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Atomic, Molecular And PMI Database In Current Edge Plasma Transport Codes, And Forward Sensitivity Analysis

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IAEA Technical Meeting on Uncertainty Assessment and Benchmark Experiments for Atomic and Molecular Data for Fusion Applications, Vienna, December 19-21, 2016

TEC

ITER: Balance of power

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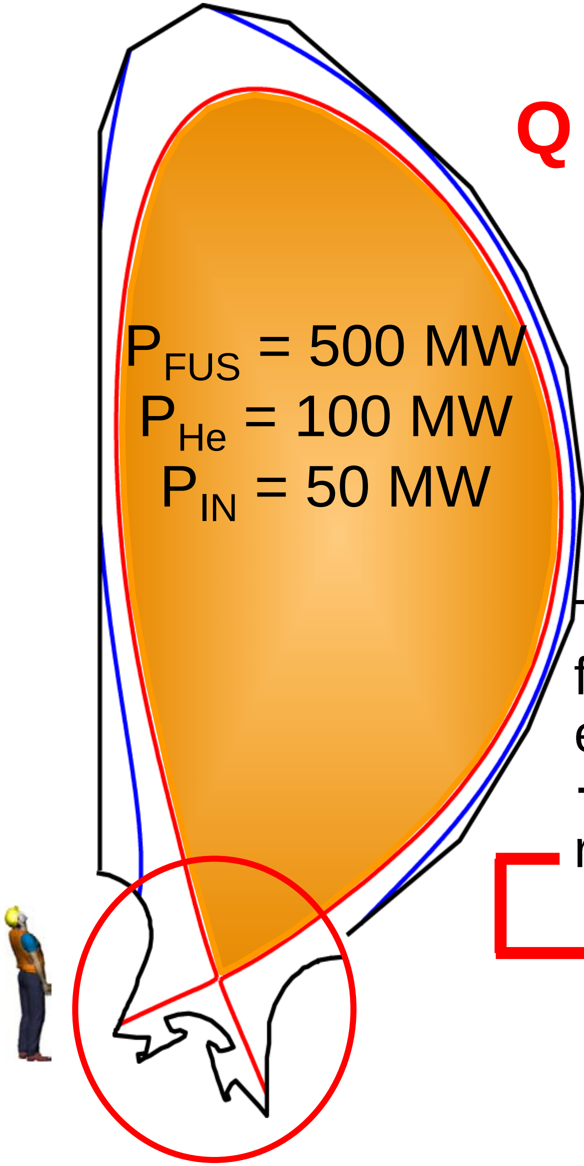
$$Q = \frac{\text{Fusion power}}{\text{Input power}} = \frac{500\ \text{MW}}{50\ \text{MW}} = 10$$



D + T → He + neutron

100 MW

Trapped by the magnetic field (He^{2+}) → gives its energy up to the plasma → maintains the fusion reactions

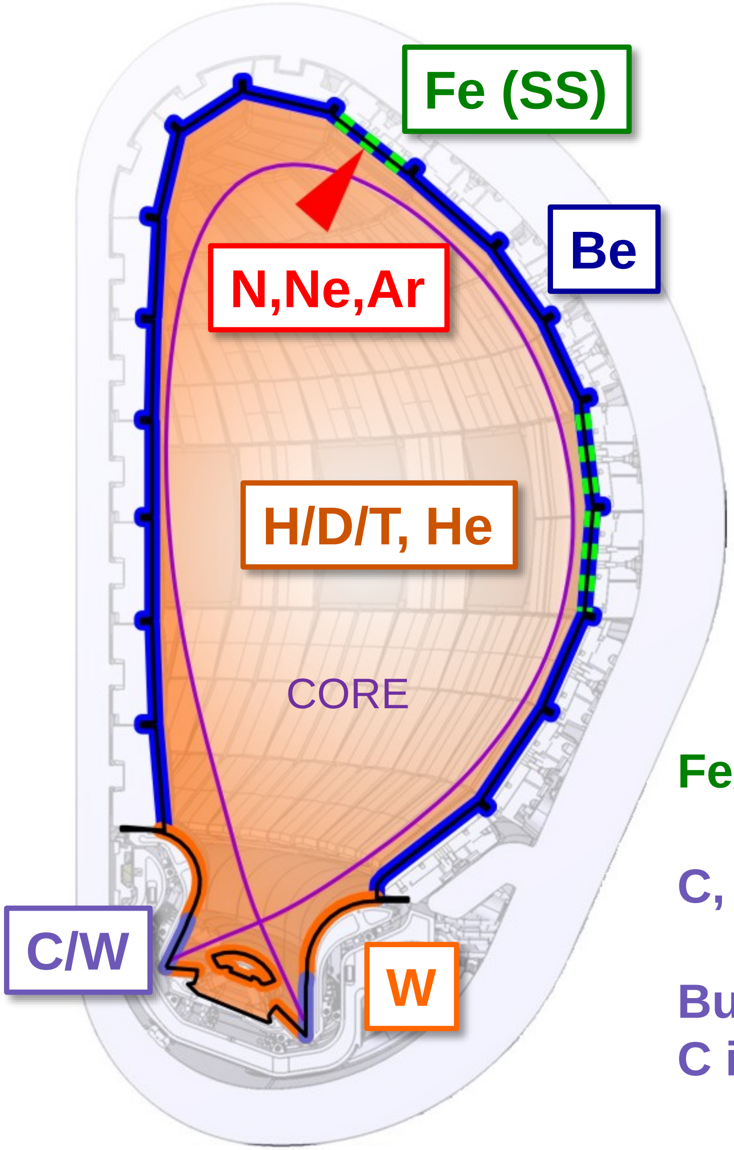
400 MW

Escapes from the plasma (no electric charge) → absorbed in the blanket surrounding the plasma

Must be exhausted from the plasma

The "divertor"

List of the main elements relevant to the ITER plasma



Fe/SS, 2011: armour at
diagnostics port plugs

C, 2013: replaced by
all W divertor

But:

C in: W7X (2016),
JT-60SA (2019),…

Outline

A: Core plasma: (beam-) spectroscopy
strongly stripped ions, often: H, He-like

B: Plasma boundary: spectroscopy plus: powerful plasma flows, particle exhaust, heat exhaust, machine availability

C: Typical parameters (electron density, temperature)

D: A&M data sensitivity (→ uncertainty propagation)

- 1: status: A&M data: sensitivity analysis in 0D plasma chemistry models.
- 2: outlook: A&M data: sensitivity analysis in current edge plasma flow models ???

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ITER, 500 MW fusion power, n_e, T_e

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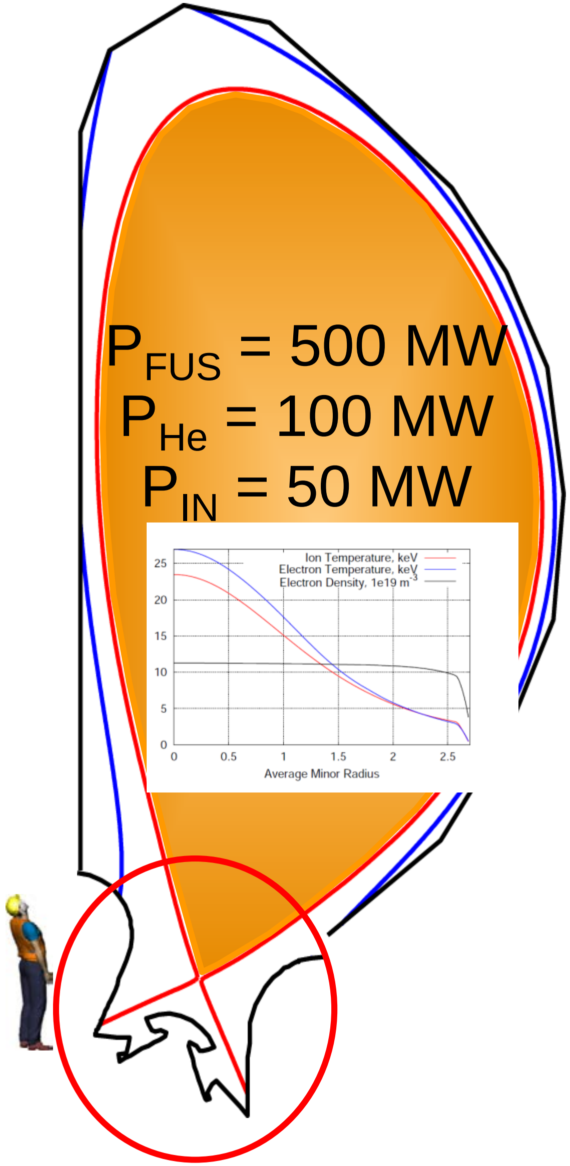
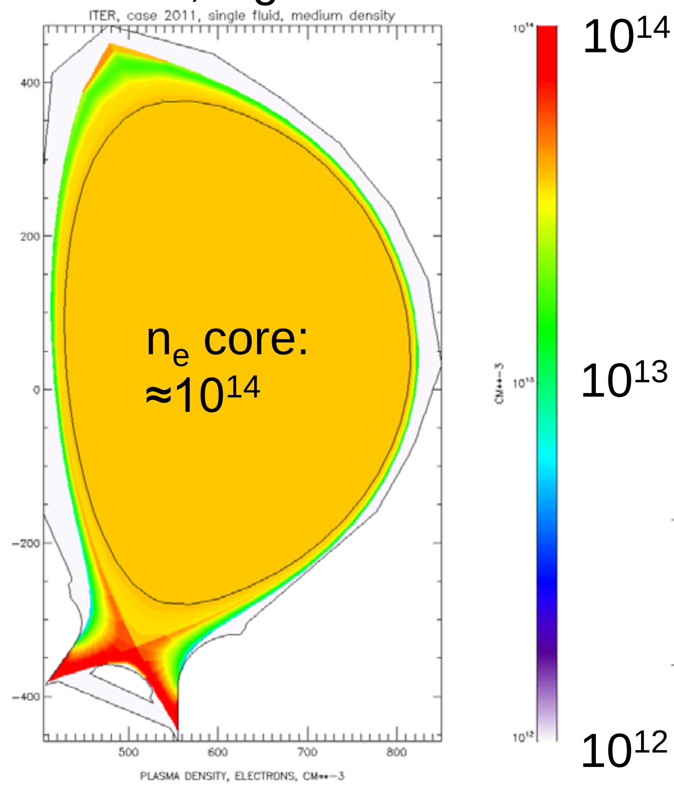
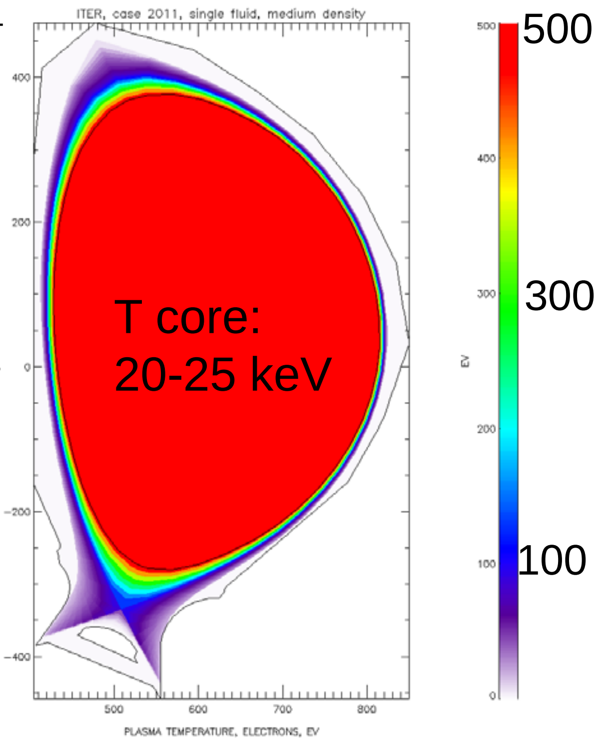


Plasma density
cm^{-3}, log scale



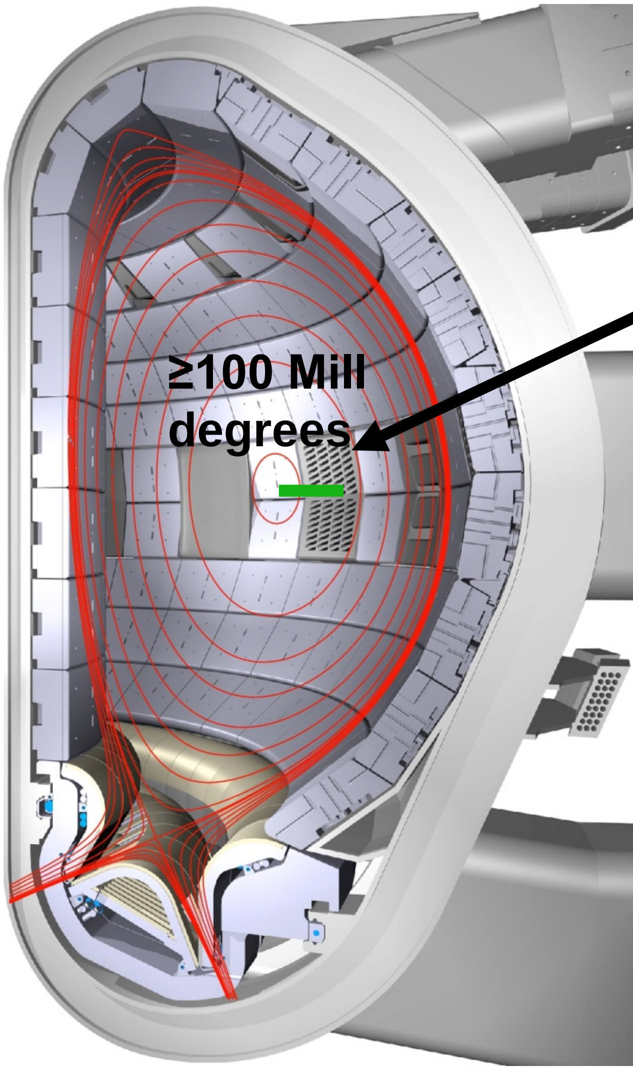
Electron temperature
eV, lin. scale



Relative importance of plasma flow forces over chemistry and PWI

$$\frac{\partial}{\partial t} n_i + \vec{\nabla} \cdot \left(n_i \vec{V}_i \right) = S_{n_i}$$

div(nv$_\parallel$)+div(nv$_\perp$)= ionization/recombination/charge exchange



Core

- **All chemical bonds broken,**
- **(turbulent) cross field flow, $D_\perp$, $V_\perp$**

(advanced plasma scenario development)

ionization/recombination/CX.

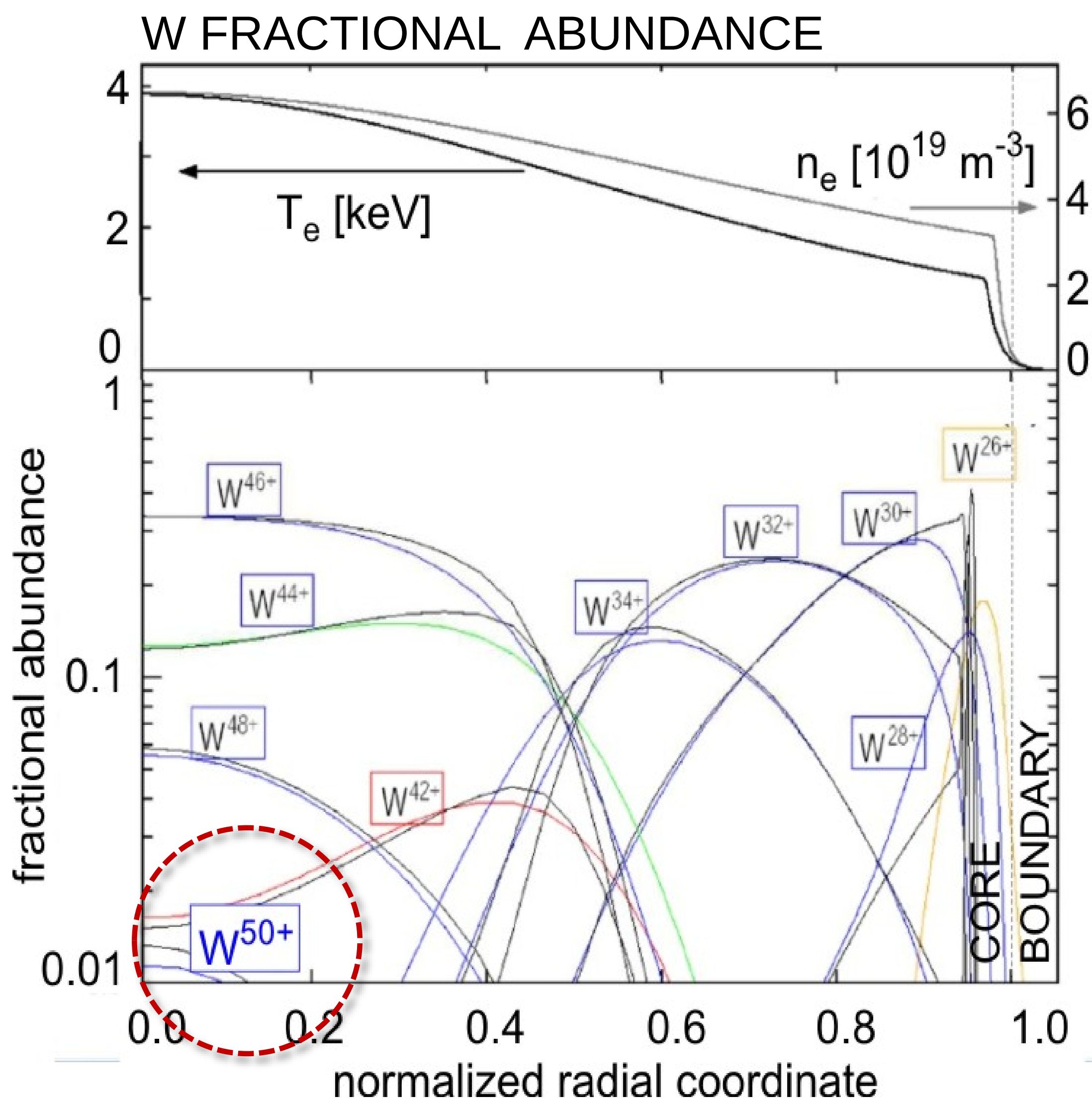
Atomic data models for hot plasma spectroscopy

- **interpretation,**
- **line shape modelling:**

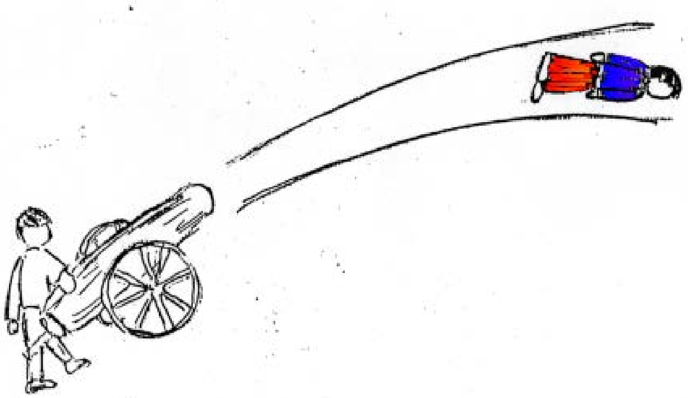
Spectroscopy : nZ*
CR Model : nZ* → nZ
Transport Model : nZ → $D_\perp$, $V_\perp$

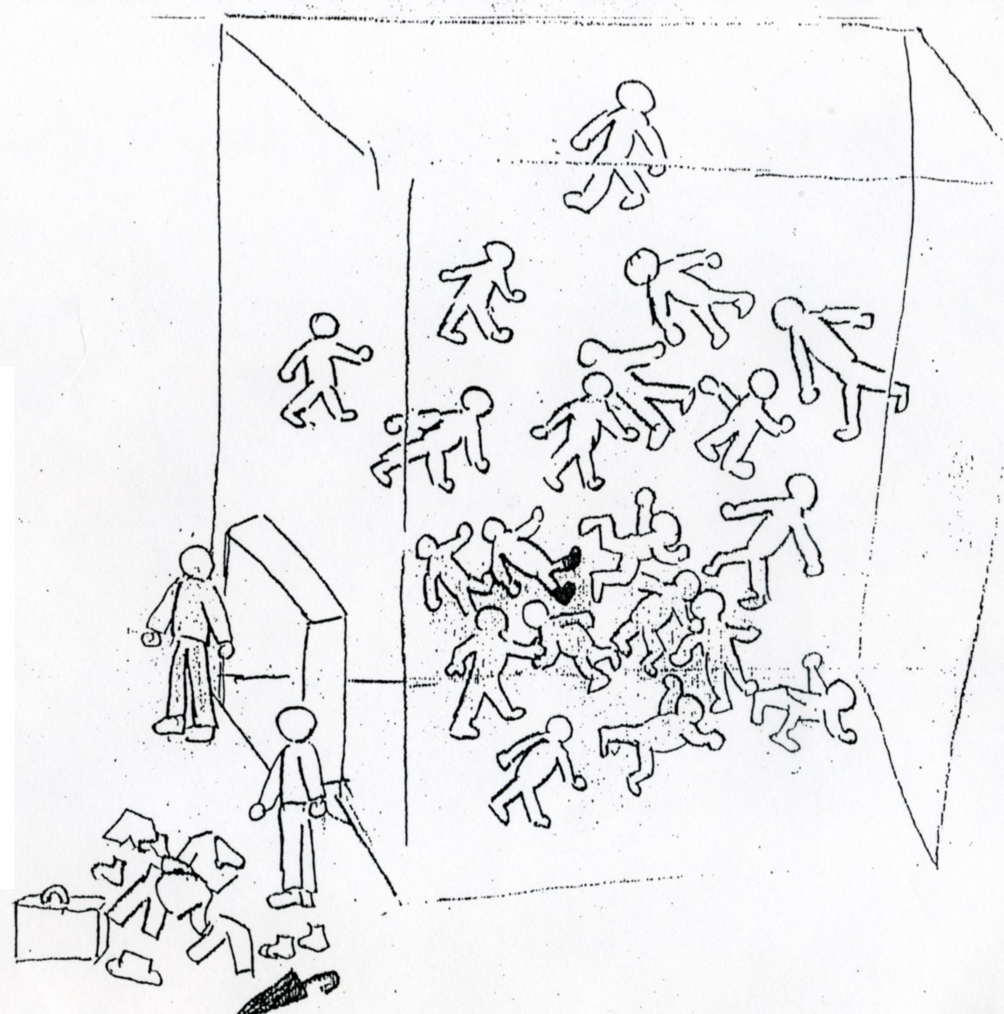
W atomic data development requested

- Understanding W behaviour in the plasma core is very important for ITER and future high-performance, high-duty cycle devices
  - W is a strong radiator at fusion core energies → concentration must be very low (< 0.001% in ITER)



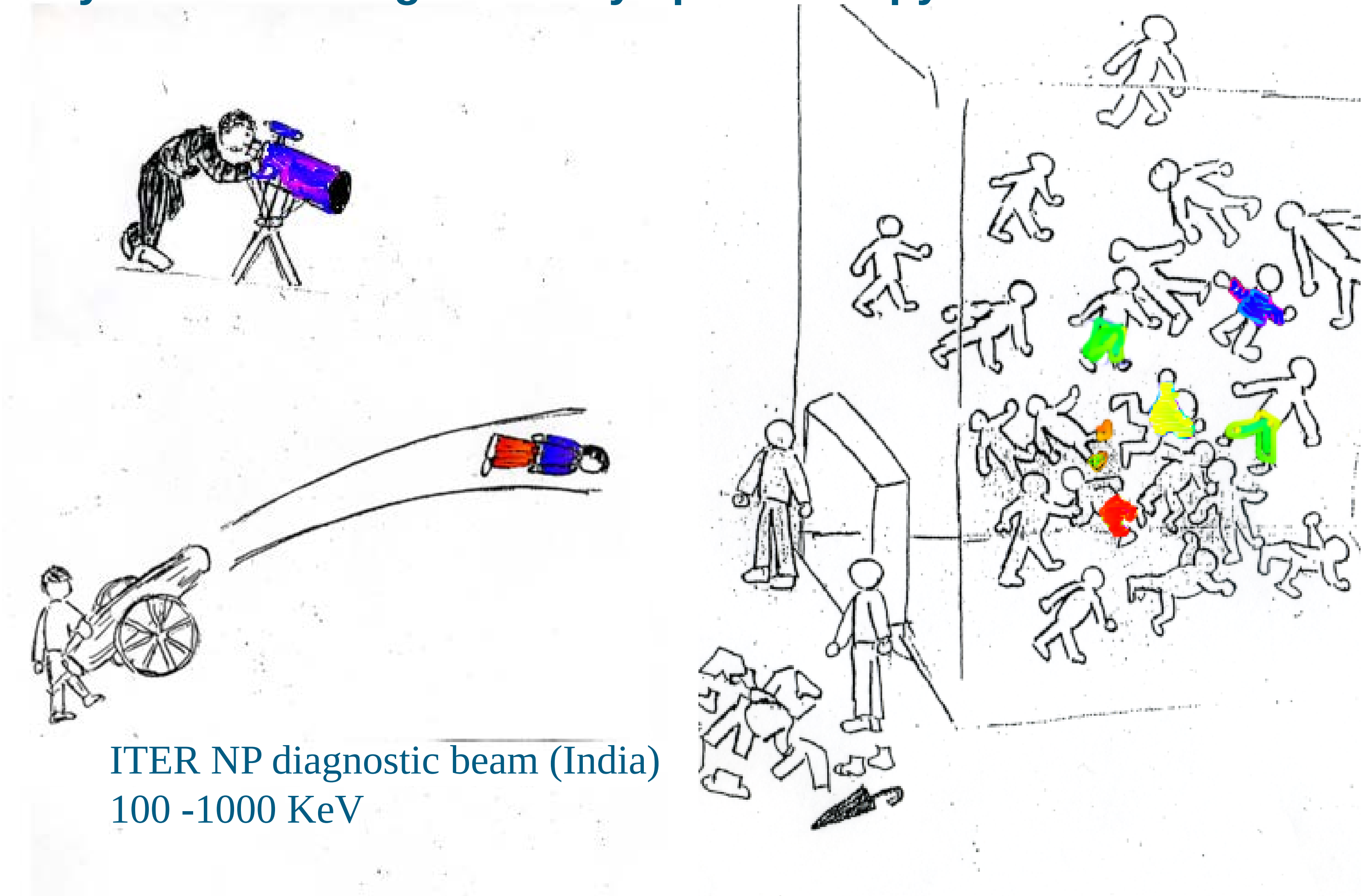
All relevant elements other than W are fully stripped of their electrons, except in the edge region





In the late 1970's Afrosimov suggested to inject high energy neutrals (hydrogen) which can pass through the magnetic field, primarily to heat the plasma by momentum transfer, but more importantly, passing electrons to fully stripped plasma ions.

Neutral (H) Beam (100 keV) injection provides electrons to elements, so they can be distinguished by spectroscopy



All elements (cooling gases, wall materials) become subject to plasma spectroscopy in fusion devices, because they are made “distinguishable” by H-diagnostic beams.

M. von Hellermann

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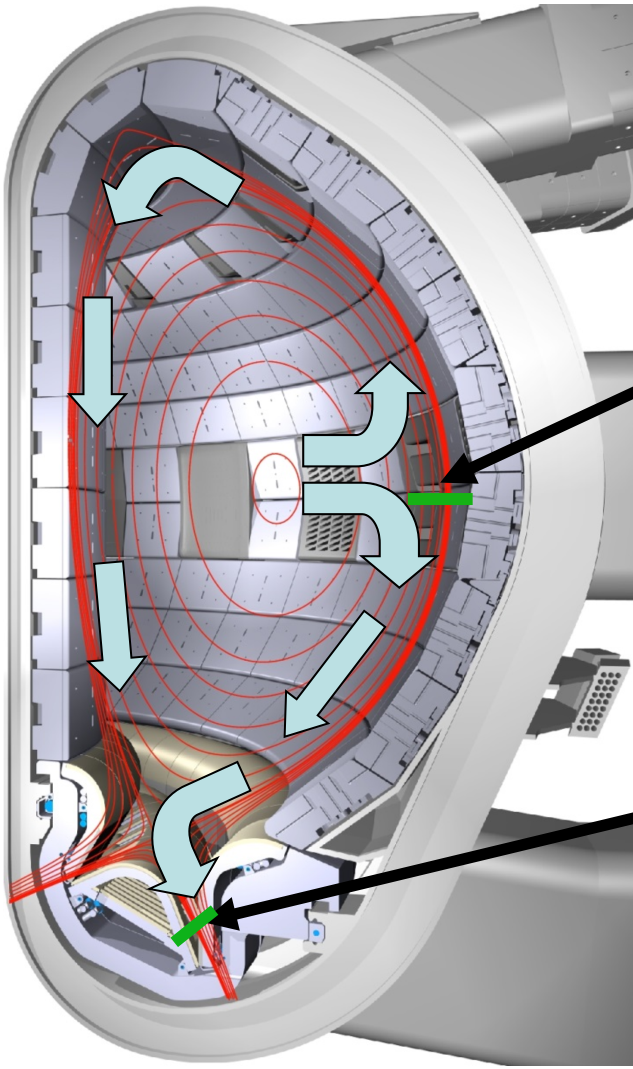
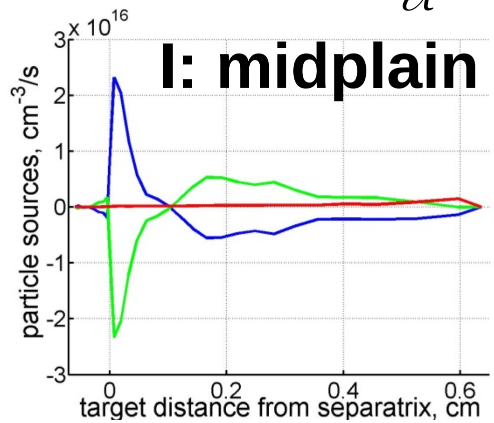
Relative importance of plasma flow forces over chemistry and PWI: I edge region → II divertor

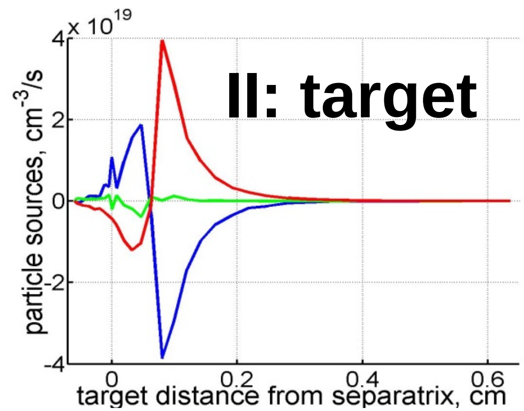
div(nv$_{\parallel}$)+div(nv$_{\perp}$)= ionization/recombination/charge exchange

$$\frac{\partial}{\partial t} n_i + \vec{\nabla} \cdot \left(n_i \vec{V}_i \right) = S_{n_i}$$





parallel vs. **(turbulent) cross field flow**



parallel vs. **chemistry and PWI driven flow**

H, He, Be, W,… dominant process:
vol. recomb., & friction: p + H_2, "detachment"

Atomic & molecular processes: boundary plasma

e,p + H, $H_2(v_i)$ → …, $e+H_2^+(v_i)$ → H + H*

- divertor detachment dynamics, final states? Isotopes?

www.amdis.iaea.org, database & data center network,

e,p + C, C_xH_y →…., $e+C_xH_y^+$ → …. C erosion and migration, tritium retention in remote areas,…. Excited states of products (CH(A→X)) ?

R. Janev et al., Phys. Plasma (2004) 11, www.hydkin.de, IAEA: www.amdis.iaea.org

e $+H_3^+(v_3)$ → …., DR, DE,….

- H_3^+ probably irrelevant in fusion plasmas

M. Larsson et al., PRL (1993) 70, S. Datz et al., PRL (1995) 74, and: Conference series: DR 1-9

e,p + Be, BeH/BeH^+ → …. possible role on spectroscopy and on material migration: Formation rates ?? 10% of Be sputtering?

J.B. Roos et al. Phys. Rev A (2009) 80, IAEA Atomic Molec. data unit CRP 2012-2015

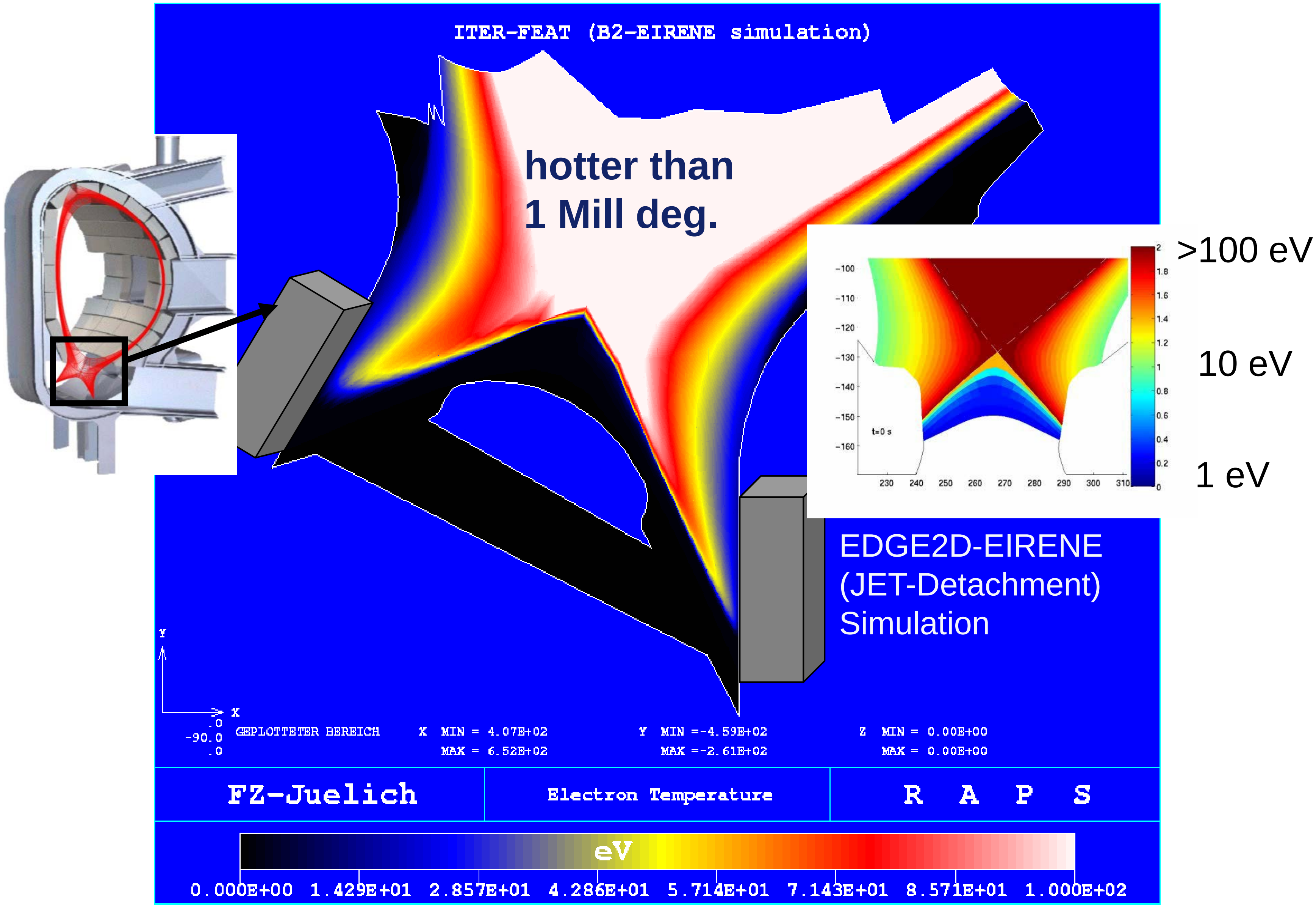
Exp.: UC Louvain, Theory: I. Schneider et al., Univ. Du Havre, J. Tennyson et al. (Quantemol), R. Celiberto et al. (Bari)

e,p + Ne, Ar, N, N_2, N_2^+ → …. ??

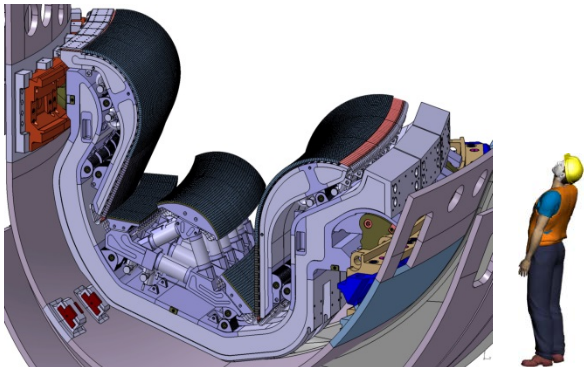
- N_2-seeding, edge plasma cooling: molecular effects not yet studied in fusion plasmas, only resulting atomic ions N, N^+, N^{++},….

Extensive database exists, See planetary atmospheric entries research, e.g. A. Bultel et al, Universite de Rouen, France

Divertor detachment: ITER, simulation, detached, T_e field. Movie (JET): T_e during n_e ramp up, transition to detachment.



Narrowing down on the divertor plasma



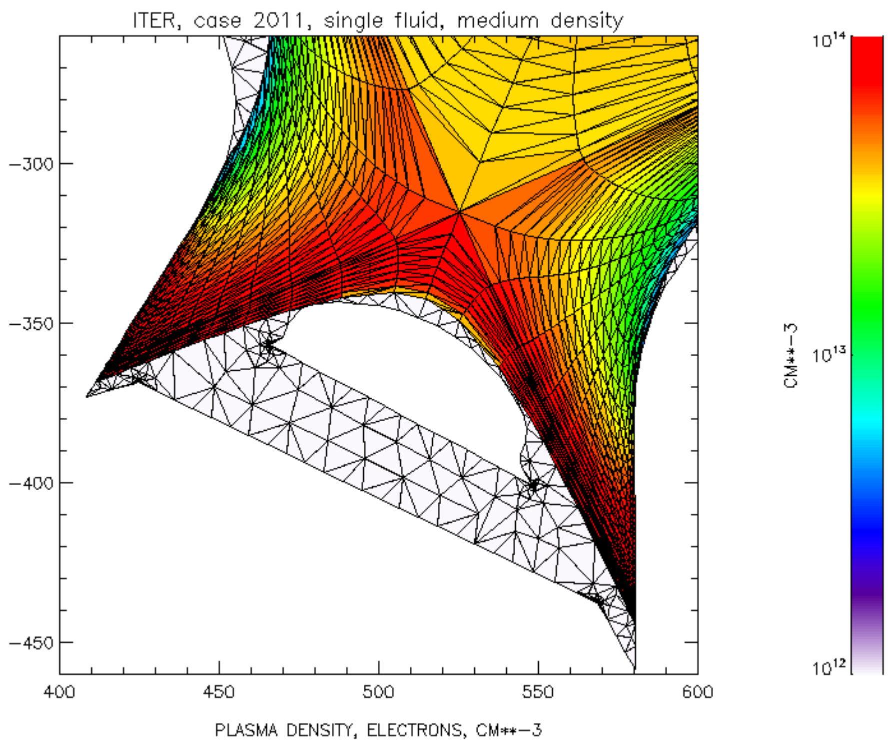
Electron thermalization time

$$\tau_{ee} \approx 3.3 \times 10^{-13} \left(\frac{T_e}{100\ \text{eV}}\right)^{3/2} \left(\frac{10^{21}\ \text{cm}^{-3}}{n_i\ \log\Lambda}\right) \quad \text{s}$$

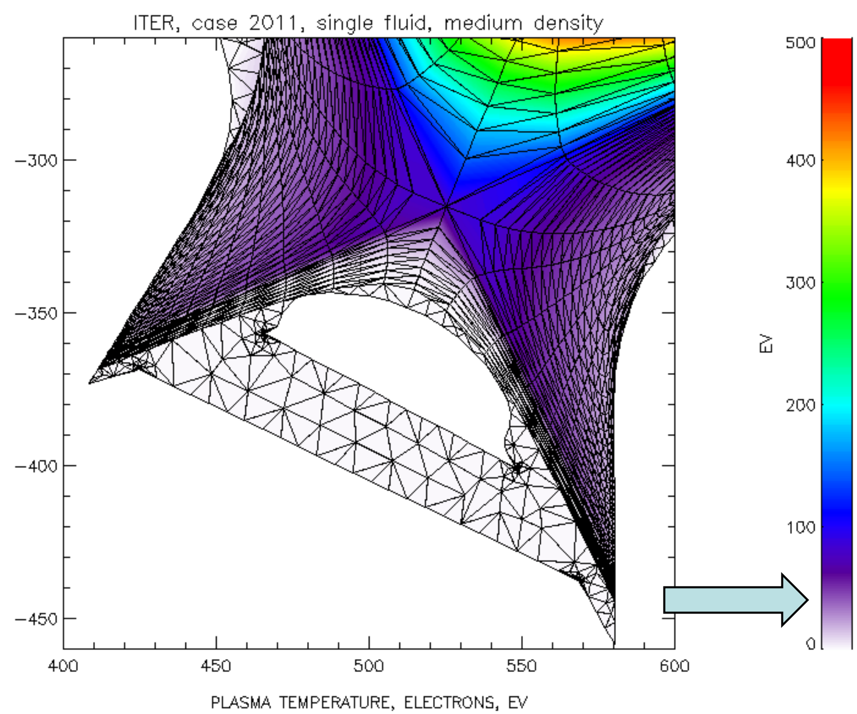
→ Electrons well thermalized in divertor

→ no need for EEFD considerations there

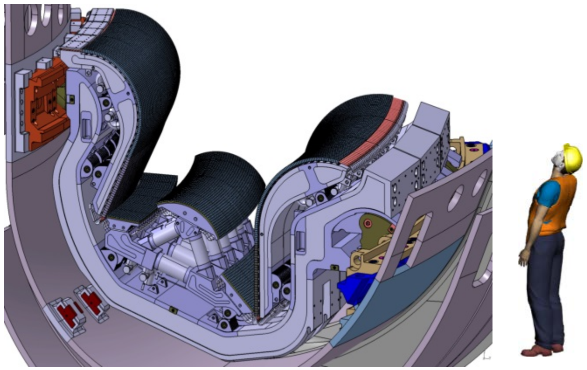
Divertor plasma density
cm^{-3}, log scale, 10^{12} -10^{14}



Divertor electron temperature
eV, lin. scale, 0 – 500 eV



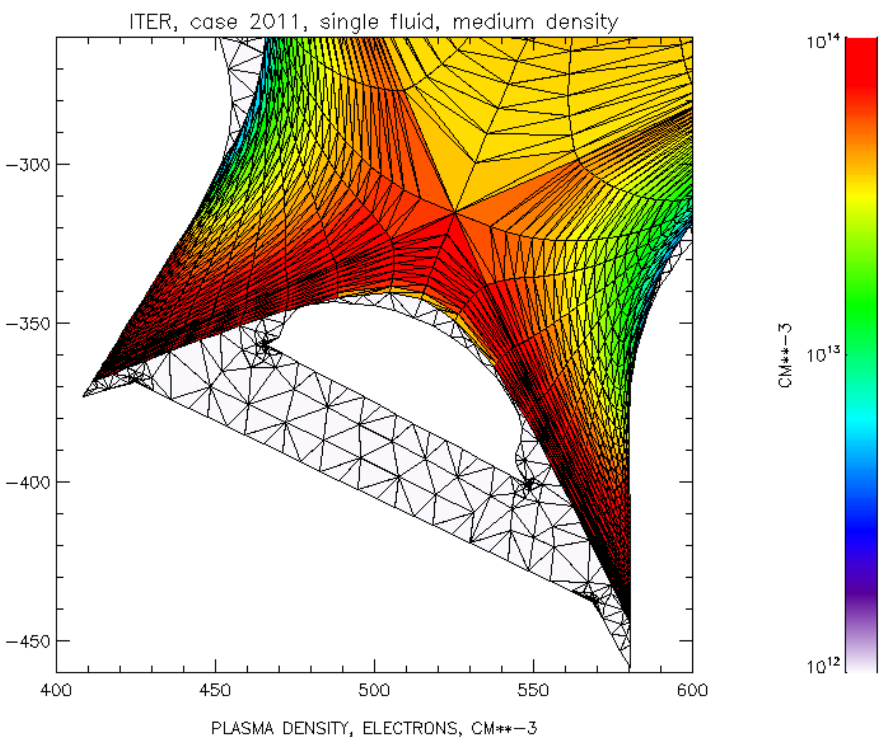
Plasma in "weakly detached" ITER divertor
n_e: > 1e14, T_e < 5 eV



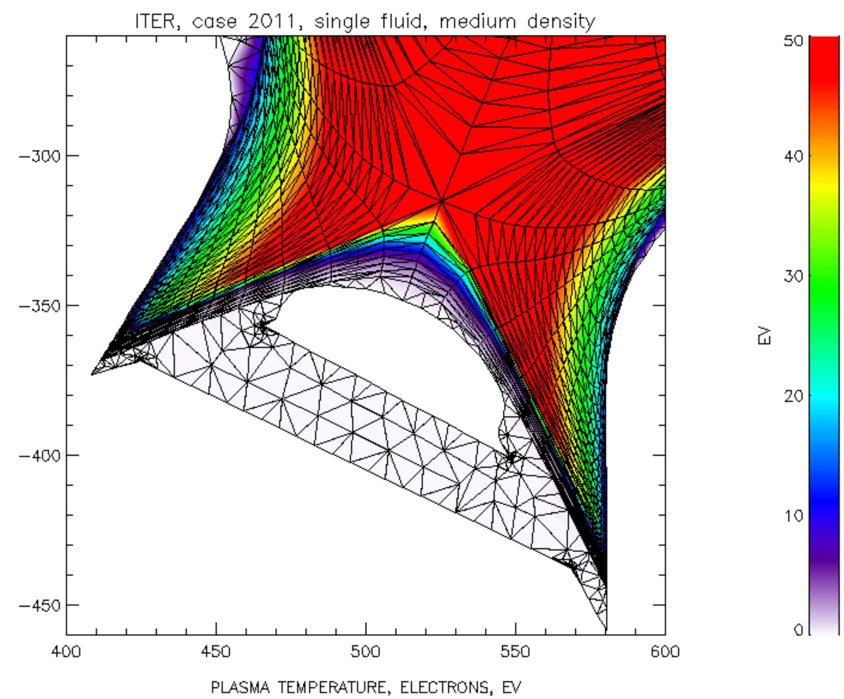
Tokamak Divertor Detachment:

- Self sustained dense, cold plasma layer (≈ 1 – 3 eV) formed in front of high heat flux components.
- Plasma flux drops, despite increased density

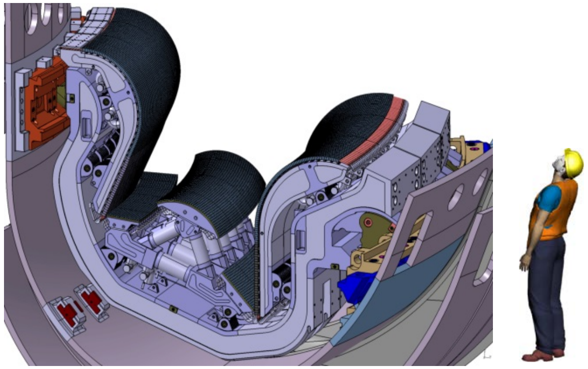
Divertor plasma density
cm^{-3}, log scale, 10^{12} -10^{14}



Divertor electron temperature
eV, lin. Scale, 0 – 50 eV



Electron – ion temperature equilibration:
→ Divertor $T_i \approx T_e$



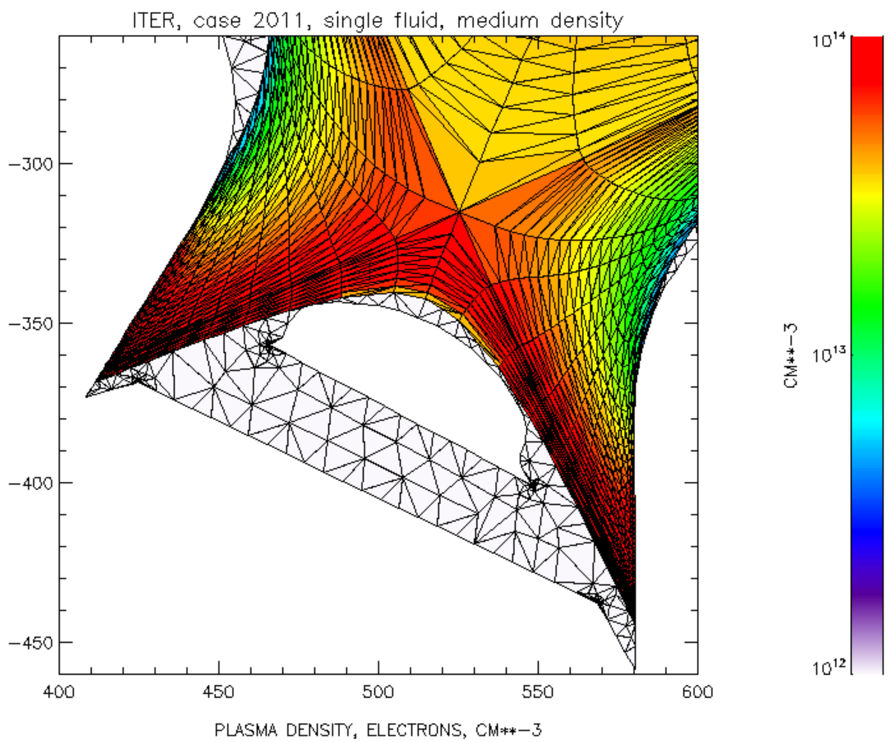
$T_e - T_i$ equilibration time

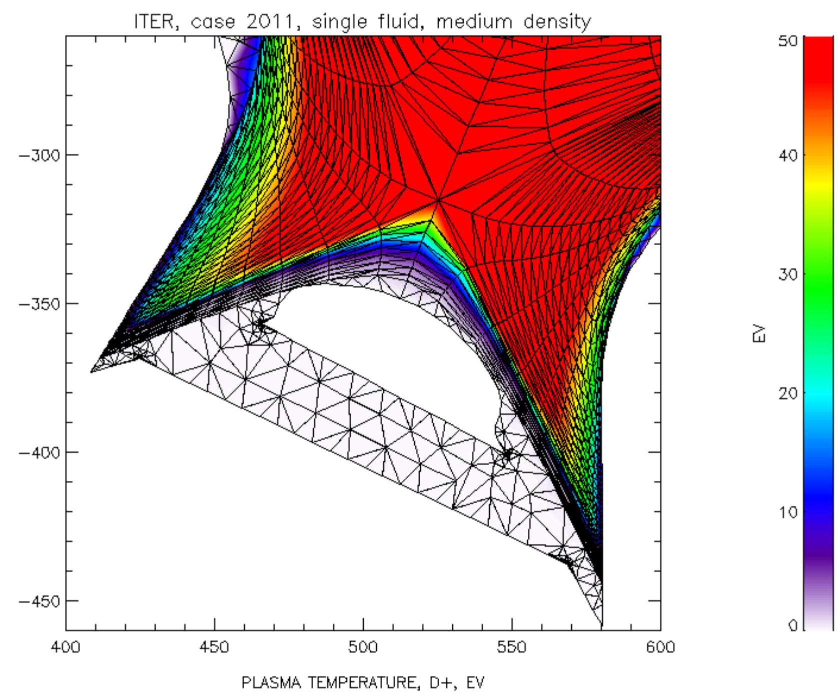
$$\tau_{eq} \approx 3.16 \times 10^{-10} \frac{A}{Z^2} \left(\frac{T_e}{100 \text{ eV}}\right)^{3/2} \left(\frac{10^{21} \text{ cm}^{-3}}{n_i \log\Lambda}\right) \quad \text{s}$$

≈ 1000 x τ_{ee} (for H plasma), but still fast.

Divertor plasma density
cm^{-3}, log scale, 10^{12} -10^{14}

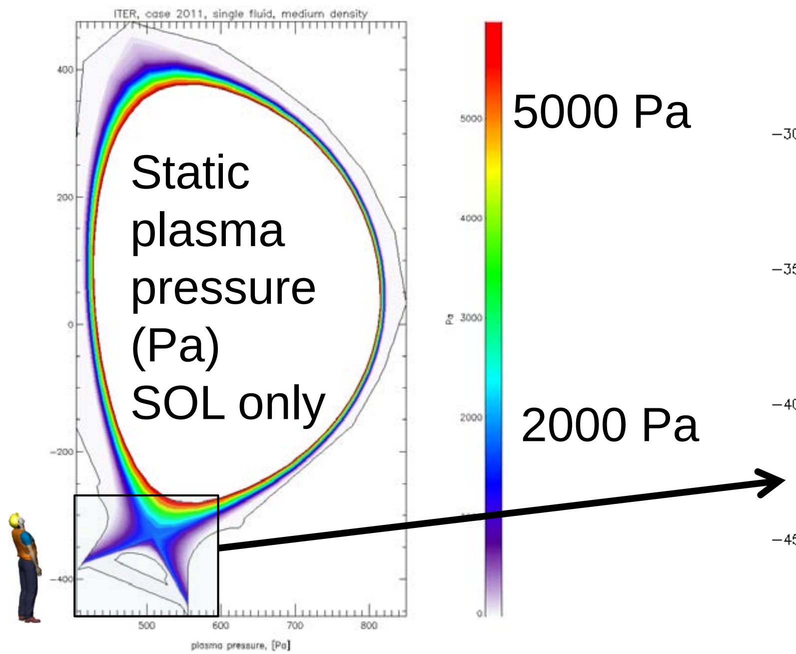
Divertor D^+ ion temperature
eV, lin. scale, 0 – 50 eV

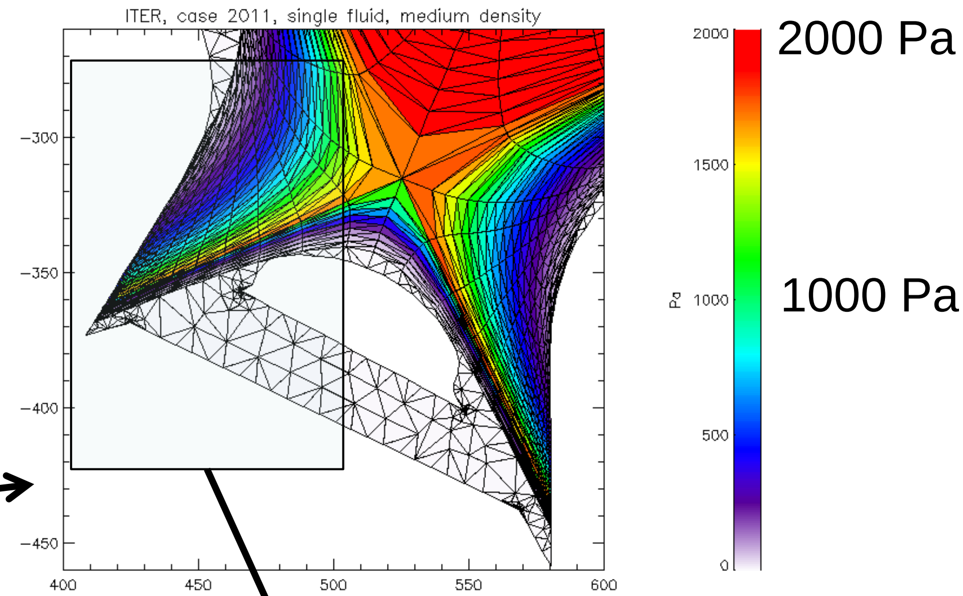




(static) plasma pressure (Pa)

- Inside separatix (confined plasma): constant on magn. flux surf.
- In divertor: pressure drop along B-field



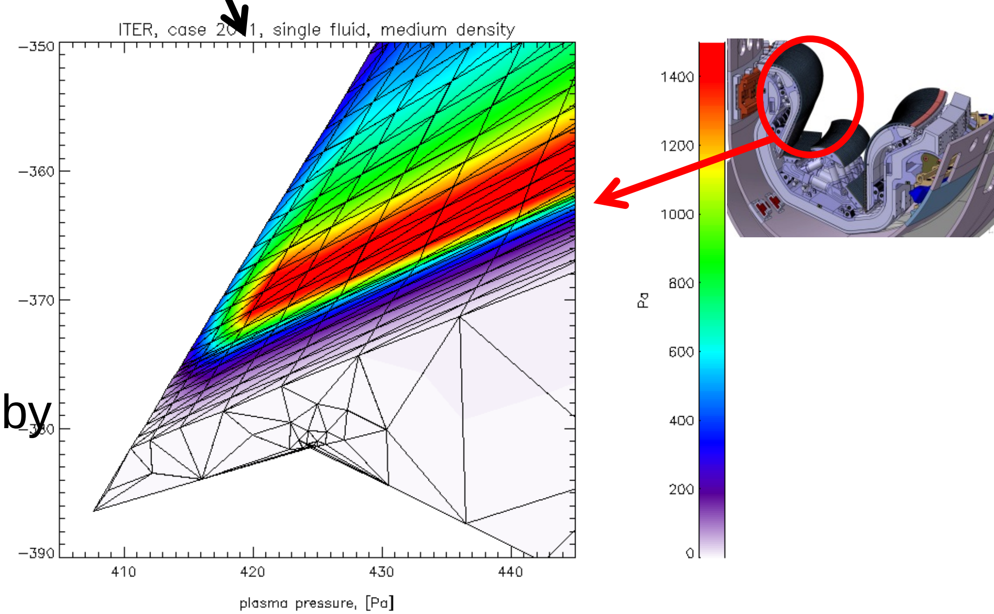


Momentum balance for H^+ ions

$$\frac{\partial}{\partial t}\left(m_i n_i \vec{V}_i\right) + \vec{\nabla}\cdot\left(m_i n_i \vec{V}_i \vec{V}_i\right) = -\vec{\nabla} p_i - \vec{\nabla}\cdot\overleftrightarrow{\Pi}_i + Z_i e n_i\left(\vec{E}+\vec{V}_i\times\vec{B}\right) + \vec{R}_i + \vec{S}_{m_i\vec{V}_i}$$

Near target pressure gradient balanced by momentum sinks:

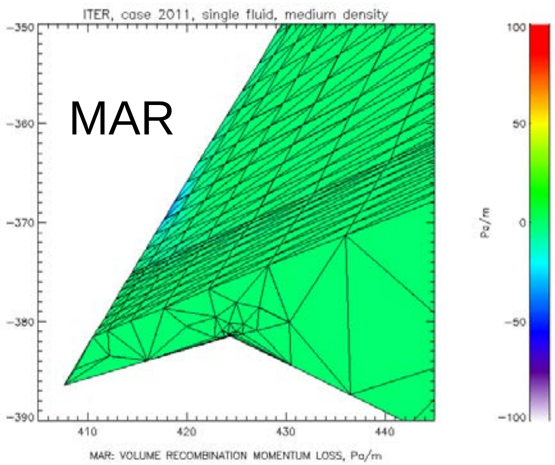
- e + H^+ plasma volume recombination
- Neutral gas – plasma friction



ITER divertor detachment:

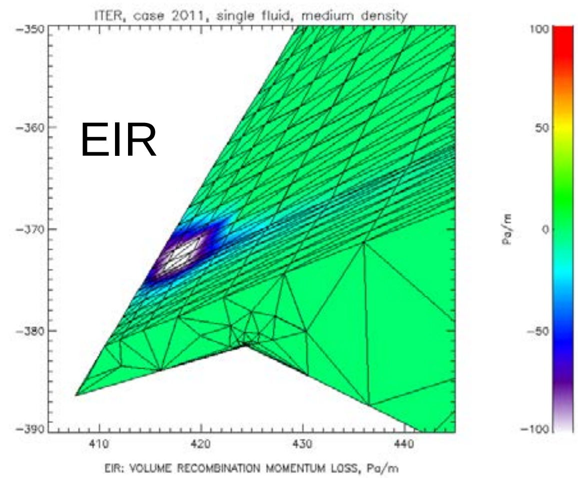
Plasma pressure gradient [Pa/m] provided by:

MAR < EIR < p+H (CX) < $p+H_2$ (elastic) friction



$p+H_2(v) \rightarrow H_2^+ + H$

$e+H_2^+ \rightarrow H + H$



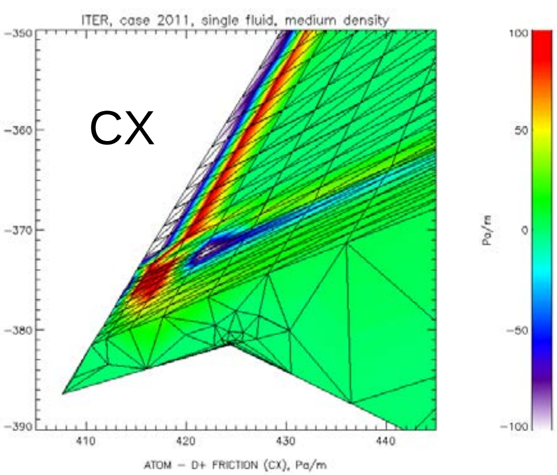
100 Pa/m

0 Pa/m

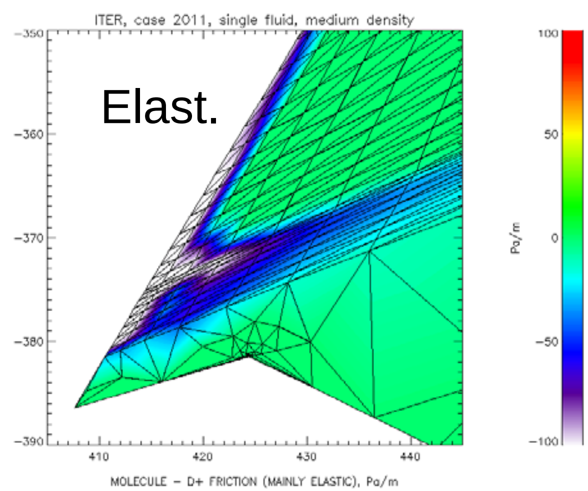
-100 Pa/m

$e+p \rightarrow H + h\upsilon$

$e+p+e \rightarrow H + e$



$p + H \rightarrow H + p$



100 Pa/m

0 Pa/m

-100 Pa/m

$p+H_2$ - elastic

Plasma chemistry is localized in divertor. Provides powerful particle, momentum and energy volumetric sources for plasma flow.

Continuity eq. for ions and electrons

$$\frac{\partial}{\partial t} n_i + \vec{\nabla} \cdot \left(n_i \vec{V}_i \right) = \boxed{S_{n_i}}$$

Momentum balance for ions and electrons

$$\frac{\partial}{\partial t} \left(m_i n_i \vec{V}_i \right) + \vec{\nabla} \cdot \left(m_i n_i \vec{V}_i \vec{V}_i \right) =$$

$$- \vec{\nabla} p_i - \vec{\nabla} \cdot \overleftrightarrow{\Pi}_i + Z_i e n_i \left(\vec{E} + \vec{V}_i \times \vec{B} \right) + \vec{R}_i + \boxed{\vec{S}_{m_i \vec{V}_i}}$$

$$- \vec{\nabla} p_e - e n_e \left(\vec{E} + \vec{V}_e \times \vec{B} \right) + \vec{R}_e = 0$$

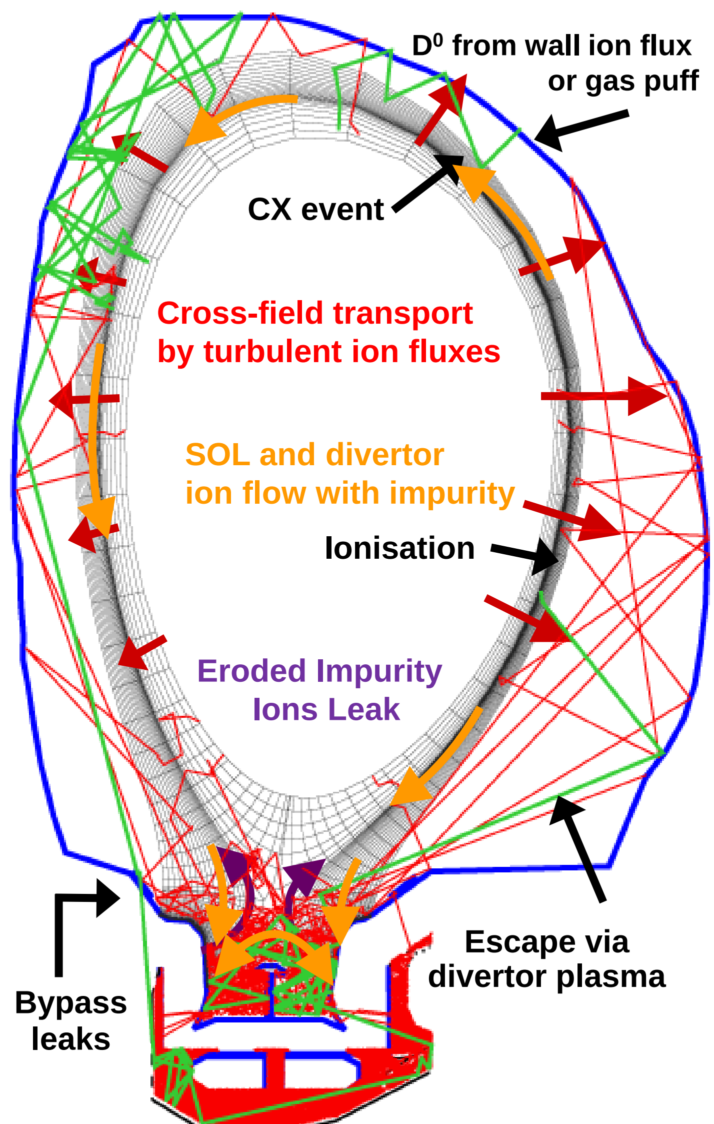
energy balance for ions and electrons

$$\frac{\partial}{\partial t} \left(\frac{3}{2} n_i T_i + \frac{m_i n_i}{2} \vec{V}_i^2 \right) +$$

$$\vec{\nabla} \cdot \left[\left(\frac{5}{2} n_i T_i + \frac{m_i n_i}{2} \vec{V}_i^2 \right) \vec{V}_i + \overleftrightarrow{\Pi}_i \cdot \vec{V}_i + \vec{q}_i \right]$$

$$= \left(e n_i Z_i \vec{E} - \vec{R} \right) \cdot \vec{V}_i - Q_{ei} + \boxed{S_E^i}$$

$$\frac{\partial}{\partial t} \left(\frac{3}{2} n_e T_e \right) + \vec{\nabla} \cdot \left(\frac{5}{2} n_e T_e \vec{V}_e + \vec{q}_e \right) = - e n_e \vec{E} \cdot \vec{V}_e + \vec{R} \cdot \vec{V}_i + Q_{ei} + \boxed{S_E^e}$$



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$$\frac{\partial}{\partial t}\left(\frac{3}{2} n_e T_e \right) + \vec{\nabla} \cdot \left(\frac{5}{2} n_e T_e \vec{V}_e + \vec{q}_e \right) = -e n_e \vec{E} \cdot \vec{V}_e + \vec{R} \cdot \vec{V}_i + Q_{ei} + \boxed{S_E^e}$$

In magnetic fusion:
focus is on plasma flow, turbulence,….
(unknown, and computational challenge),
taking the
S terms (A&M data) **as „known“, and computationally „in hand“**

Selection:
Non atomic physics experts
Disconnection between „fusion“ and atomic physics communities

Implementation:
Very time consuming
Software duplication

Results:
Comparison of results from different groups is often highly dependent on the atomic data used

See: Enrico Landi (CHIANTI), on atomic database for astrophysical plasmas (IAEA-NFRI, 2012, Daejeon)

Atomic & molecular processes: boundary plasma

e,p + $H_2(v_i)$ → …, e+$H_2^+(v_i)$ → H + H*

- divertor detachment dynamics, final states? DR, DE ?

H. Takagi, Phys. Scr. (2002) 52, and: Conference series: DR 1-9

e,p + C, C_xH_y →…., e+$C_xH_y^+$ → …. C erosion and migration, tritium retention in remote areas,…. Excited states of products (CH(A→X)) ?

R. Janev et al., Phys. Plasma (2004) 11

e+$H_3^+(v_3)$ → …., DR, DE,….

- H_3^+ probably irrelevant in fusion plasmas

M. Larsson et al., PRL (1993) 70, S. Datz et al. (1995) 74, and: Conference series: DR 1-9

e+ Be, BeH/BeH^+ → …. possible role on spectroscopy and on material migration: Formation rates ?? 10% of Be sputtering ??

J.B. Roos et al. Phys. Rev A (2009) 80, IAEA Atomic Molec. data unit CRP 2012-201

e+ N, N_2, N_2^+ → …. NN

- N_2-seeding, edge plasma cooling: not yet studied in fusion plasmas, only resulting atomic ions N, N^+, N^{++},….

See planetary atmospheric research

Proposed ITER divertor strategy: decision at the end of 2013

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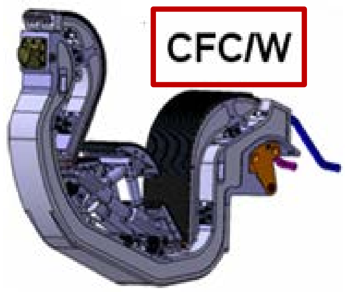
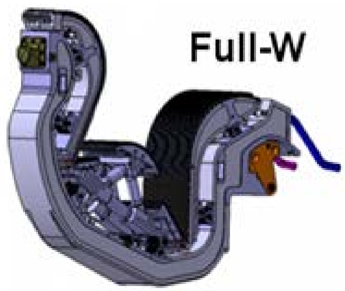
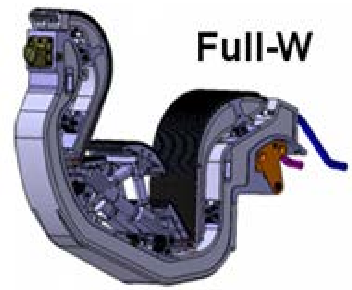
H/He

D/DT

BASELINE







CFC monoblocks at 10 MW m^{-2},
W monoblocks at 5 MW m^{-2}

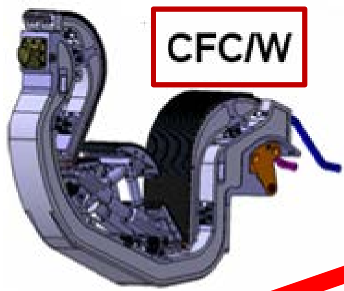
21.11.2013; The ITER Council approved the IO proposal and decided to commence operations with a **full tungsten divertor**...

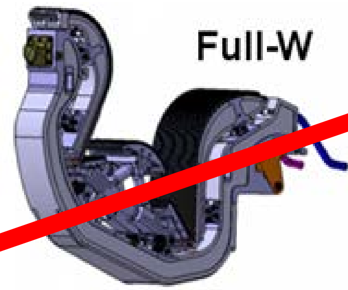
Proposed divertor strategy: decision at the end of 2013

BASELINE

H/He

D/DT



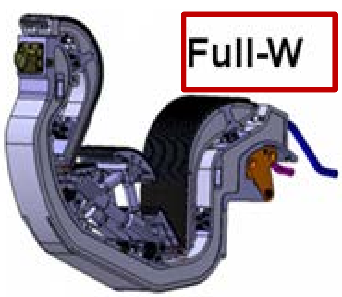


CFC monoblocks at 10 MW m^{-2}, W monoblocks at 5 MW m^{-2}

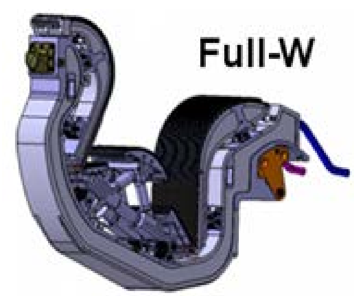
FULL-W START

H/He

D/DT



~10 years



W monoblocks at 10 MW m^{-2}

Tokamak/Stellarator boundary: hybrid plasma (fluid) neutral/impurity (kinetic)

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- **Status:**

  transition from computational science to computational engineering currently ongoing (e.g. divertor design for ITER, DEMO, W7X,JT-60SA…)

  despite many deficits still

- **But: long list of deficient understanding:**

  In particular: plasma material interaction (empirical laws only)

  but also: sources, parallel flows, cross field turbulent fluxes….

- **Goal:** separate all known (ab initio) model parts from the still unknown (ad hoc) parts, often by detailed computational bookkeeping.

  Ultimately: isolate anomalous cross field transport as only remaining unknown, to make it accessible experimentally.

→ **sub-Goal: at least: turn A&M&S data issues from unkown to known (at least to: “evaluated”, “publicly exposed”, “ITER reference data set”)**

Thank you for your attention!

Outline

A: Core plasma: (beam-) spectroscopy

strongly stripped ions, often: H, He-like

B: Plasma boundary: spectroscopy plus: powerful plasma flows, particle exhaust, heat exhaust, machine availability

C: Typical parameters (electron density, temperature)

D: A&M data sensitivity (→ uncertainty propagation)

- 1: status: A&M data: sensitivity analysis in 0D plasma chemistry models.
- 2: outlook: A&M data: sensitivity analysis in current edge plasma flow models ???

Uncertainty propagation and sensitivity analysis

Atomic structure

collision codes

experimental data

fundamental data

Velocity distribution:
Boltzmann solver,
Maxwellian

Processed data (rate coef.)

CR transition matrix A =
A_excit+
A_radiative+
A_ionis+
A_cx+
A_recomb+….

Linear algebra,
ODE solvers

effective rates,
population coefficients
cooling rates,
beam stopping rates,….

Uncertainty propagation and sensitivity analysis:

journey of data…

A&M experts

Evaluation, …
Data centers

Data centers
and/or
user community

Atomic structure

collision codes

experimental data

fundamental data

→ PMI, and kinetic models

Processed data (rate coef.)

CR transition matrix A =
A_excit+
A_radiative+
A_ionis+
A_cx+
A_recomb+….

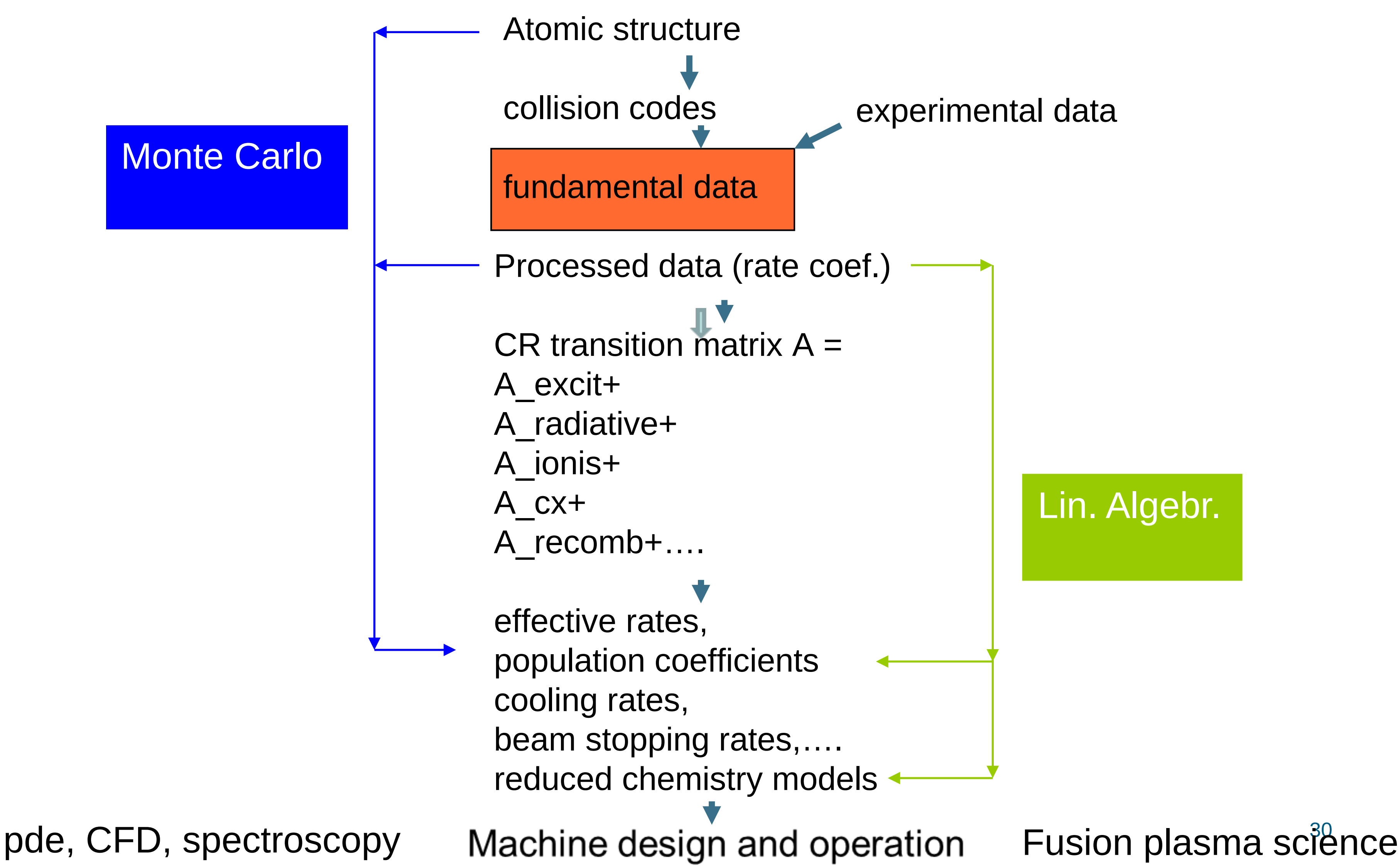
effective rates,
population coefficients
cooling rates,
beam stopping rates,….

near
edge plasma
far

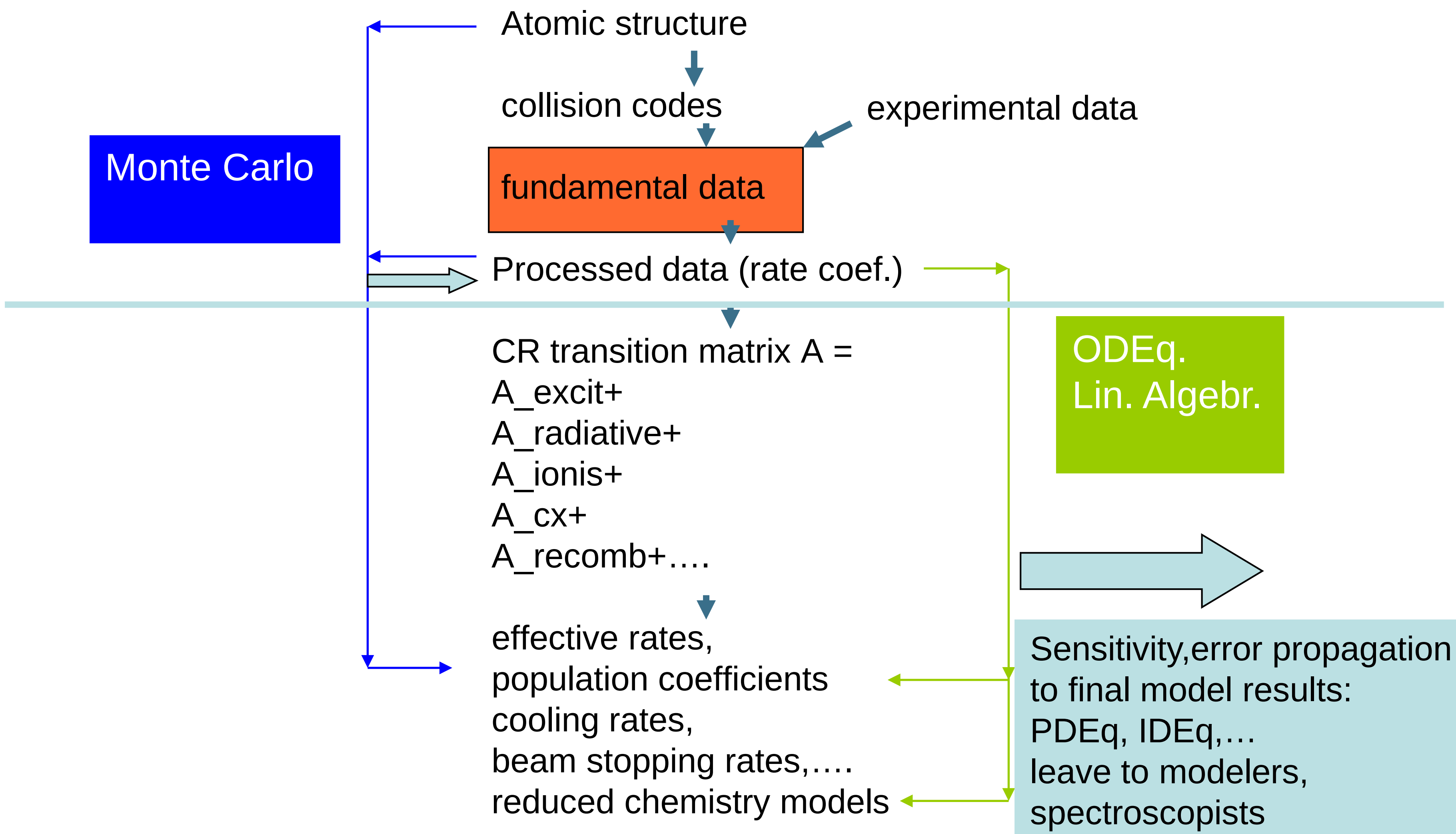
core plasma

Machine design and operation

Uncertainty propagation and sensitivity analysis

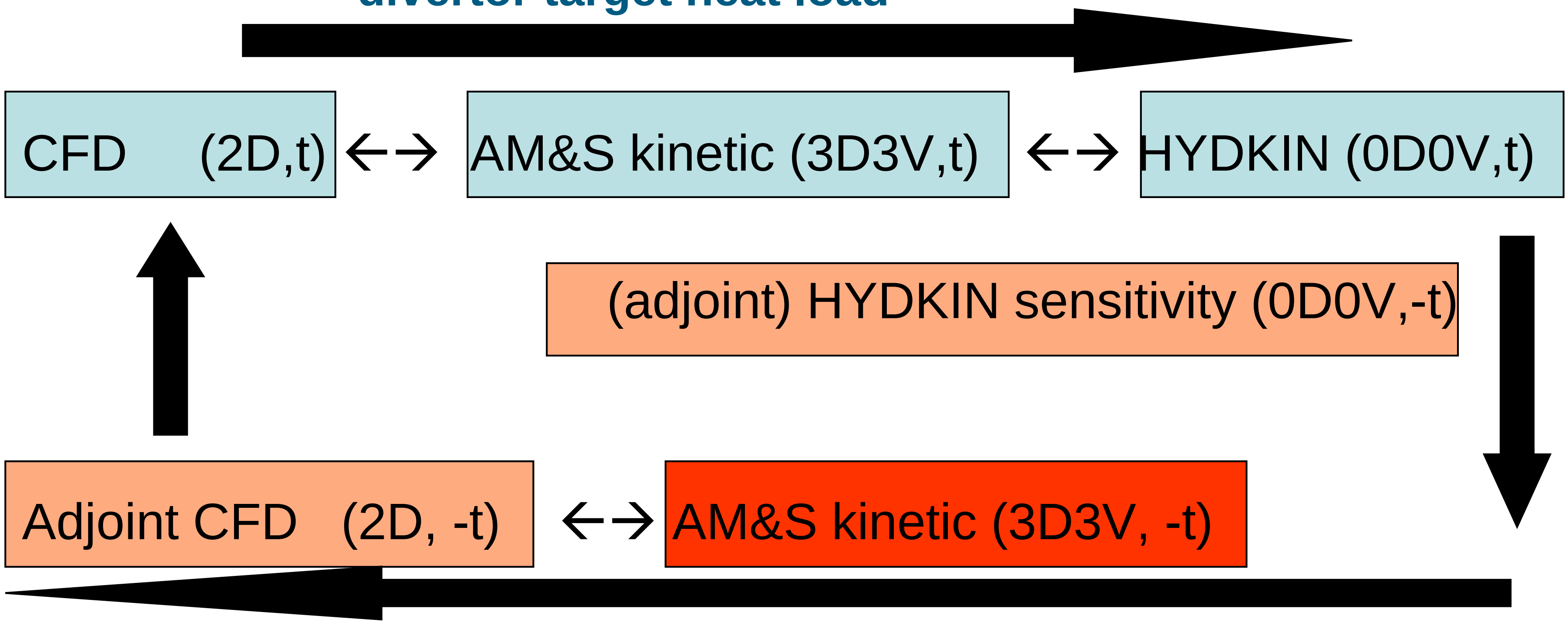


Uncertainty propagation and sensitivity analysis



A&M sensitivity, uncertainty propagation in fusion reactor design and operation:

How do uncertainties in A&M data propagate to divertor target heat load

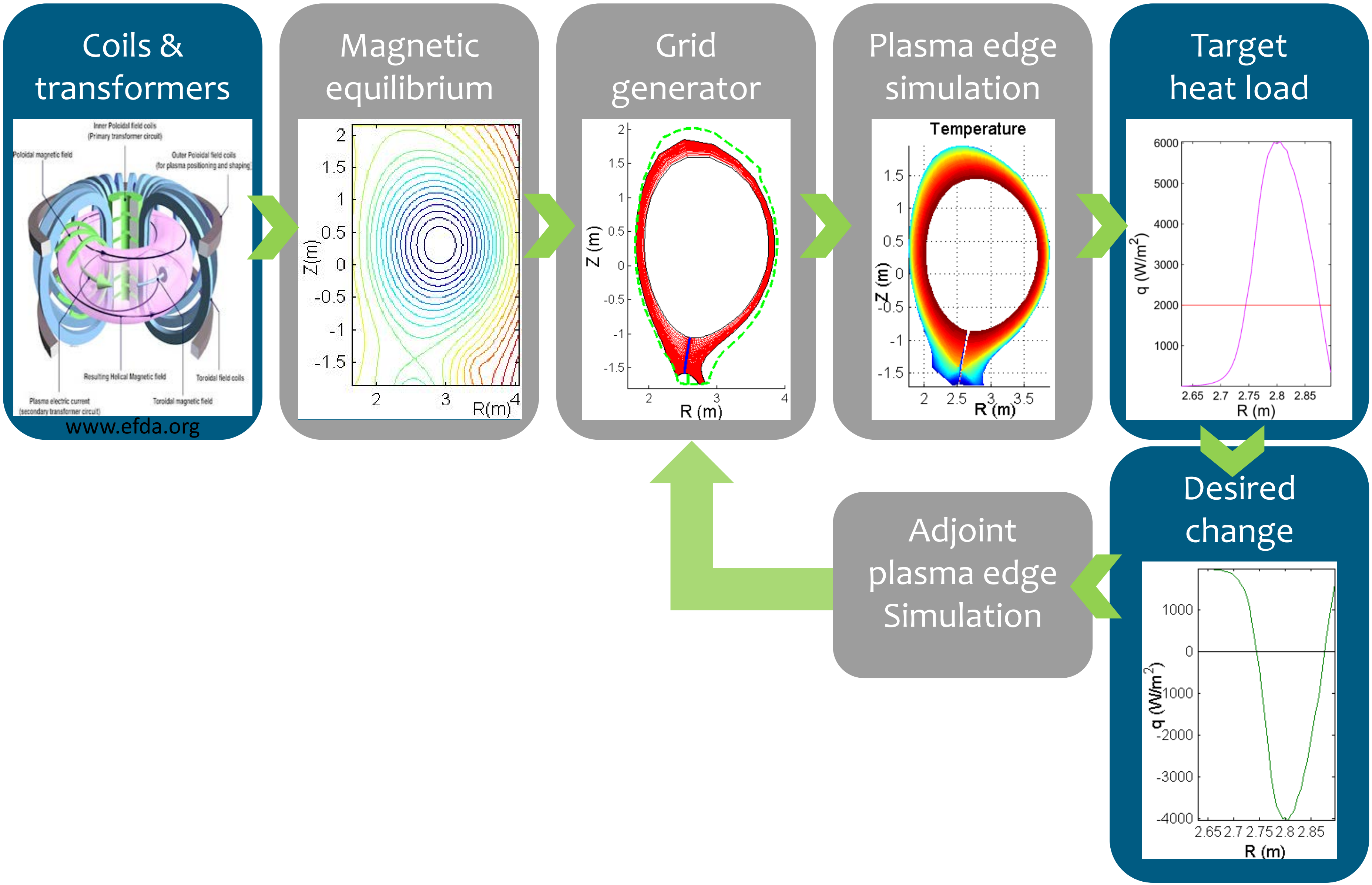


Available since 30 years

Recent development

By-product from "adjoint" based automated divertor design approaches
(adaptations from methodology in automotive and aeronautic applications)

Introducing adjoint sensitivities



Sensitivities from adjoint flow simulation

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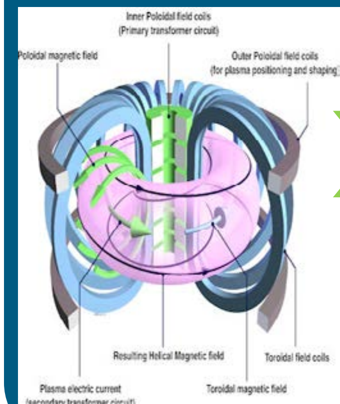
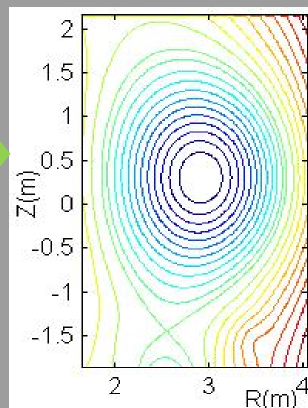
Coils & transformers

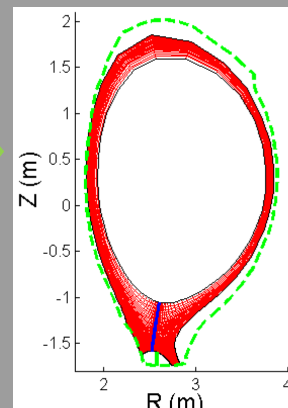


www.efda.org

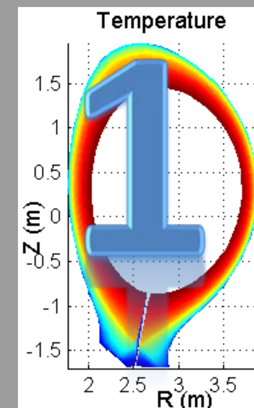
Magnetic equilibrium



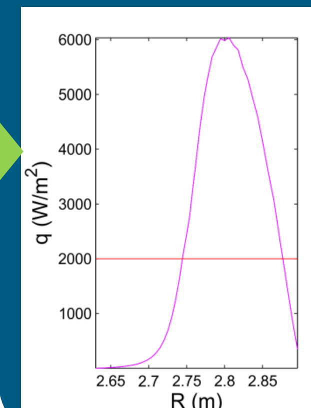
Grid generator



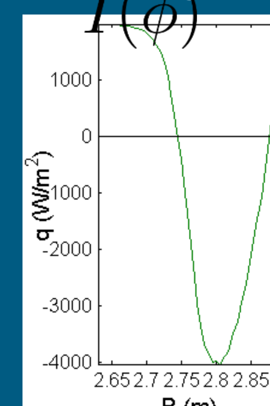
Plasma edge simulation



Target heat load



Desired change $\hat{I}(\phi)$



Adjoint plasma edge Simulation

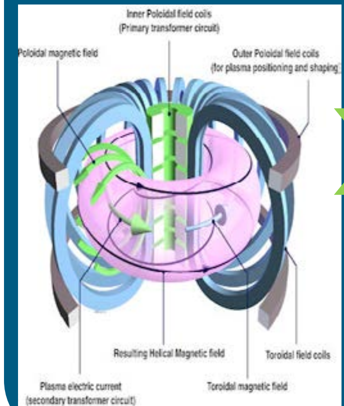
$$\phi + t \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\nabla_\phi \hat{I} = \begin{pmatrix} 2 \\ -1 \\ 1 \\ 3 \\ -2 \end{pmatrix}$$

Mitglied der Helmholtz-Gemeinschaft

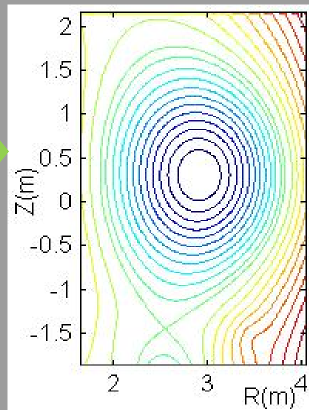
Sensitivities in practice

Coils & transformers

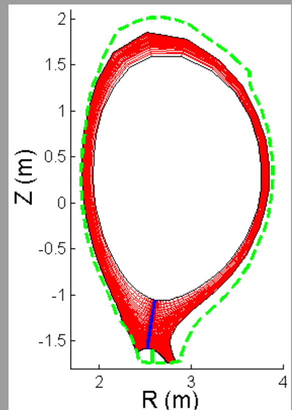


www.efda.org

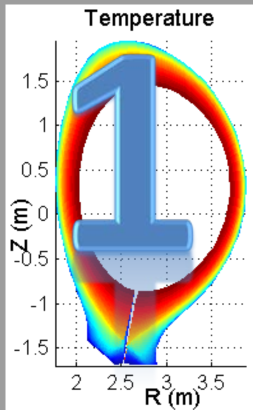
Magnetic equilibrium



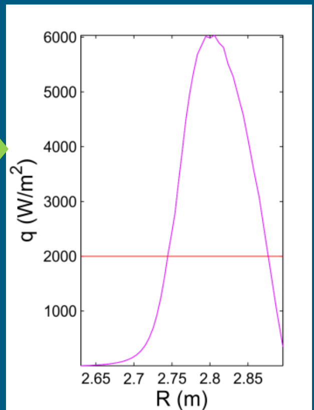
Grid generator



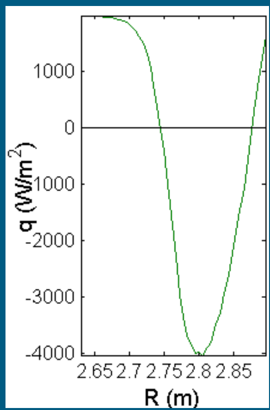
Plasma edge simulation



Target heat load



Desired change



Adjoint plasma edge Simulation

1

$$\mathrm{cost}(\nabla_\phi \hat{I}) \approx 2\ \mathrm{cost}(\hat{I})$$

Details:

M. Blommaert et al. “A Novel Approach to Magnetic Divertor Configuration Design,” Journal of Nuclear Materials, 2014.

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