E+00
   -1        0.00000E+00 0.00000E+00 0.00000E+00
  6 AMJUEL H.4 2.2.10   DS   0  2 0.00000E+00 0.05000E+00 0.00000E+00
   -1        0.00000E+00 0.00000E+00 0.00000E+00
  7 AMJUEL H.4 2.1.8    RC   0  1 0.00000E+00 0.10000E+00 0.00000E+00
   -1        0.00000E+00 0.00000E+00 0.00000E+00
  8 AMJUEL H.102.1.8    RC   0  1 1.36000E+01 0.10000E+00 0.00000E+00
   -1        0.00000E+00 0.00000E+00 0.00000E+00
  9 AMJUEL H.2 3.2.3    CX   1  2 0.00000E+00 0.00000E+00 1.00000E+03
    4        0.00000E+00 0.00000E+00 0.00000E+00
 10 AMJUEL H.4 2.2.11   EI   0  2 0.00000E+00 0.00000E+00 1.00000E+03
    4        0.00000E+00 0.00000E+00 0.00000E+00
 11 AMJUEL H.4 2.2.12   DS   0  2 0.00000E+00 0.00000E+00 1.00000E+03
    4        0.00000E+00 0.00000E+00 0.00000E+00
 12 AMJUEL H.4 2.2.14   DS   0  2 0.00000E+00 0.00000E+00 2.00000E+04
    4        0.00000E+00 0.00000E+00 0.00000E+00
 13 AMJUEL H.8 2.2.14   DS   0  2 0.00000E+00 0.00000E+00 0.00000E+00
 14 AMJUEL H.0 0.3T     EL   1  2 0.00000E+00 0.00000E+00 0.00000E+00
 14 AMJUEL H.1 0.3T     EL   1  2 0.00000E+00 0.00000E+00 0.00000E+00
 14 AMJUEL H.2 0.3T     EL   1  2 0.00000E+00 0.00000E+00 0.00000E+00
* NEUTRAL ATOMS SPECIES CARDS:  NATMI SPECIES ARE CONSIDERED, NATMI=
     1
 1 H          1  1  1  0  1 -1  0  2  0  0
     1   115   114     0 30000     0     0
 2.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
     3   114   111   114 01000   000
 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E 00
* NEUTRAL MOLECULES SPECIES CARDS:  NMOLI SPECIES ARE CONSIDERED, NMOLI=
     1
 1 H2         2  2  2  0  0  1  0  5  0  0
     4   115   113     0     0
-1.54000E+01 0.00000E+00 1.00000E+00 0.00000E+00 0.00000E+00
     5   115   121     0     0
```

STYX diagnostics example



"Short –cycling" calls to EIRENE

- **Monte-Carlo solver typically slower** than plasma time-stepper (factor 2 to 3)
  - But plasma evolves very little from one step to another
- Solution: call Monte-Carlo only every so often and keep constant some info = **short-cycling**



Branch at fixed interval or depending on automatic strategy

*Plasma **state** (particles density, temperature, momentum density)*

SOLEDGE3X Mean-field fluid plasma solver
(plasma species)

« Short-cycling »
Return sources without running Monte Carlo
(e.g. keep sources constant, simple rescale…)

Cheap !

EIRENE
Kinetic neutrals Monte Carlo
(neutral* species)

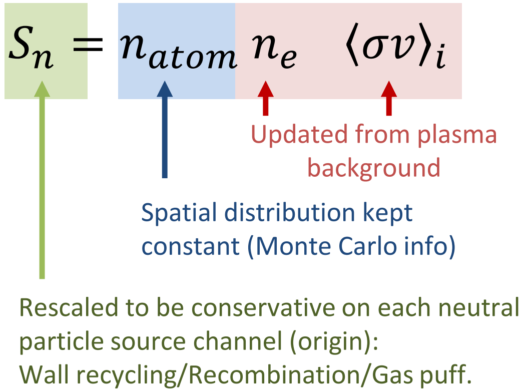
Costly !
(x2-3 vs a SOLEDGE3X timestep)

*Plasma **sources** (particle source, energy source, momentum source)*

Short-cycling strategies and their pros/cons

- Several “levels” of short-cycling:
  - **Level 1**: **keep sources** constant
  - **Level 2**: **scale sources with ion flux** to the wall $S_n = S_n^{last\ call} \frac{\Gamma_i}{\Gamma_i^{last\ call}}$
  - **Level 3**: **keep neutrals density** distribution, **recompute sources based on new plasma background** and scale integral with ion flux to the wall

Example of ionization: $S_n = n_{atom}\, n_e \ \langle \sigma v \rangle_i$



Updated from plasma background

Spatial distribution kept constant (Monte Carlo info)

Rescaled to be conservative on each neutral particle source channel (origin):
Wall recycling/Recombination/Gas puff.

- Level 2 and level 3 have to be done “strata-wise”, i.e. dependent on origin of atoms in EIRENE (handled by STYX)

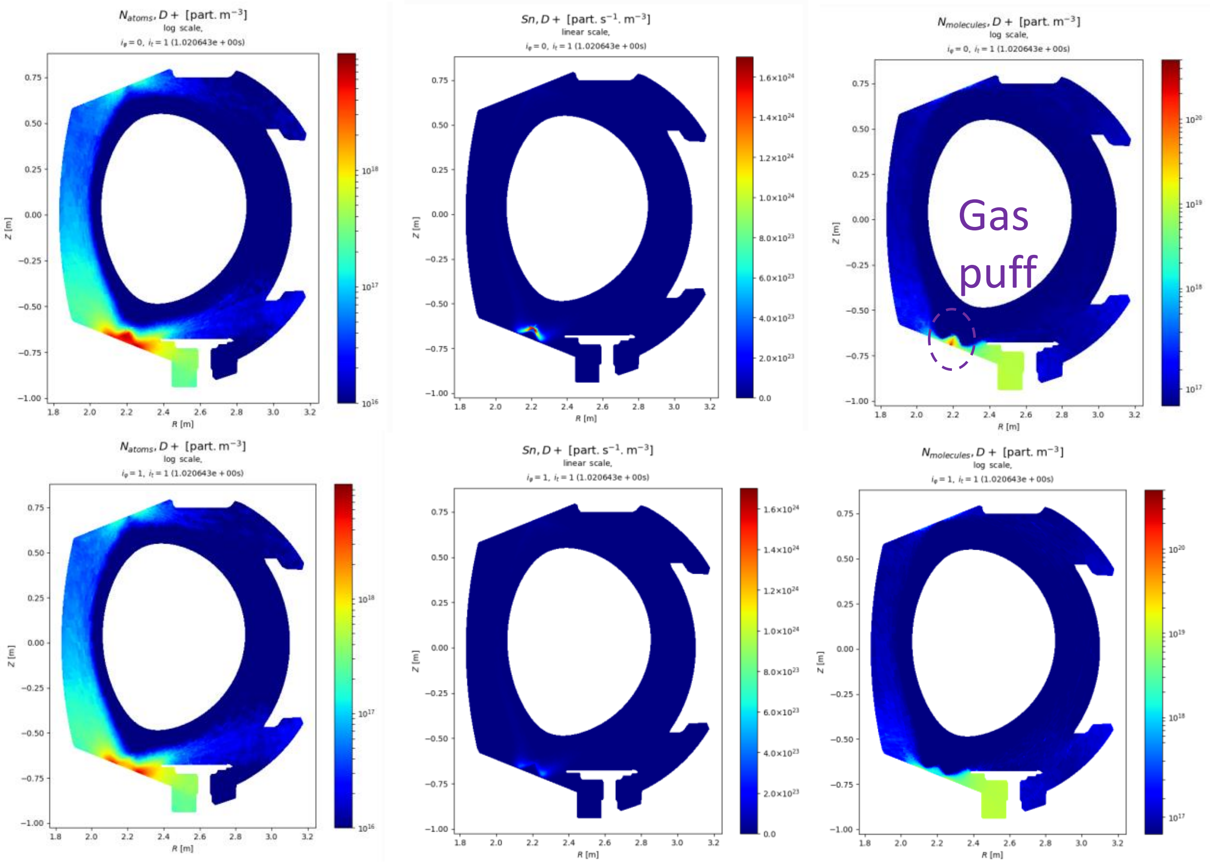
Short-cycling strategies and their pros/cons

- Several “levels” of short-cycling:
  - **Level 1**: **keep sources** constant
  - **Level 2**: **scale sources with ion flux** to the wall $S_n = S_n^{last\ call} \frac{\Gamma_i}{\Gamma_i^{last\ call}}$
  - **Level 3**: **keep neutrals density** distribution, **recompute sources based on new plasma background** and scale integral with ion flux to the wall

Level	Pros	Cons
1	Fast and very simple	**Non conservative** **Poor stability** in stiff regimes Fully **explicit**
2	Fast and simple **Conservative**	**Poor stability** in stiff regimes Fully **explicit**
3	**Conservative** **Improved stability** Opens way to **partial implicitation**	Complex to code and understand (handled by STYX) A bit slower

Coupling to EIRENE in 3D available in SOLEDGE3X

- After move to SOLEDGE3X, kinetic neutrals used only in 2D
- On-going effort to revive 3D version of coupling
- First **3D WEST case and full kinetic neutrals** obtained recently



Making Soledge3X kinetic neutrals module available

- **SOLEDGE3X-STYX-EIRENE** currently **intricated**
  - Cross-dependencies between modules and functions
  - Compilation performed as a single code, not as separate libraries

- On-going effort to **make a clean separation between the 3 codes**

- Once done, **STYX could be made available as a library** to the rest of the community to couple 2D / 3D fluid edge plasma codes to EIRENE
  - Readily planned for HDG code

Summary and prospects

- Progress on fluid neutrals side:
  - SOLEDGE3X simulations with **simplistic fluid neutrals running routinely** up in low to high-ish recycling regime => soon to be standard way of running SOLEDGE3X (to get the sources right self-consistently)
  - Extension of plasma solver and fluid neutrals to handle **3D PFC configurations**
  - More **advanced fluid neutrals model** mandatory for dissipative regimes, implementation on-going (high-priority)

- Progress on kinetic neutrals side:
  - Coupling to **EIRENE via STYX interface revived in 3D** following TOKAM3X
  - Intensive work on STYX coupling strategy via **short-cycling to improve stability and save computing time**
  - ➢ Make STYX(-EIRENE) a separate module from SOLEDGE3X to **make it available to other codes** (planned for HDG)

Additional slides

Progress in kinetic neutrals model

Recap of EIRENE Atomic & Molecular models setup in SOLEDGE3X

Species	Reaction Name	Reaction	SOLEDGE3X Standard	New "Advanced" SOLPS-ITER-like (~Kotov model)
Atoms H	Ionisation	$e + H(1s) \rightarrow e + H^+ + e$	✓	✓
	Recombination	$H^+ + e \rightarrow H(1s)$	✓	✓
	Charge Exchange	$p + H(1s) \rightarrow H(1s) + p$	✓	✓
Molecules H_2	Dissociative Ionisation	$e + H_2 \rightarrow 2e + H + H^+$	✓	✓+
	Dissociation	$e + H_2 \rightarrow e + H + H$	✓	✓+
	Molecule Ionisation	$e + H_2 \rightarrow 2e + H_2^+$	✓	✓+
	Charge Exchange	$p + H_2 \rightarrow H + H_2^+$	✗	✓
	Elastic Collision	$p + H_2 \rightarrow p + H_2$	✗	✓
Molecule Ion H_2^+	Dissociative Ionisation	$e + H_2^+ \rightarrow 2e + H^+ + H^+$	✓	✓+
	Dissociation	$e + H_2^+ \rightarrow e + H + H^+$	✓	✓+
	Dissociative Recombination	$e + H_2^+ \rightarrow H + H$	✓	✓+

"✓+" : other molecule reactions **rates coefficients fits now include dependency in n** (pop. effects)

- **2 new reactions** have been shown to be important in JET [1]:
  - Molecule CX
  - Ion-Molecule elastic collision
- Posed strong numerical stability issues, especially in cold plasma regions
- **Now fixed**

[1]: V. Kotov (2008) Plasma Phys. Control. Fusion 50 105012

Strong impact of additional reactions on predictions

- Key role of elastic collisions with molecules in divertor target fluxes