The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA
International Atomic Energy Agency

**2327-8**

**Joint ICTP-IAEA Workshop on Fusion Plasma Modelling using Atomic and Molecular Data**

***23 - 27 January 2012***

**Introduction to Edge Plasma Modelling**

TELMINI Mourad

*LSAMA, Department of Physics*
*Faculty of Science of Tunis, El Manar 2092*
*Tunis*
*TUNISIA*

Detlev REITER

*Forschungszentrum Juelich GmbH, Institute for Energy & Climate Research,*
*52425 Juelich*
*GERMANY*

# Introduction to edge plasma modelling

Detlev Reiter

Forschungszentrum Jülich GmbH, Institute for Energy and Climate Research
52425 Jülich, Germany

# FZ Jülich:
# in Germany fusion research is organized in the Helmholtz Association

## Germany

Helmholtz Association

DFG / Universities

## Europe

TEC: Trilateral Euregio Cluster (B, Nl, Jül)

EURATOM Association

EFDA (JET, Technol.)

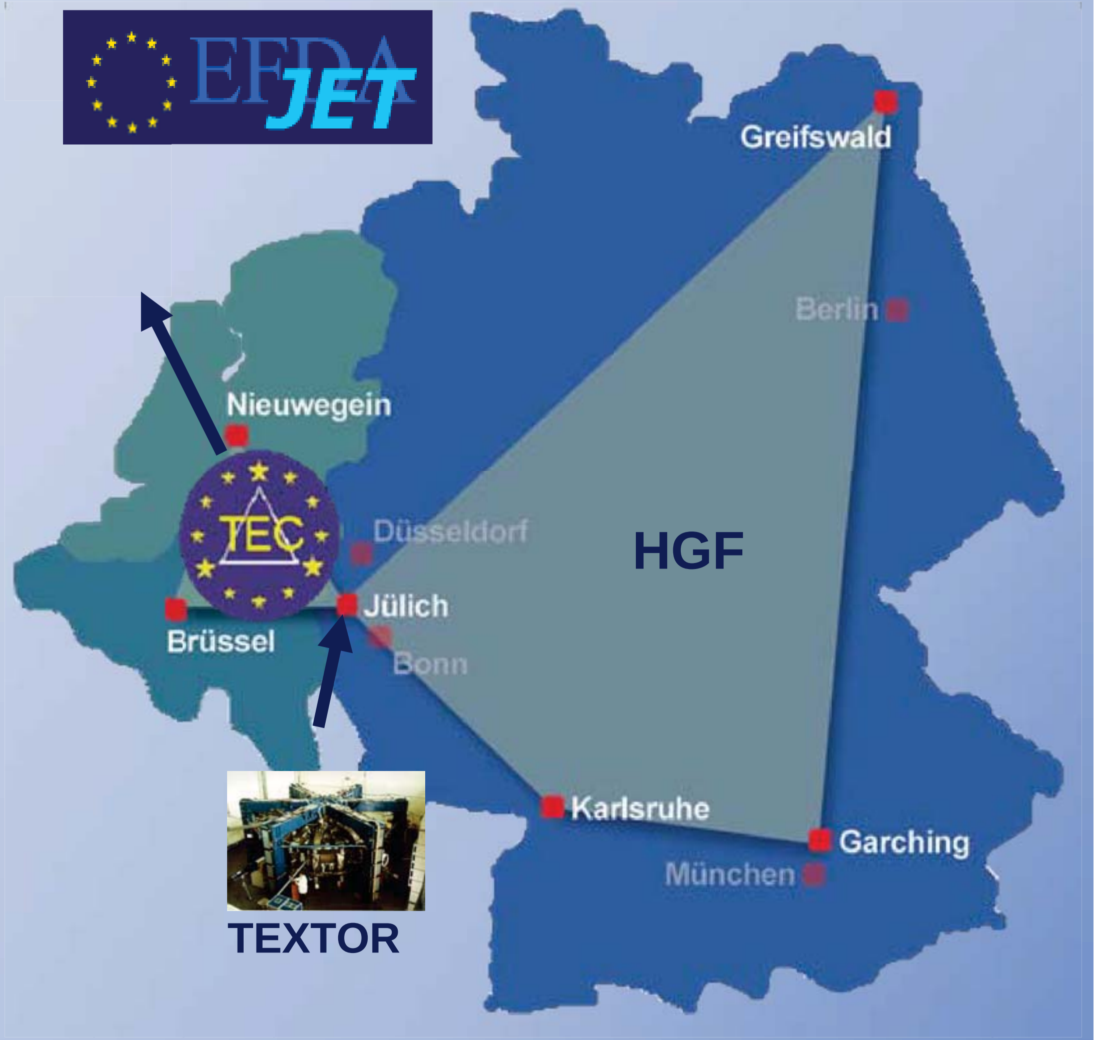
F4E (ITER)

## World

IEA Implementing Agreement

“Plasma-Wall Interaction” (J, USA, Canada)

ITPA International Expert Groups



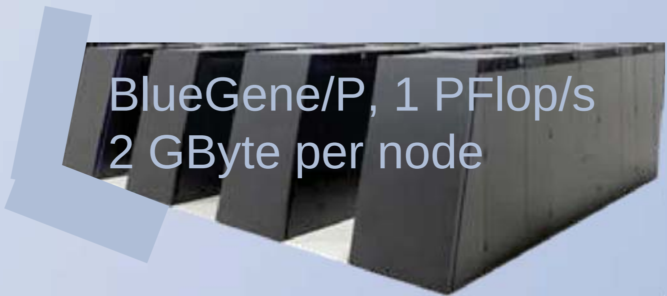
# Supercomputer Environment FZ Juelich, by Aug. of 2009

EFDA-
Supercomputer for
Fusion Science
HPC-FF

Jülich‘s General Purpose Supercomputer
installed in 2009

- 2048 nodes @ 8 cores
- 24 GByte per node
- Intel NEHALEM
- Network: $QSnet^{III}$
- Peak Performance about 200 TFlop/s

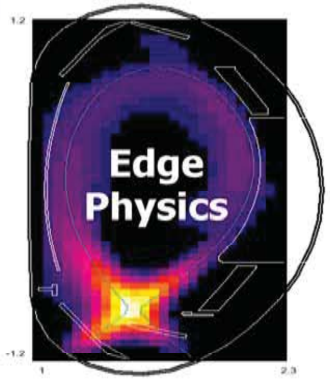
- 1000 nodes @ 8 cores
  of same architecture
- Estimated Peak Performance
  about 100 TFlop/s

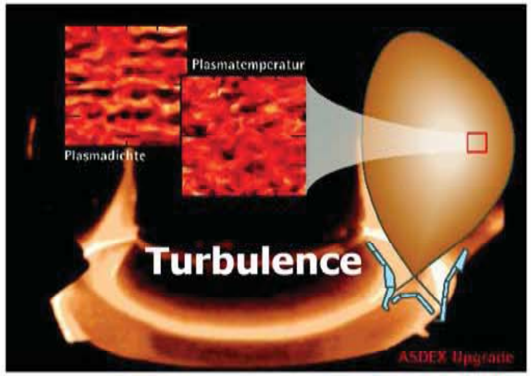


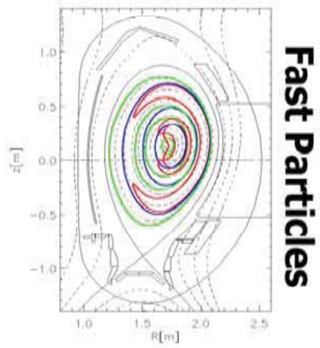

Storage
Environment

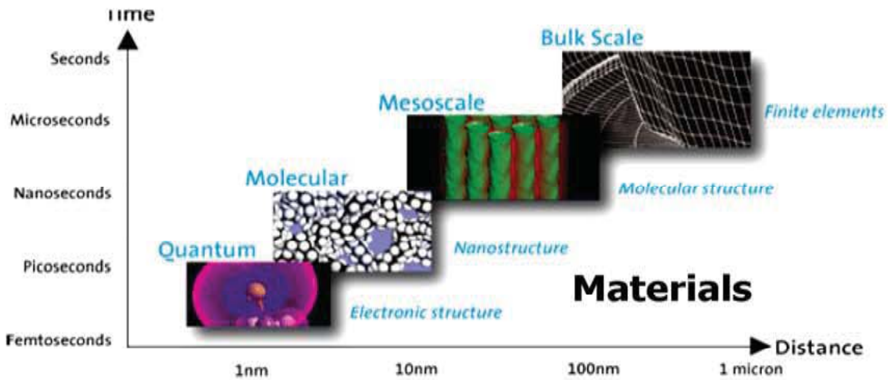
## The EU 100 TF HPC-FF has started operation on Aug. 5$^{th}$ 2009

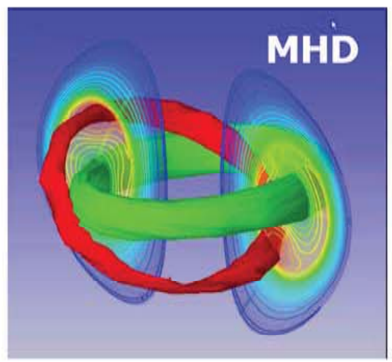
# Fusion and materials modeling: Various HPC needs



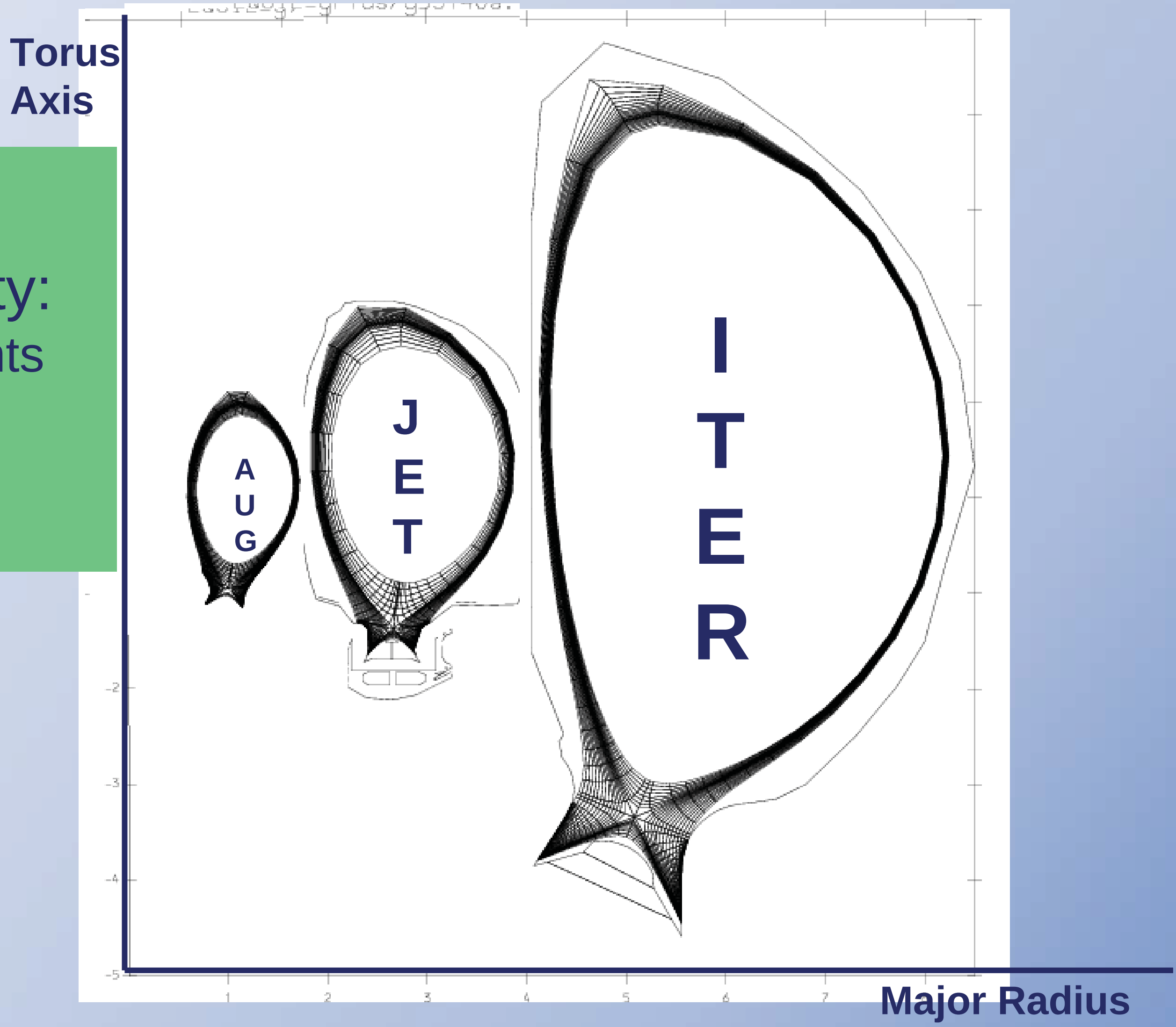



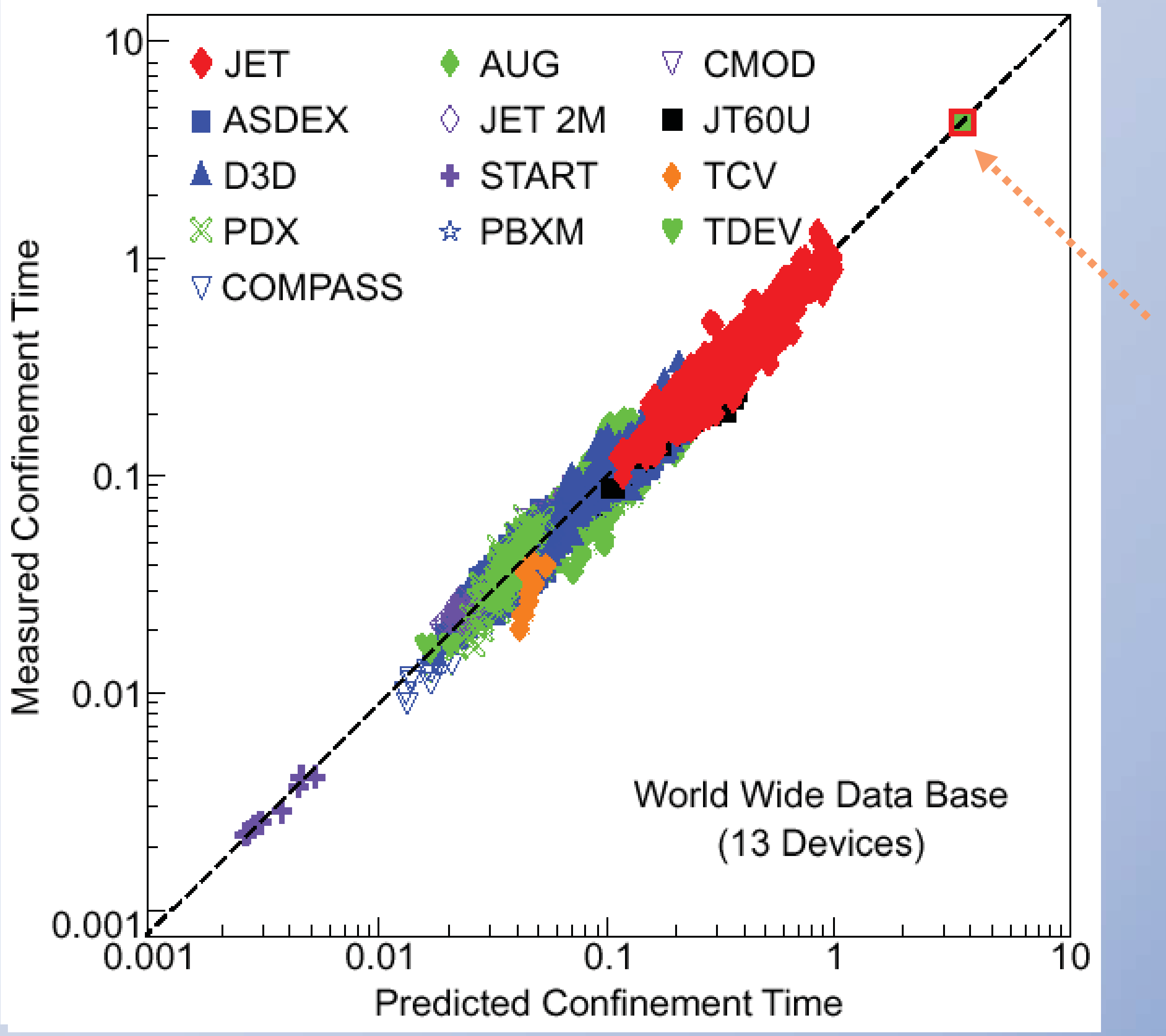



## Extrapolation: present experiments ⇒ ITER

Core:
plasma similarity:
present experiments are "wind tunnel experiments" for ITER

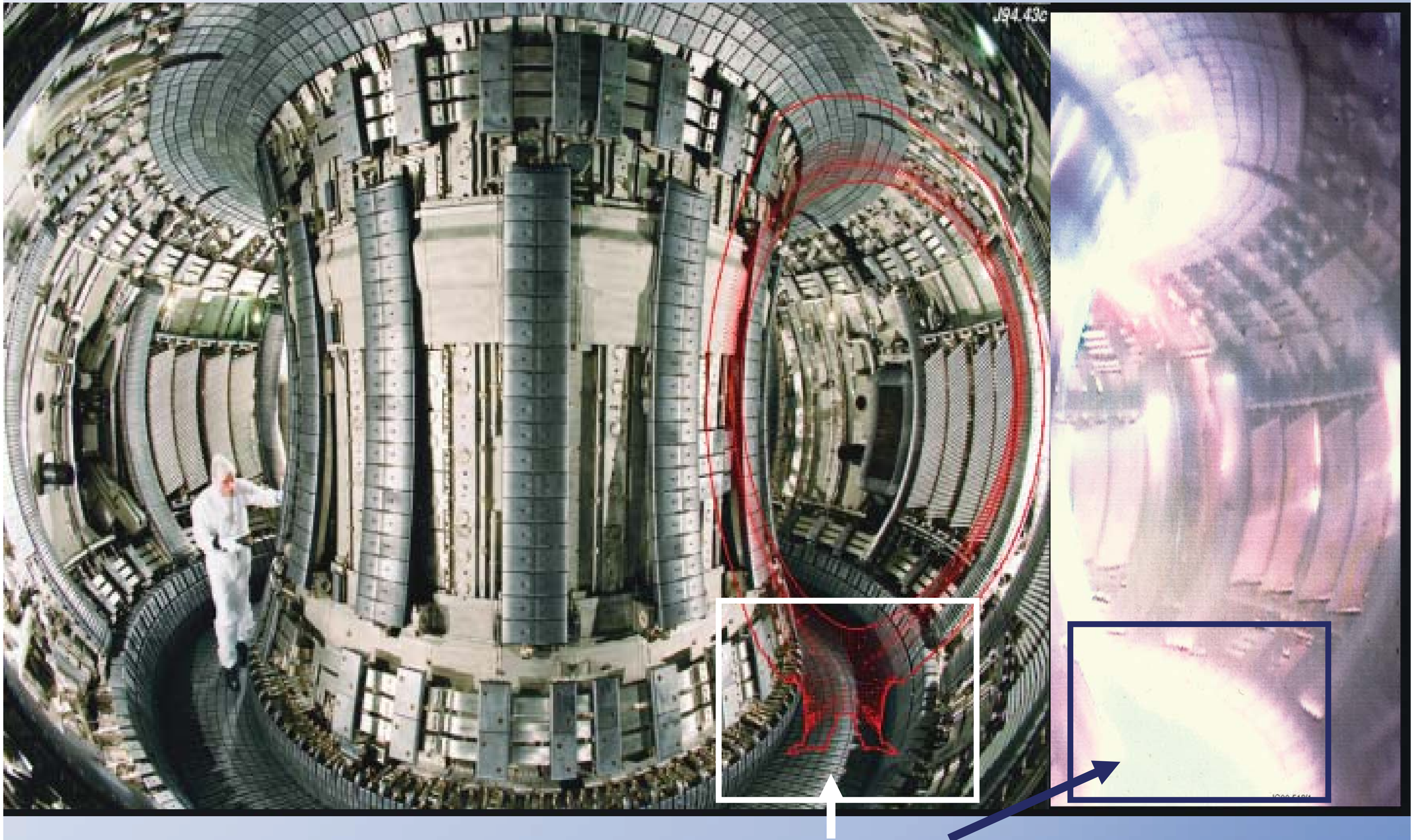


Extrapolation of core plasma confinement to ITER




**ITER reference scenario**

**JET (Joint European Torus) :**
**Ø 8.5 m,   2.5 m high,  3.4 T,   7 MA, 1 min**

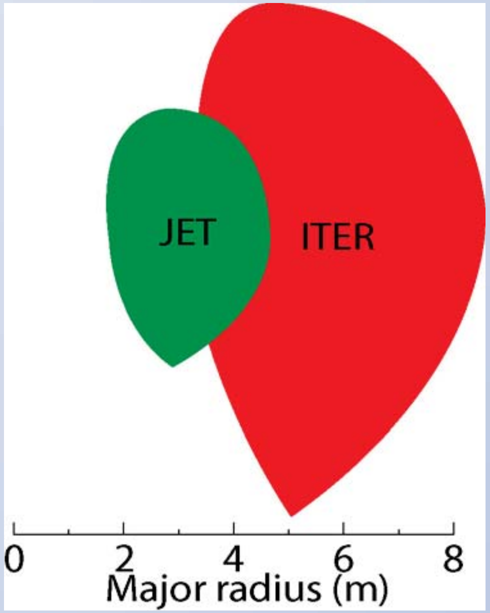



**The edge plasma challenge: Key area for plasma wall interaction**

# Edge plasma science: Upscale to ITER is a big step

| Parameter | JET MkIIGB (1999-2001) | ITER |
|---|---|---|
| Integral time in diverted phase | 14 hours | 0.1 hours |
| Number of pulses | 5748 | 1 |
| Energy Input | 220 GJ | 60 GJ |
| Average power | 4.5 MW | 150 MW |
| Divertor ion fluence | $1.8x10^{27}$ | $*6x10^{27}$ |

*Code calculation




1 ITER pulse ~ 0.5 JET years energy input

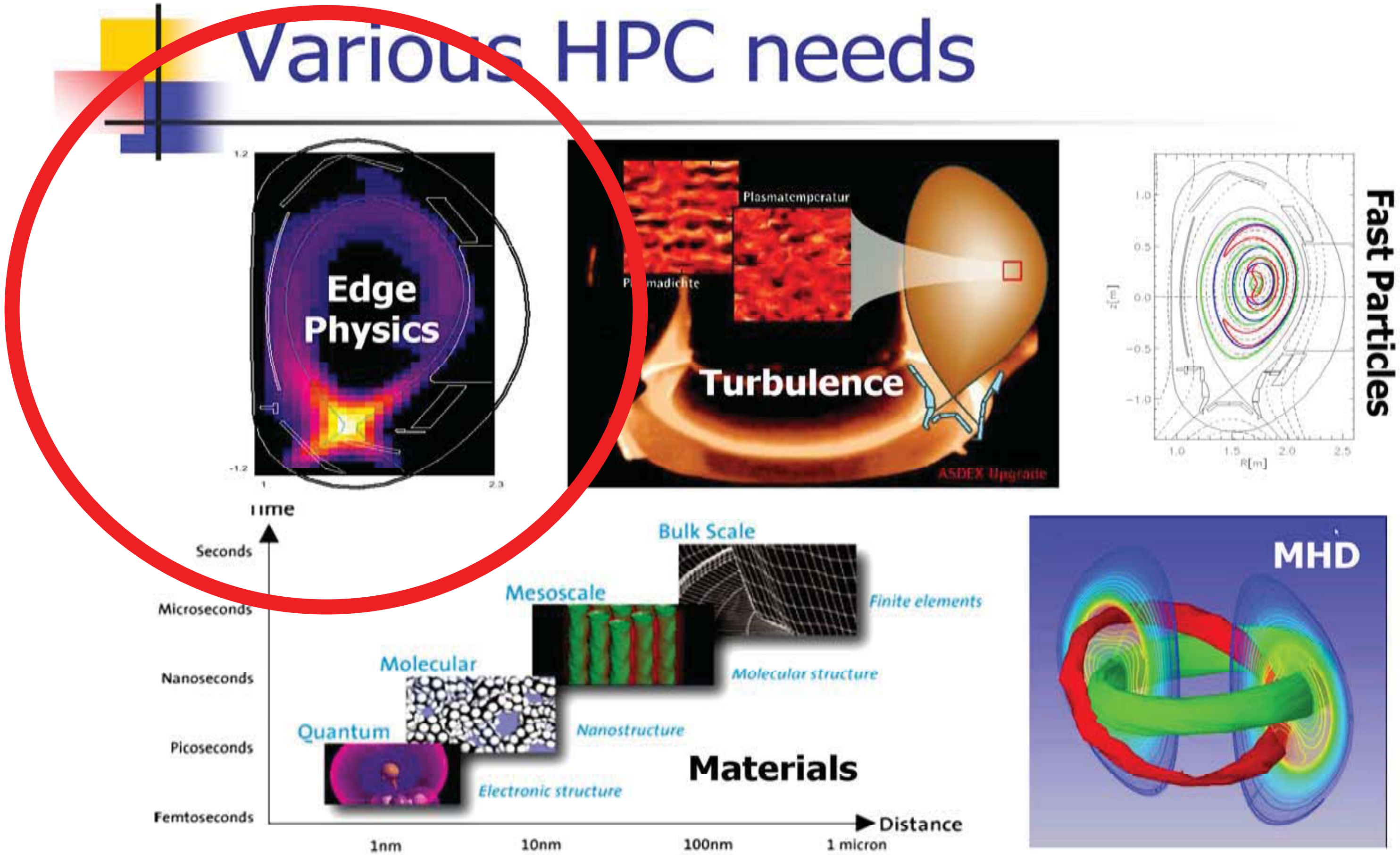
1 ITER pulse ~ 6 JET years divertor fluence

**The edge plasma will "work on" the wall surfaces in ITER 3-5 orders of magnitude stronger than in JET**

Courtesy: G. Matthews, JET

**The EU 100 TF HPC-FF has started operation on Aug. 5th 2009**

# Fusion and materials modeling: Various HPC needs



# Role of Edge Plasma Science

**Early days** **of magnetic fusion (sometimes still today?):**

**Hope that a fusion plasma would not be strongly influenced by boundary:**

***"The edge region takes care of itself".***

**Single goal: optimize fusion plasma performance ("advanced scenarios",…..)**

**Now:**

**man made fusion plasmas are now powerful enough to be dangerous for the integrity of the container:**

***The edge region does NOT take care of itself.***
***It requires significant attention!***

**The ITER lifetime, performance and availability will not only be influenced, it will be controlled by the edge region**

# Role of Edge Plasma Science, cont.

**The layman's response to the idea:**

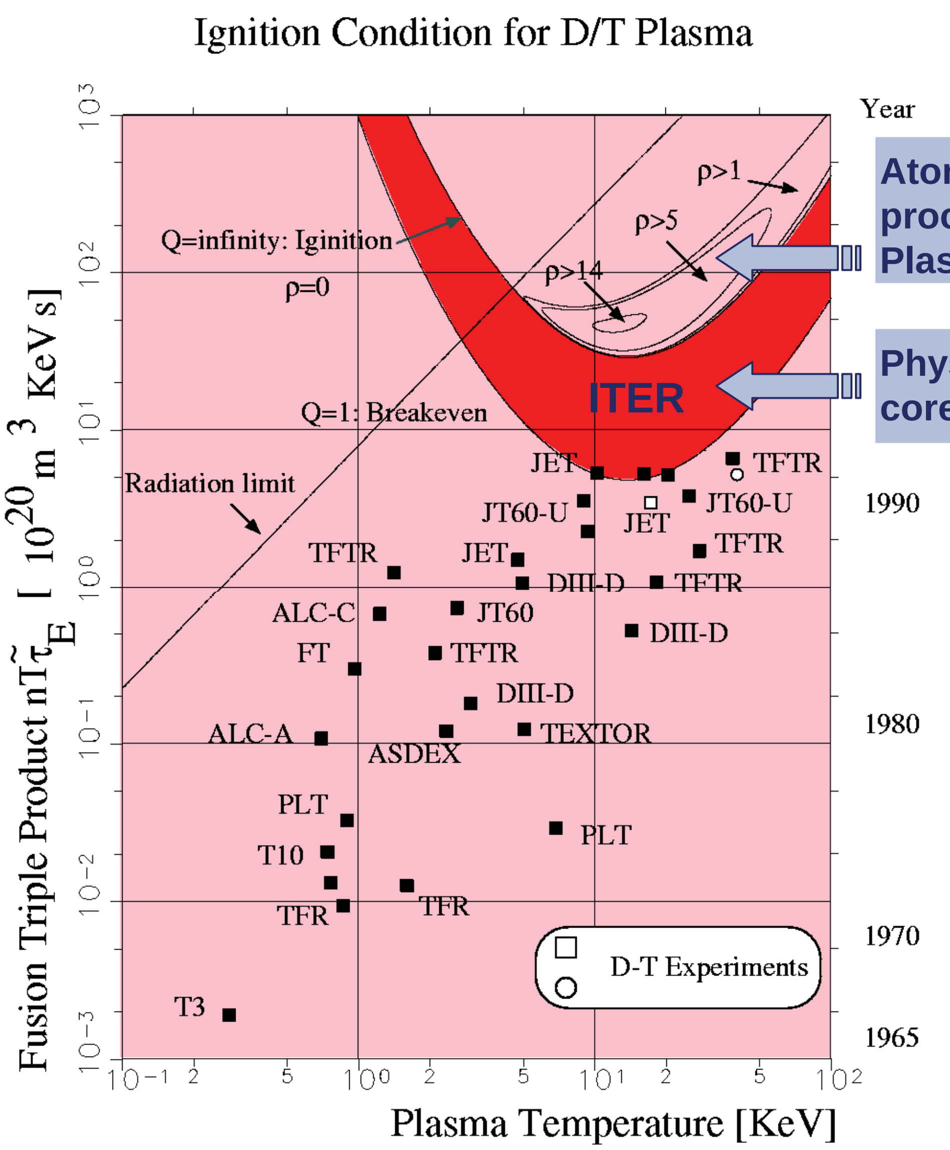
**"A miniature star (100 Mill degrees) in a solid container":**

**THIS MUST BE IMPOSSIBLE !**

**It turned out unfortunately (early 1990th):**

**THE LAYMAN IS RIGHT !**

**Almost...**




Atomic/Molecular processes,
Plasma material interaction

Physics of hot plasma core

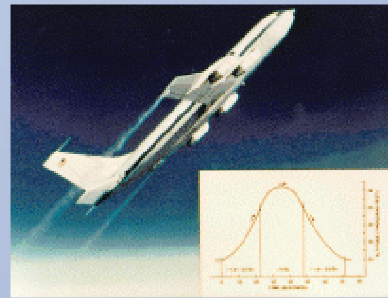
**Can we hope that magnetic confinement core plasma physics progress will mitigate plasma-surface problems ?**

Candle, on earth


Convection,

driven by buoyancy
(i.e. gravity)

Candle, under mircogravity



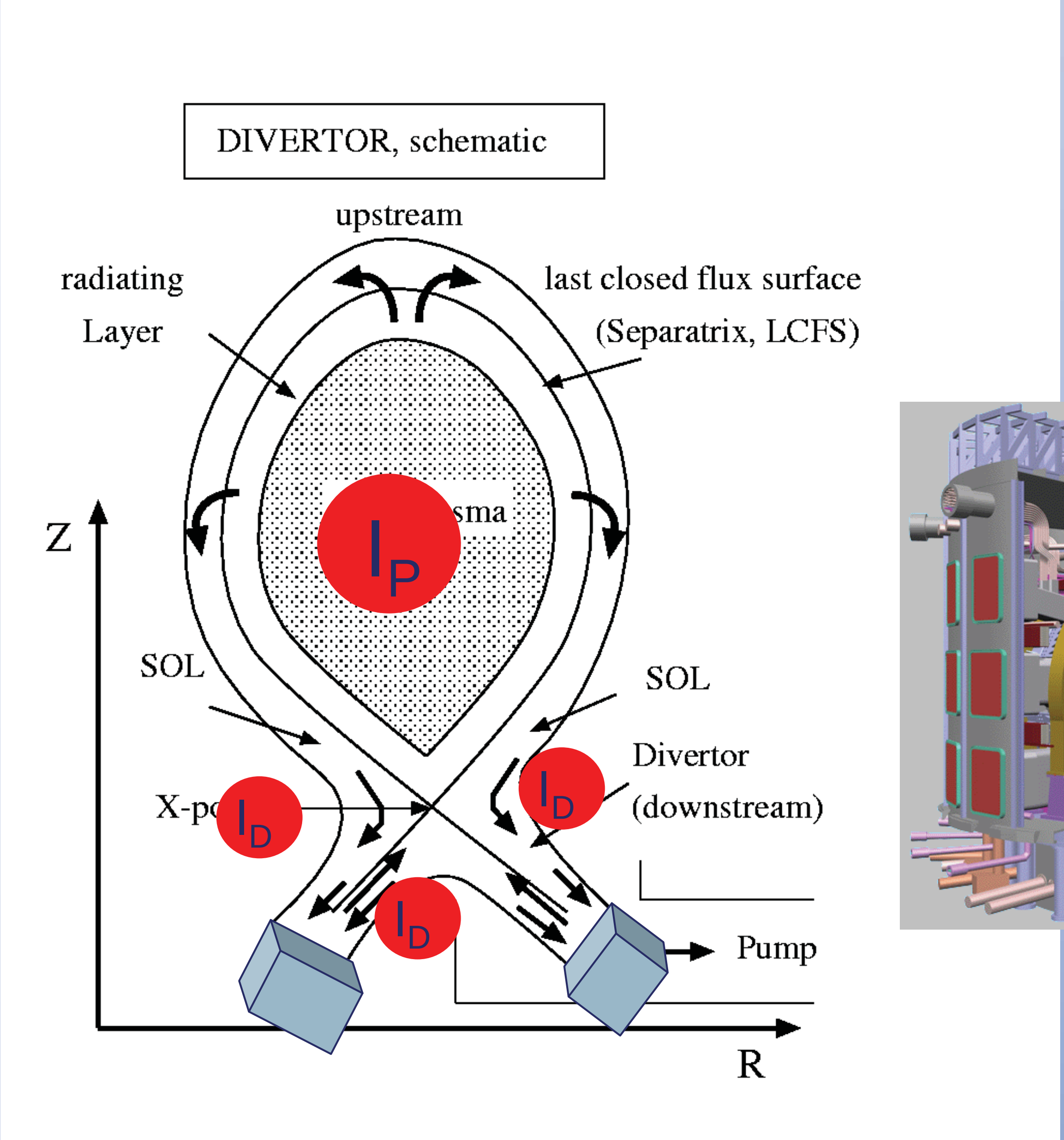
**e.g.: parabola flight,**
**g ≈ 0**

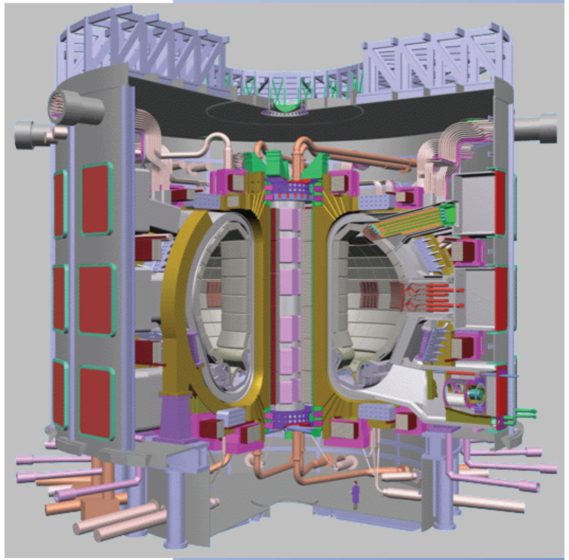
**(only small,**
**dim burn,**
**at best)**

Only Diffusion

(no convection)

## Magnetic Fusion: how to produce convection ? DIVERTOR

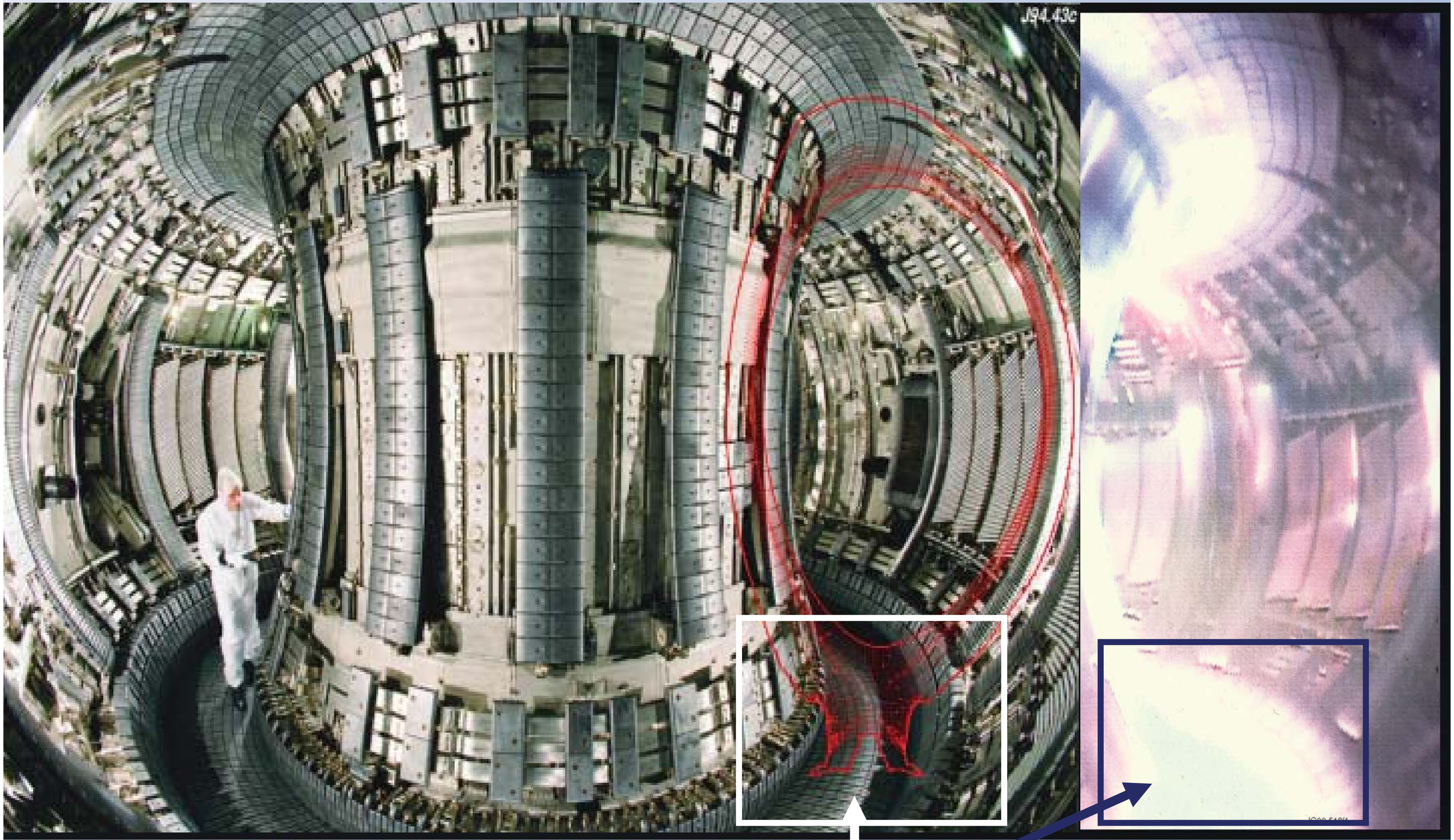


Increase convection → increase plasma surface interaction: operational window?

**JET (Joint European Torus) :**

**Ø 8.5 m,   2.5 m high,  3.4 T,   7 MA, 1 min**

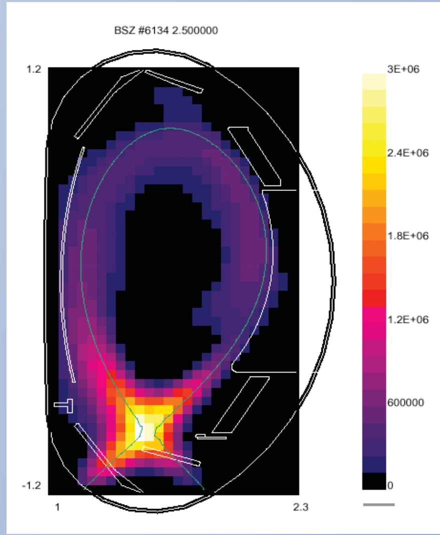


**Key area for plasma wall interaction**

# Numerical edge/divertor modelling

- interdisciplinary
- already a highly integrated field
  - plasma physics ⟷ fusion, technical, astro
  - CFD ⟷ fluid-dynamics
  - rarefied gas dynamics ⟷ aero-dynamics, vacuum
  - opacity ⟷ lighting, inertial fusion
  - plasma wall interaction
  - atomic physics
  - molecular physics

  ⟷ currently through IAEA
  - .....

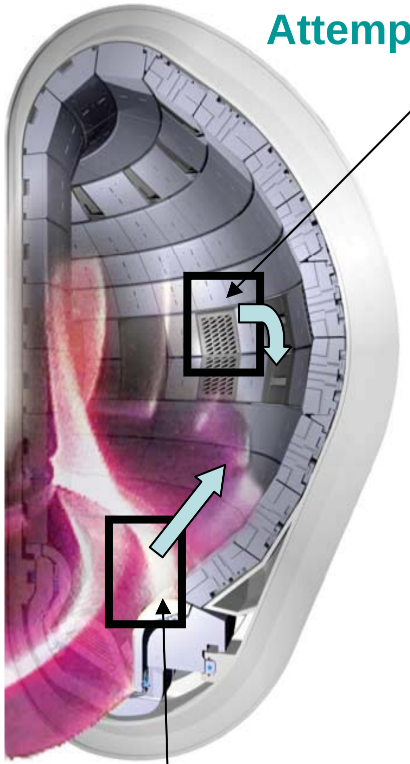



FZJ - KU Leuven activities in edge plasma simulation:

**EIRENE** : gas dynamics, radiation, gyro-averaged impurities
**ERO** : PWI, microscopic: Erosion and re-deposition
edge **code integration**: B2-EIRENE (a.k.a. SOLPS….),
EMC3-EIRENE, EDGE2D-EIRENE
OSM-EIRENE
atomic and molecular **databases** (with IAEA, Vienna)

# Integrated edge plasma simulation at FZJ: "From the barrier to the target"

**ITER**



**Drift-Fluid turbulence: Attempt**

Input:
Transp. Coeff.

EMC3 (& B2)
CFD, 2D & 3D
Charged fluid parcels
m – 100 m scale

EIRENE
3D kinetic
Gyro centers,
Entire SOL and Core
mm - m scale

ERO, PEPC
"Real" ions (and electrons)
PSI in plasma, near solid
(sub-) cm scale

MACRO

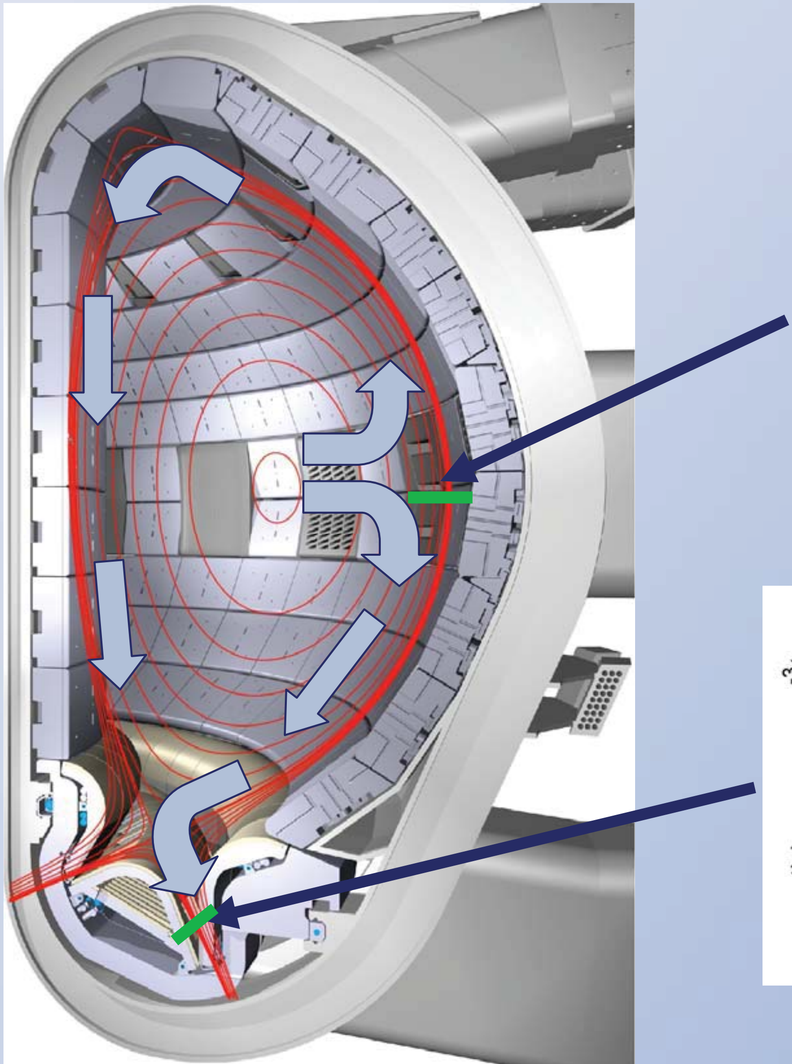
MICRO

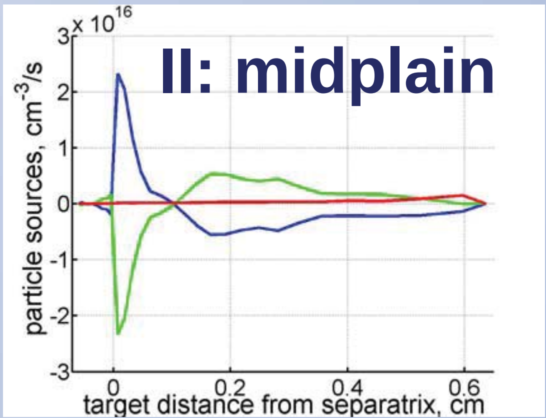
**PSI inside solid: TRIM.xxx, Material science etc…, nm-scale**

Input:
Kinetic boundary conditions

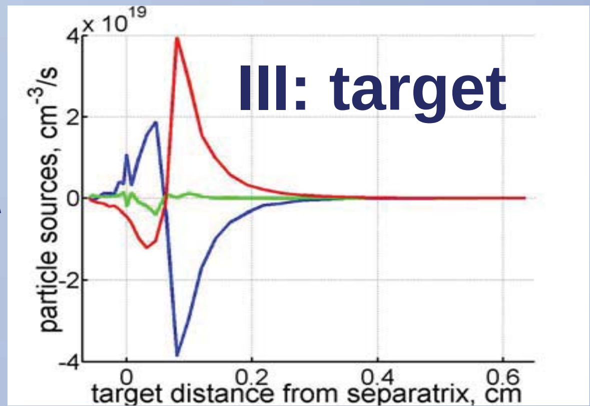
## Relative importance of plasma flow forces over chemistry and PWI
## II edge region → III divertor

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






parallel vs. (turbulent) cross field flow




parallel vs. chemistry and PWI driven flow

# The EDGE plasma challenge (same for tokamaks and stellarators) :

- **Broad range of space and timescales**
- **no clearly separated timescales, → no natural separation into reduced sub-models.**

- **large variation of collisionality**
- **multitude of physical processes**
- **near sonic flow**
- **large number of species**
- **three states of matter (at least) involved, strong exchange**
- **complex magnetic fields (2D → 3D)**

- **computational boundary plasma engineering needed now (not in 10 years)**

**Need for mature edge codes defines work packages for next years.**

# The work horse for tokamak edge modelling: B2-EIRENE

- **Status:**

  transition from computational science to computational engineering despite many deficits still

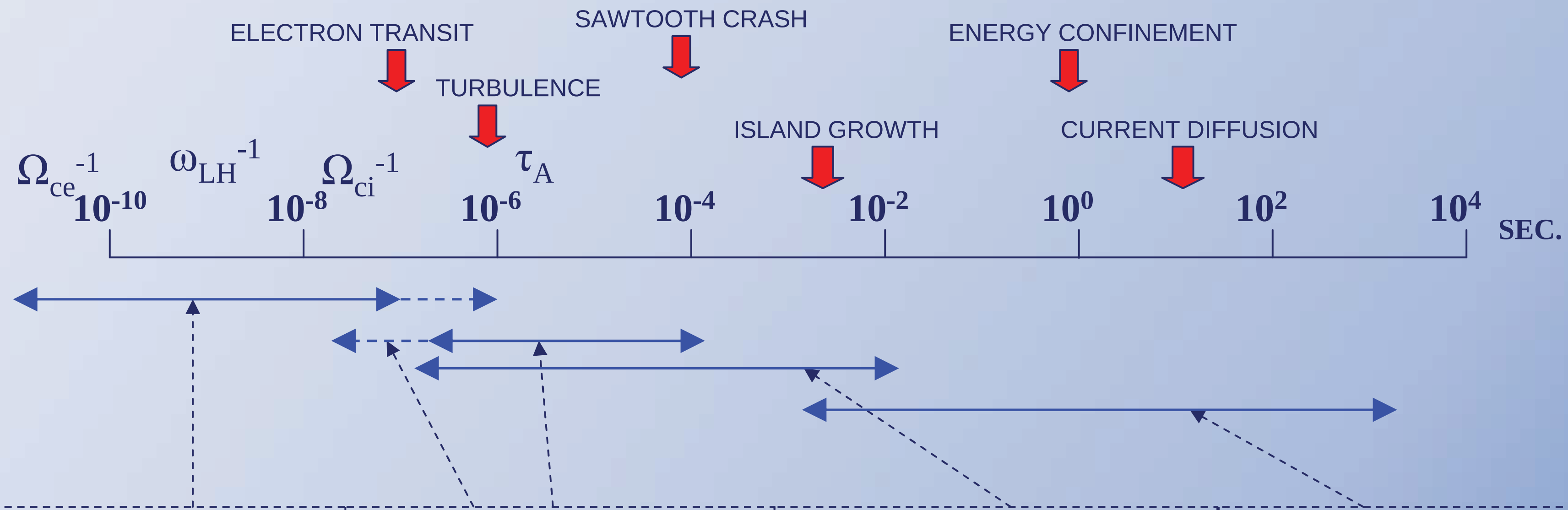
- **But: long list of deficient understanding:**

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

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

# core plasma

## Typical Time Scales in a next step experiment with B = 10 T, R = 2 m, $n_e = 10^{14}\ cm^{-3}$, T = 10 keV



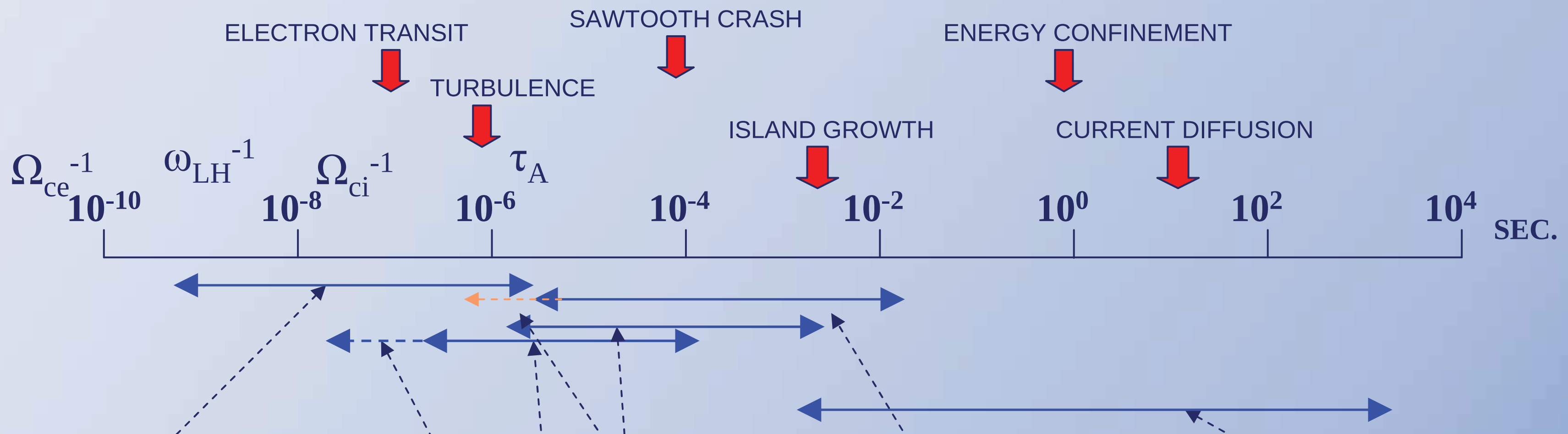

| | | | |
|---|---|---|---|
| Single frequency and prescribed plasma background | Neglect displacement current, average over gyroangle, (some) with electrons | Neglect displacement current, integrate over velocity space, neglect electron inertia | Neglect displacement current, integrate over velocity space, average over surfaces, neglect ion & electron inertia |
| RF Codes | Gyrokinetics Codes | Extended MHD Codes | Transport Codes |
| wave-heating and current-drive | turbulent transport | device scale stability | discharge time-scale |

Fusion Simulation Project Vol.2, FESAC ISOFS Subcommittee Final Report, Dec. 2002

core plasma
edge plasma

**Well separated: transport – turbulence: good !**

## Typical Time Scales in a next step experiment with B = 10 T, R = 2 m, $n_e = 10^{14}\ cm^{-3}$, T = 10 keV




Atomic & molecular processes

Neutral particle codes, kinetic imp. transport codes

plasma chemistry

Neglect displacement current, average over gyroangle, (some) with electrons

Gyrokinetics Codes

turbulence

Ideal drift waves
Transients (ELMs)

ITM

Edge transport

Parallel dynamics:
Ion transit,
Ion collisions
Parallel sound wave
Ditto, electrons

2D transport codes

Neglect displacement current, integrate over velocity space, average over surfaces, neglect ion & electron inertia

Core Transport Codes

discharge time-scale

Now first:

**lets assume: main edge plasma components: electrons, hydrogen ions, are known (from experiment, or from reliable CFD calculations)**

How do neutrals, trace-impurity ions, and radiation behave in this plasma (recycling, helium removal, wall erosion, plasma purity, .....

→ plasma performance, machine lifetime/availability
cost of electricity....

Then next:

**What if the edge plasma state (host medium) is not known from experiment (e.g.: ITER ??)**

## Generic kinetic (transport) equation (L. Boltzmann, ~1870)

- for particles travelling in a background (plasma) between collisions
- with (ions) or without (neutrals) forces (Lorentz) acting on them between collisions

Basic dependent quantity: distribution function $f(\vec{r},\vec{v},t)$

V-space: $(\vec{v}) \longrightarrow (E,\vec{\Omega})$ to accommodate also photons (radiation)

---

$$\frac{\partial f\left(E,\vec{\Omega}\right)}{\partial t} + v\vec{\Omega}\cdot\nabla f\left(E,\vec{\Omega}\right) + Forces = S\left(E,\vec{\Omega}\right) - v\sigma_a(E) f\left(E,\vec{\Omega}\right)$$

Free flight External source Absorption

$$+\int_0^\infty dE' \int_{4\pi} d\vec{\Omega}' \left[v'\sigma_s\left(E' \rightarrow E, \vec{\Omega}'\cdot\vec{\Omega}\right) f\left(E',\vec{\Omega}'\right) - v\sigma_s\left(E \rightarrow E', \vec{\Omega}\cdot\vec{\Omega}'\right) f\left(E,\vec{\Omega}\right)\right]$$

Collisions, boundary conditions

Altogether, just a balance in phase space

This kinetic  equation is algebraically very complex, but it has a very simple physical content (conservation in phase space)

There are numerous applications:

- neutron migration in nuclear reactors
- radiative transfer
- neutrino flow in astrophysics
- trace particle particle transport in plasmas
- Knudsen flow
- gamma-ray transport in shielding studies
- .....

## Particles Photons („DICTIONARY“)

Simple transformations of variables:

| | | | |
|---|---|---|---|
| velocity $v$ | ⟷ | const. velocity $c$ |
| energy $E = \frac{1}{2} m v^2$ | ⟷ | energy $E = h\nu$ |
| flux $\Psi = v \cdot f(\vec{r}, \vec{v})$ | ⟷ | spec. intensity $I = h\nu \cdot c \cdot f(\vec{r}, E, \vec{\Omega})$ |

## Equation of radiation transfer

$$\frac{1}{c}\frac{\partial I\left(\nu,\vec{\Omega}\right)}{\partial t} + \vec{\Omega}\cdot\nabla I\left(\nu,\vec{\Omega}\right) + \sigma_a(\nu) I\left(\nu,\vec{\Omega}\right) = q(\nu)$$

$$+\int_0^\infty d\nu' \int_{4\pi} d\vec{\Omega}' \frac{\nu}{\nu'} \sigma_s\left(\nu' \to \nu, \vec{\Omega}'\cdot\vec{\Omega}\right) I\left(\nu',\vec{\Omega}'\right) - \int_0^\infty d\nu' \int_{4\pi} d\vec{\Omega}' \sigma_s\left(\nu \to \nu', \vec{\Omega}\cdot\vec{\Omega}'\right) I\left(\nu,\vec{\Omega}\right)$$

(just a strangely normalized Boltzmann equation)

- In case of many particle species: each one has ist own kinetic equation. The system is then coupled via the collision terms on the right hand side).

- In case of many different types of interactions (collisions) the „ Boltzmann collision term“ (r.h.s) is a sum:

$$\sum_b C_b = \sum_b \int dx' \left[ v'\sigma_s(x' \to x) f(x') - v\sigma_s(x \to x') f(x) \right]$$

in-scattering, gain | out-scattering, loss

over all individual collision processes „b“

# The collision term can be one of two types:

A: jump process (wide angle scattering), n-n, n-e, n-i

$$C_b(x) = \int dx' \left[ v' \sigma_s \left( x' \rightarrow x \right) f\left( x' \right) \right] - \mu(x) f(x)$$

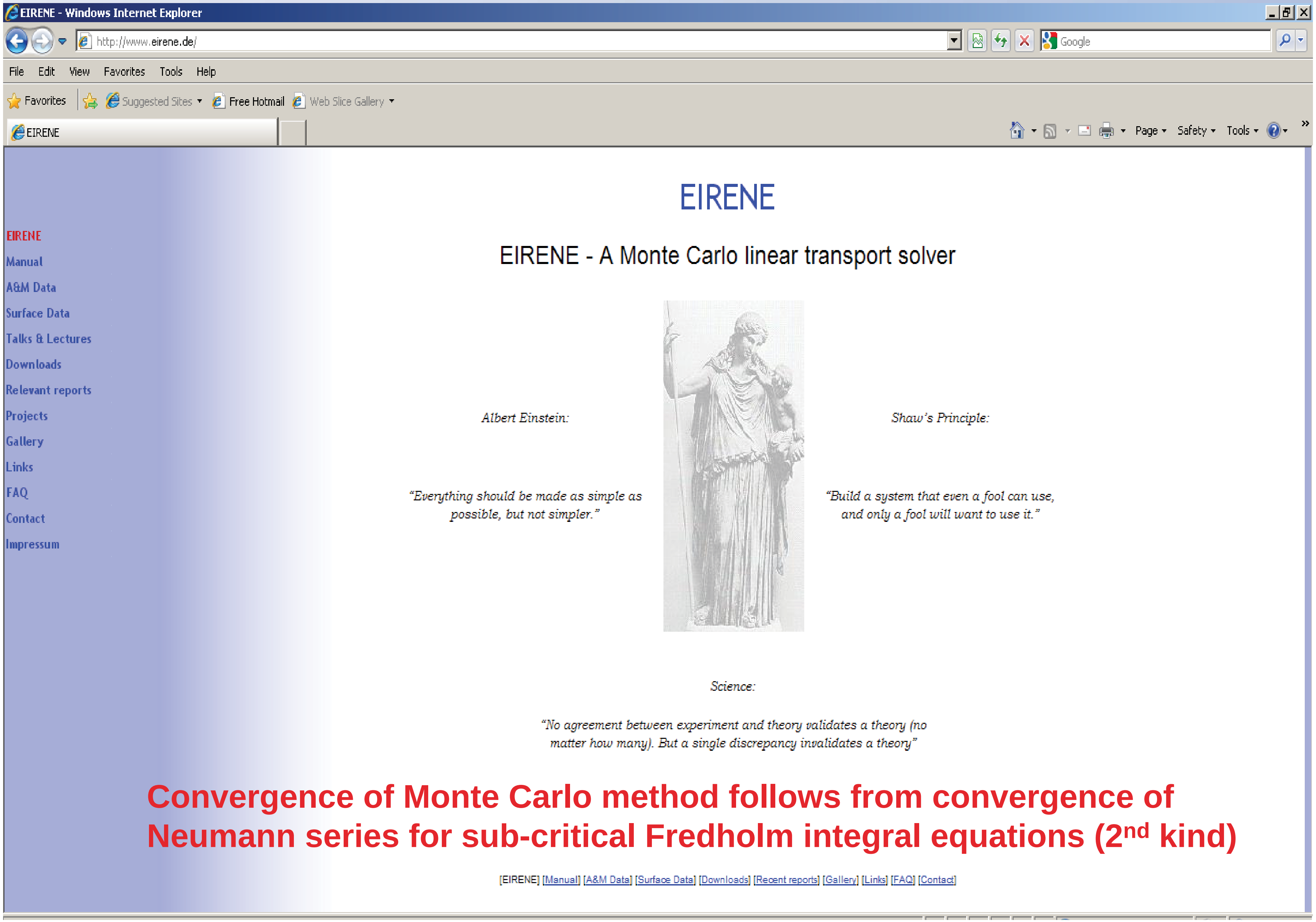
loss

B: diffusion in velocity space (small angle scattering), e-e, e-i, i-i

$$C_b = \frac{\partial}{\partial x} \left( D(x) \frac{\partial}{\partial x} f(x) \right)$$

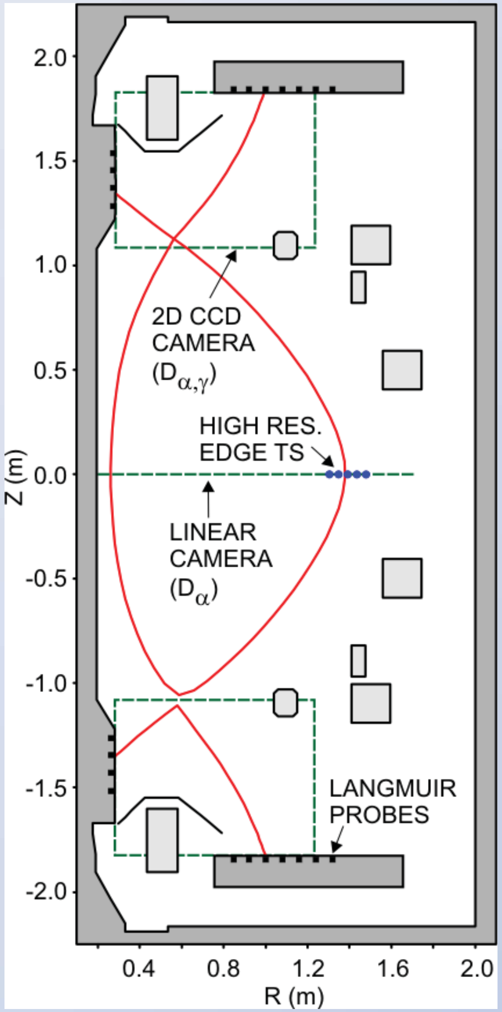
Either Boltzmann-, or Fokker Planck-, or mixed type of equation.

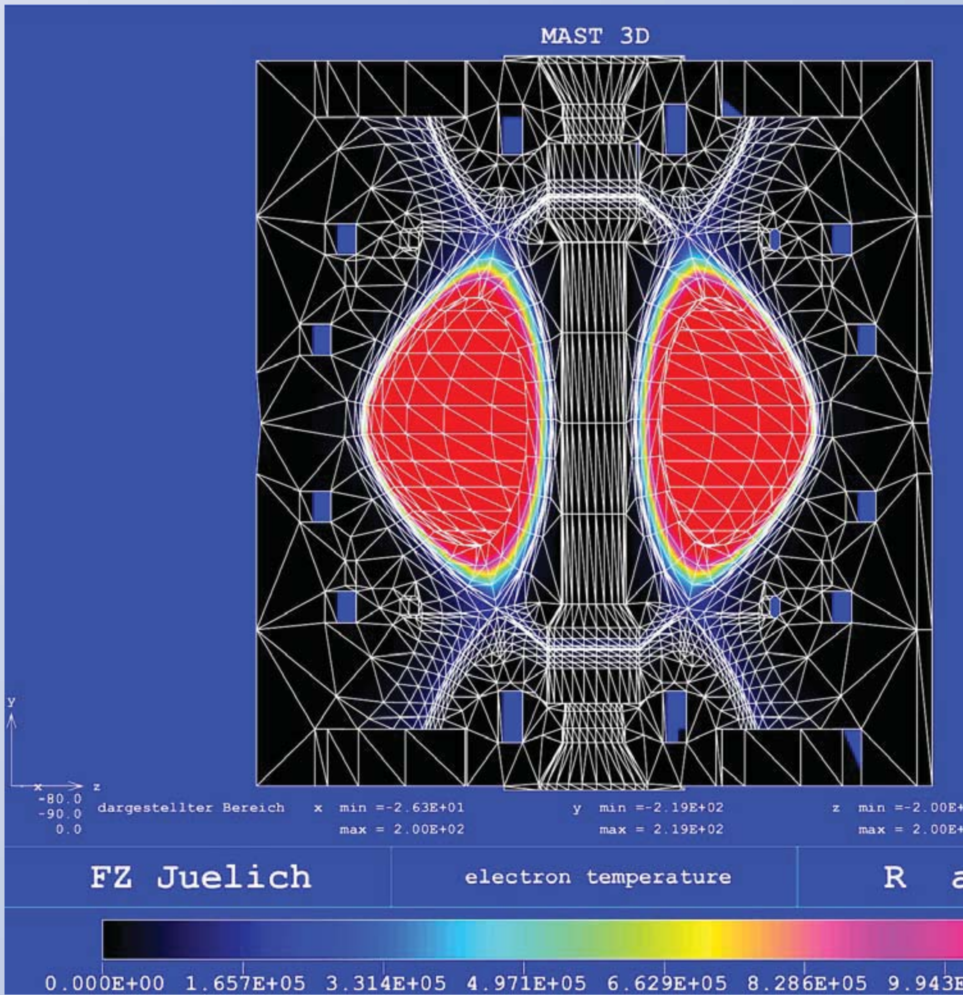
# Monte Carlo Boltzmann equation solver:  www.eirene.de

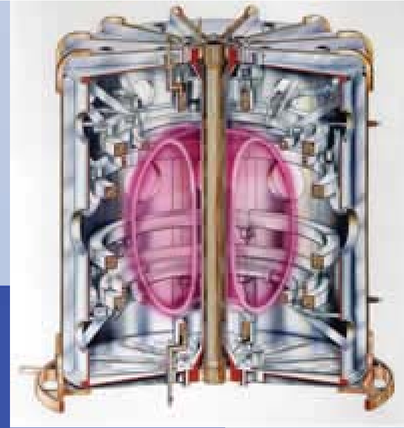



**Convergence of Monte Carlo method follows from convergence of Neumann series for sub-critical Fredholm integral equations (2nd kind)**

# Example: MAST (UK)



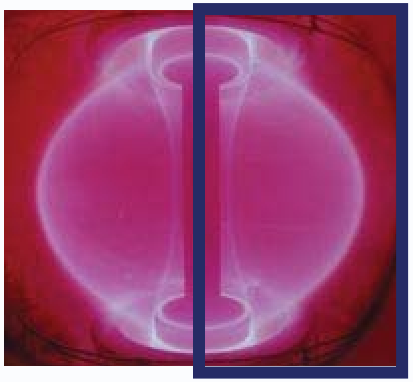



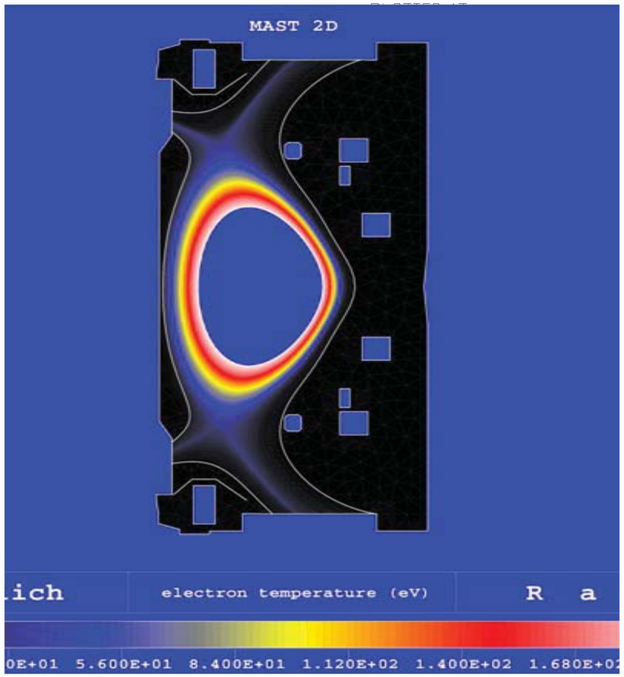



**Plasma temperature in K**

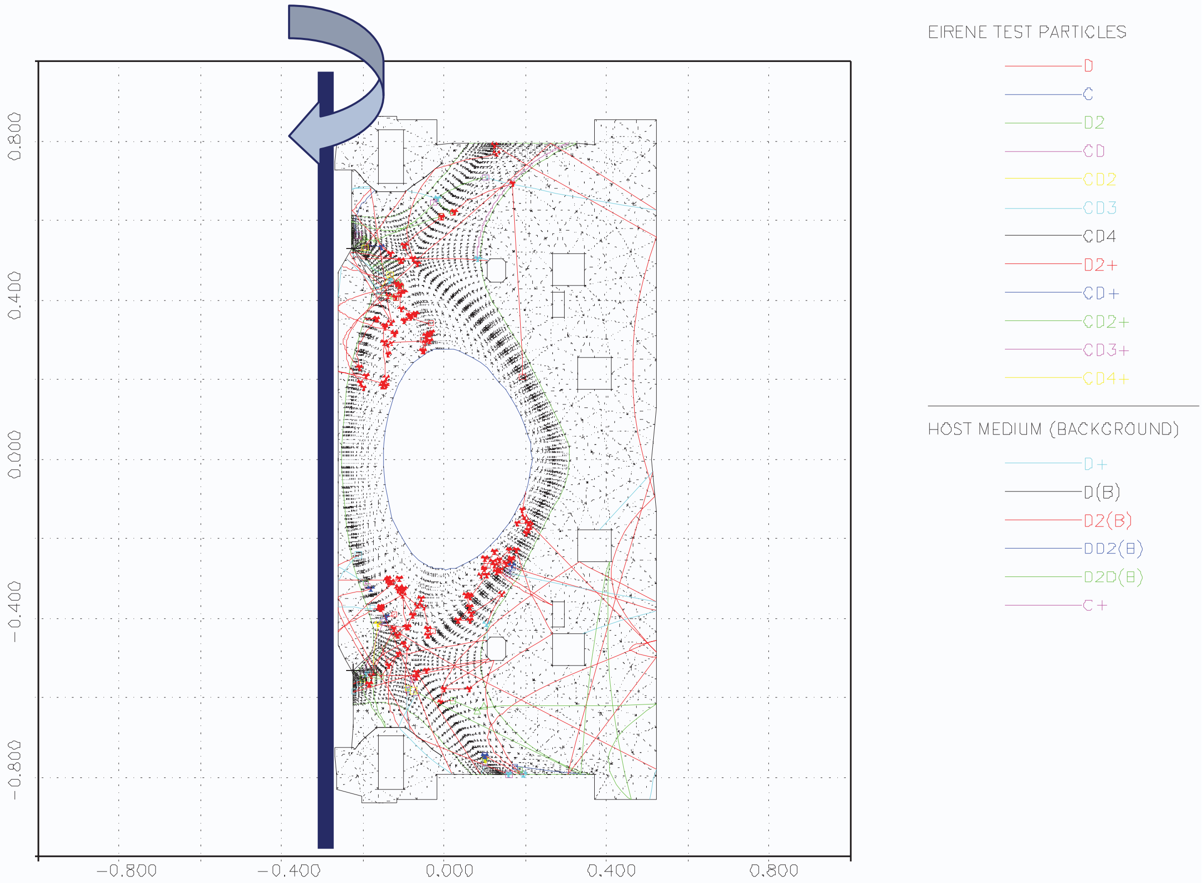
Courtesy: S. Lisgo

# Characteristics (=Trajectories) of kinetic transport equation here: MAST, Culham, UK



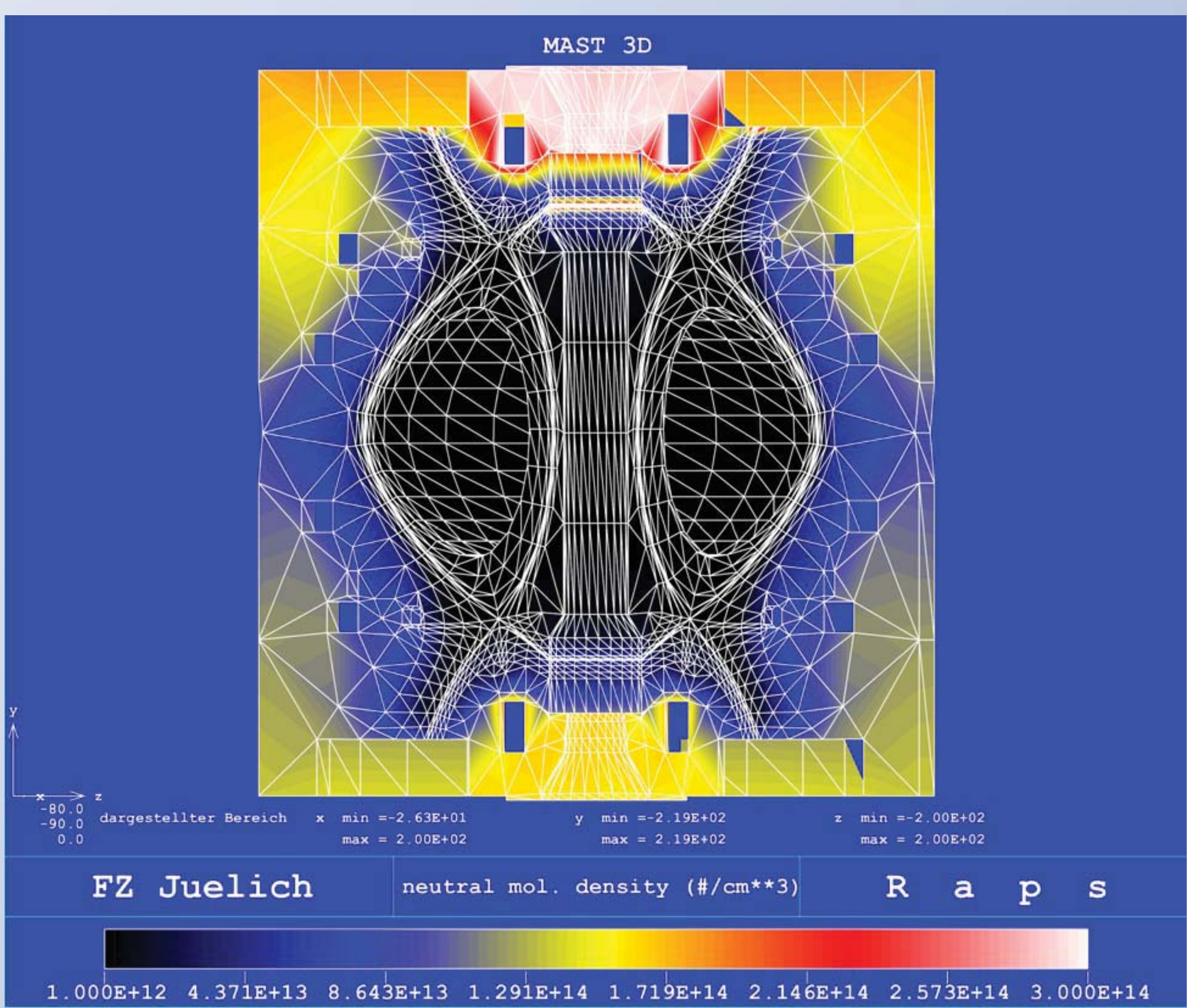



MAST: Geometry and exp. plasma data provided by S. Lisgo, UKAEA, 2007



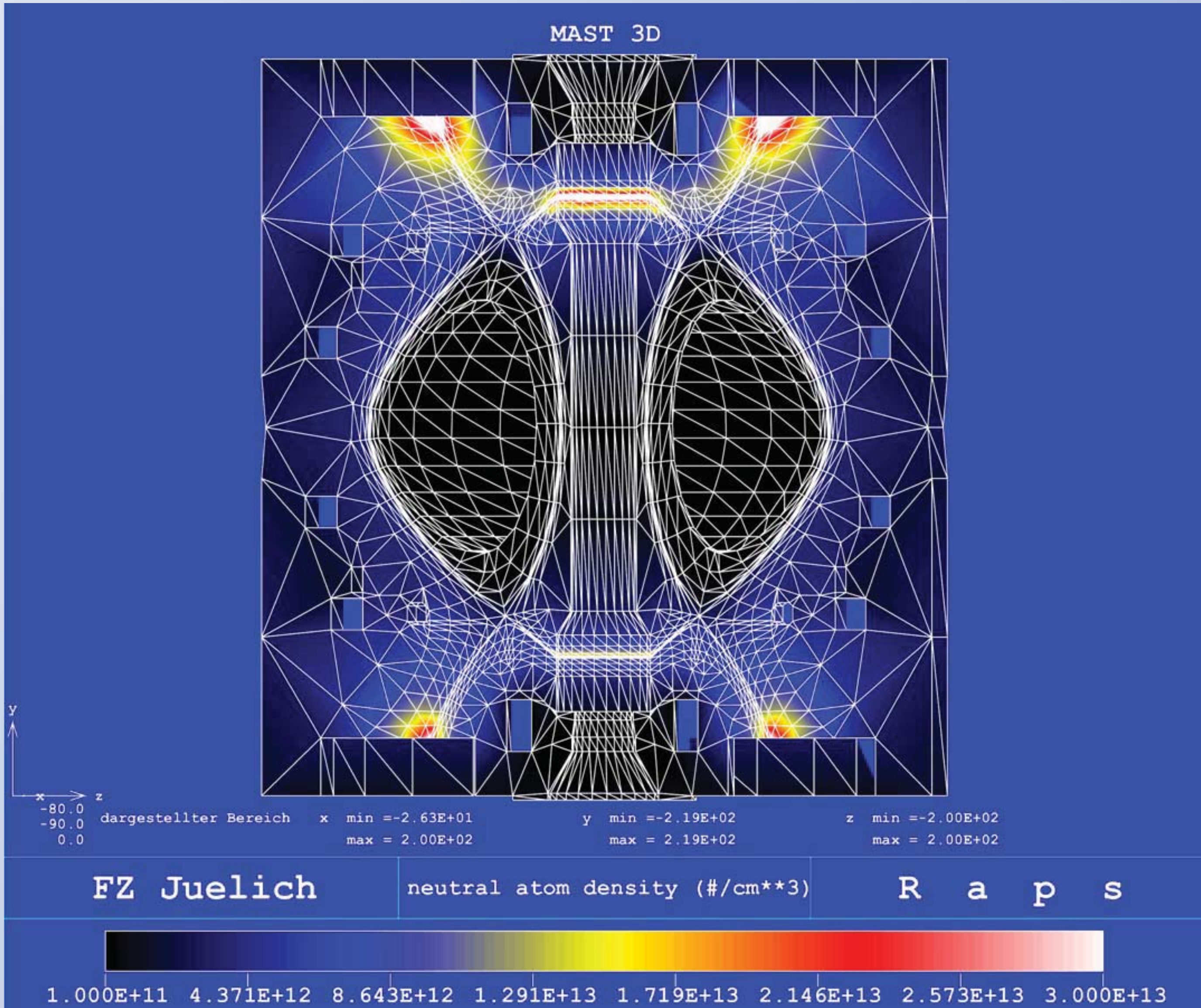

Here: mainly H, $H_2$, $C_xH_y$ neutrals

# Example: MAST (UK), 3D (filament studies)

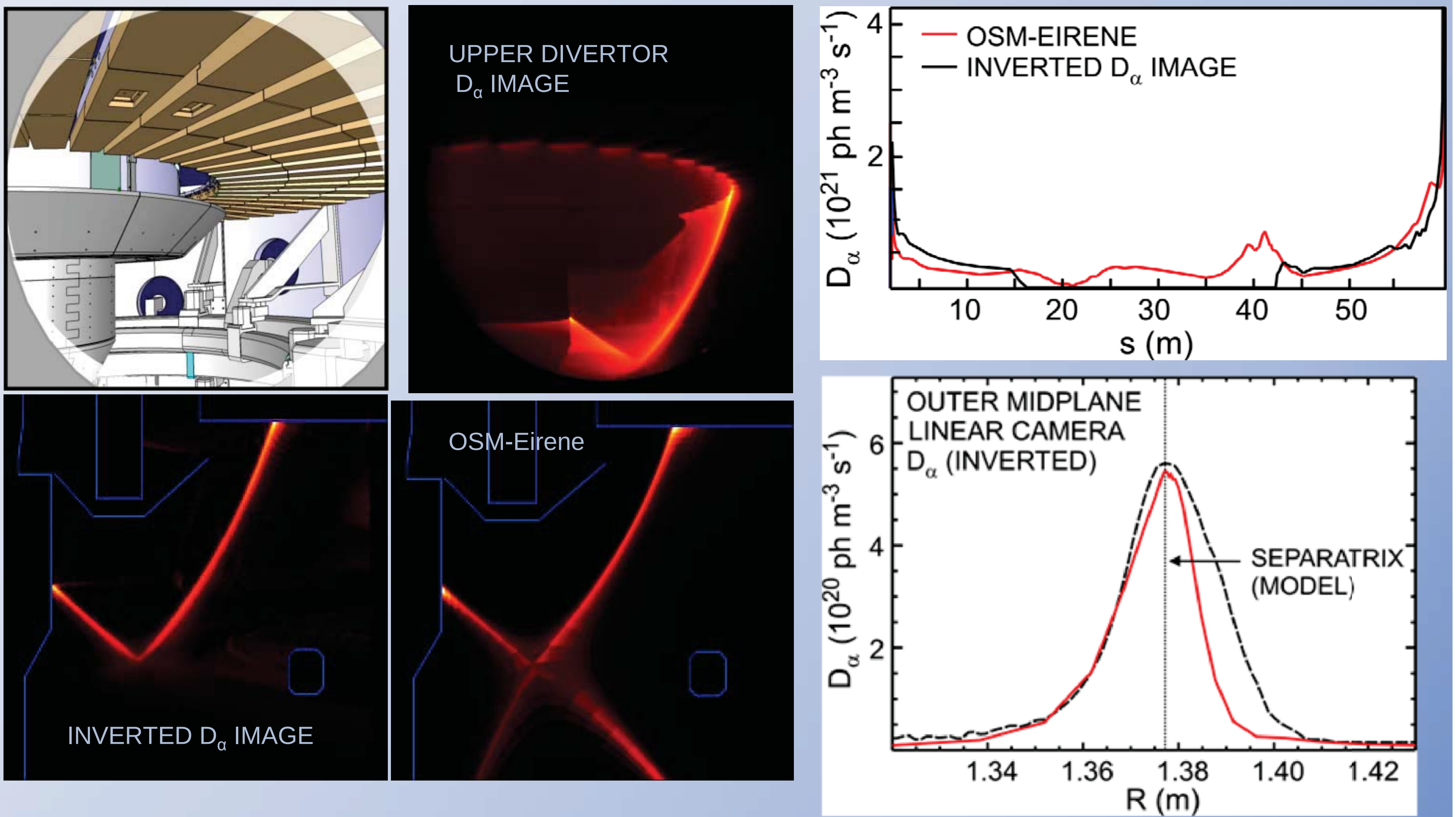



**(Molecular) Gas Density (1 – 3 E20).**

# Example: MAST (UK), 3D (filament studies)




**(Atomic) Gas Density (1—3E19**

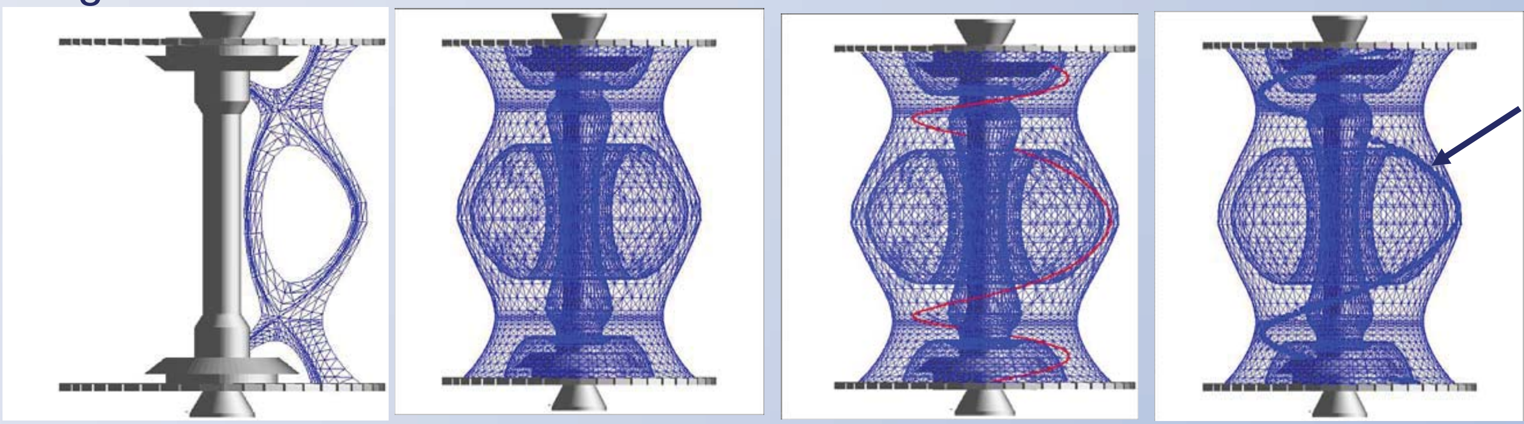



Spectroscopy → OSM transport modelling → CR plasma chemistry modelling→
→ Quantitative comparison → experimental validation of tokamak edge chemistry

Courtesy: S.Lisgo et al., MAST Team, EPS 2007

## **OSM-EIRENE (UKAEA/FZJ)** :
## Towards fully authentic 3D edge interpretation codes:

a new fully general 3D adaptive grid geometry option in EIRENE, using Tetrahedons

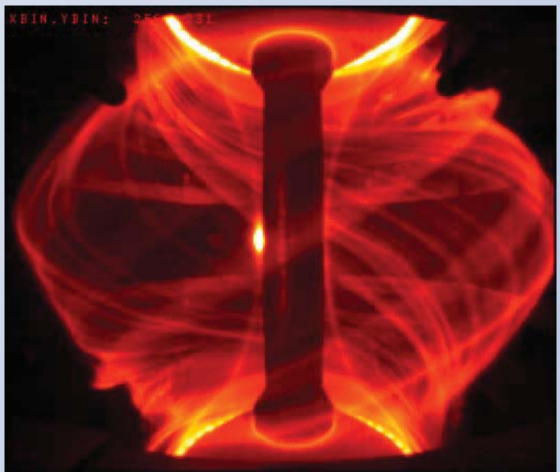


**Grid refined near ELM filament**

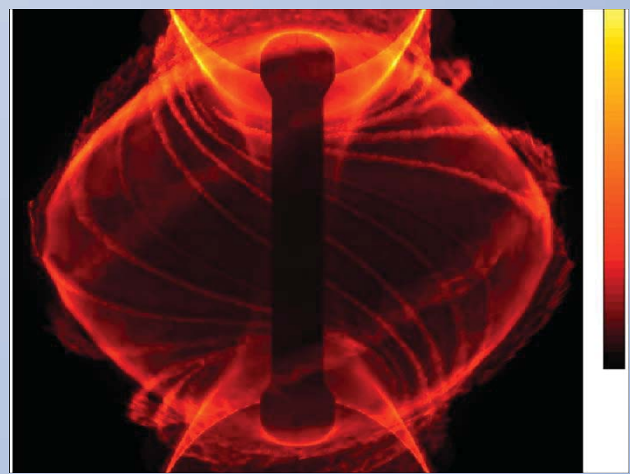
**EXAMPLE FOR A TYPICAL/REPRESENTATIVE ELM in MAST**

divertor not resolved in this example due to memory limitations

N = 6 for the simulation

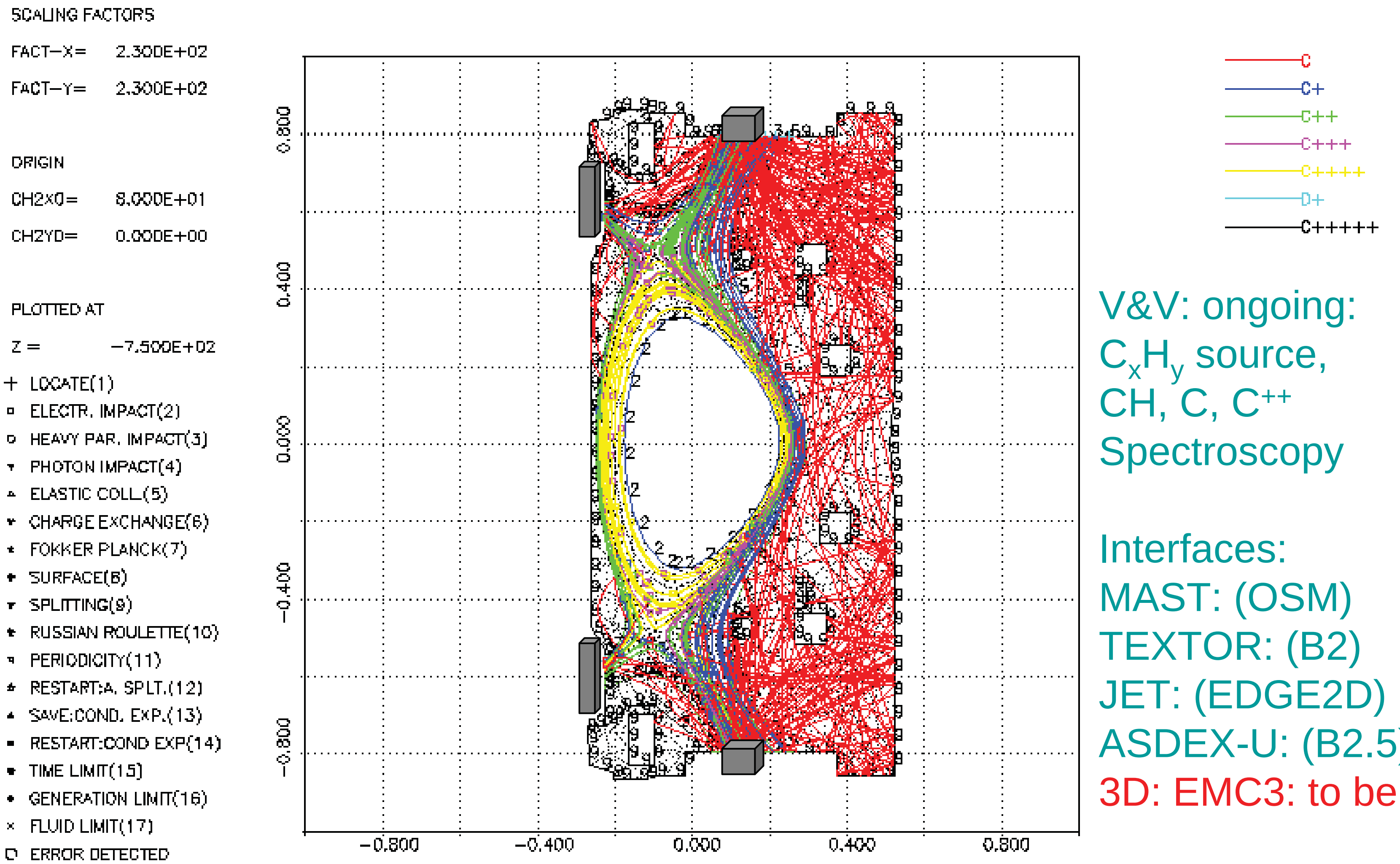


Fast Camera, unfiltered



OSM-EIRENE reconstruction: D-alpha

# Recent extension: EIRENE
## gyro averaged ion drift kinetic up to edge-core interface




V&V: ongoing:
$C_xH_y$ source,
CH, C, $C^{++}$
Spectroscopy

Interfaces:
MAST: (OSM)
TEXTOR: (B2)
JET: (EDGE2D)
ASDEX-U: (B2.5)
3D: EMC3: to be done

**Here: $C_xH_y$, C, $C^+$, $C^{2+}$, … atomic & molecular neutrals and ions**

Current numerical issues:

(guiding center-) Characteristics of trace ions are not known analytically → numerical integration (distinct from radiation, neutrals)

- Monte Carlo: favours explicit schemes (because geometrical calculations in complex boundaries are expensive)
- Accuracy requires implicit schemes (→ often simplified geometry, and simplified statistical estimation in trace ion codes)
- Can one reconcile the Boltzmann and Fokker Planck Monte Carlo procedures, or do we need separate codes (and interfaces, work flows, etc….? But then: 90% duplicating work, inconsistencies….)

Now:

What if the Plasma state (host medium) is not known from experiment (e.g.: ITER ??)

Then the problem becomes non-linear, due to powerful inelastic interactions of trace particles (e.g. neutrals) with plasma (exchange of matter)

Collisionality → plasma fluid approximation
multi-ion fluid (α ion species, $T_\alpha = T_i$, and electrons)
multi-species Boltzmann eq. for neutrals (n neutral species)
Braginskii, Reviews of Plasma Physics, 1965

**Continuity equation for ions and electrons**

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

**Momentum balance for ions and electrons**

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

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

**Energy balances for ions and electrons**

$$\frac{\partial}{\partial t}\left( \frac{3}{2} n_i T_i + \frac{m_i n_i}{2} \vec{V}_i^2 \right) + \vec{\nabla} \cdot \left[ \left( \frac{5}{2} n_i T_i + \frac{m_i n_i}{2} \vec{V}_i^2 \right) \vec{V}_i + \overleftrightarrow{\Pi}_i \cdot \vec{V}_i + \vec{q}_i \right] = \left( e n_i Z_i \vec{E} - \vec{R} \right) \cdot \vec{V}_i - Q_{ei} + S_E^i$$

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

ASIDE: eliminating turbulence from edge transport models (ab-initio→ ad hoc)

I: only external B-field
II: The cross field momentum balance is replaced by diffusion-convection ansatz
III: Coarse graining in temporal and spatial resolution

---

Momentum balance for ions and electrons (Navier Stokes „Braginskii" equations)

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

In edge codes often used only for $V_{\alpha_{\parallel}}$, the flow parallel to B-field

$$v_{\alpha\perp} = -\frac{D_n^{\alpha}}{h_{\perp}}\partial_{\perp}\left(\ln n_{\alpha}\right) - \frac{D_p^{\alpha}}{h_{\perp}}\partial_{\perp}\left(\ln p_{\alpha}\right) + V_{\perp}$$

with ad hoc (anomalous?) $D_{\perp}, V_{\perp}\ \kappa_{\perp}, \eta_{\perp},$

# Current challenge:

coupling transport approximation back to fluid turbulence models ??
(multi-scale problem of edge plasma science)

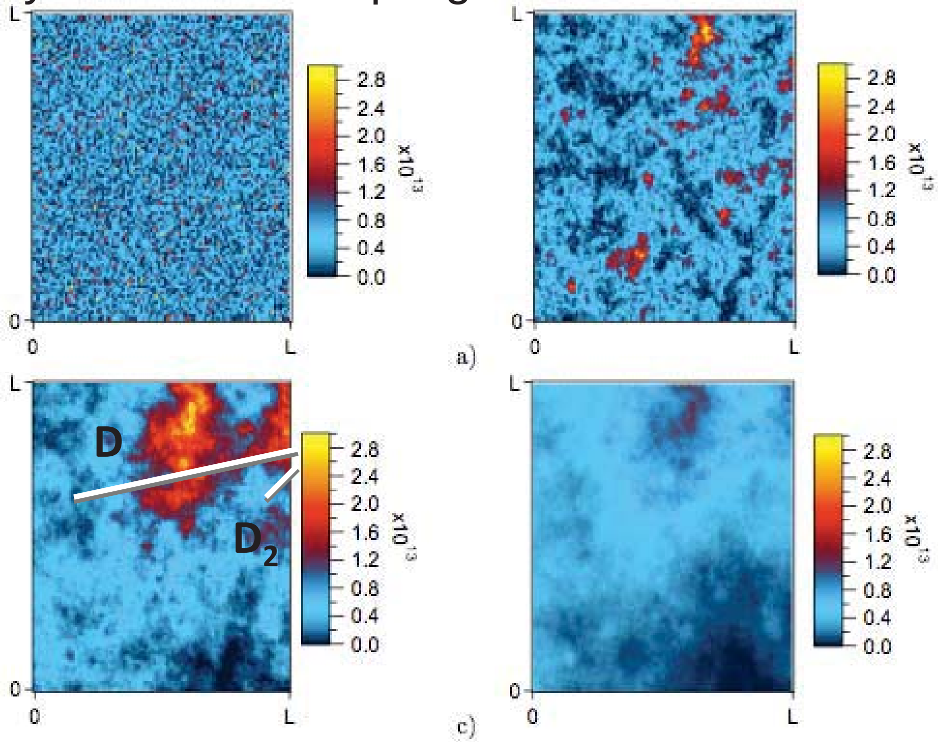
# Preparing coupling of turbulence models to edge codes: Neutral particle transport in turbulent plasmas

Y. Marandet, A. Mekkaoui, D. Reiter, et al., CCP, (2010), PSI (2010), PET (2011)
CEA Cadarache and Univ. Marseilles

("linear transport in stochastic media")

Stochastic model for turbulent fluctuations implemented in EIRENE:
Understand the physics before coupling codes

Slab geometry

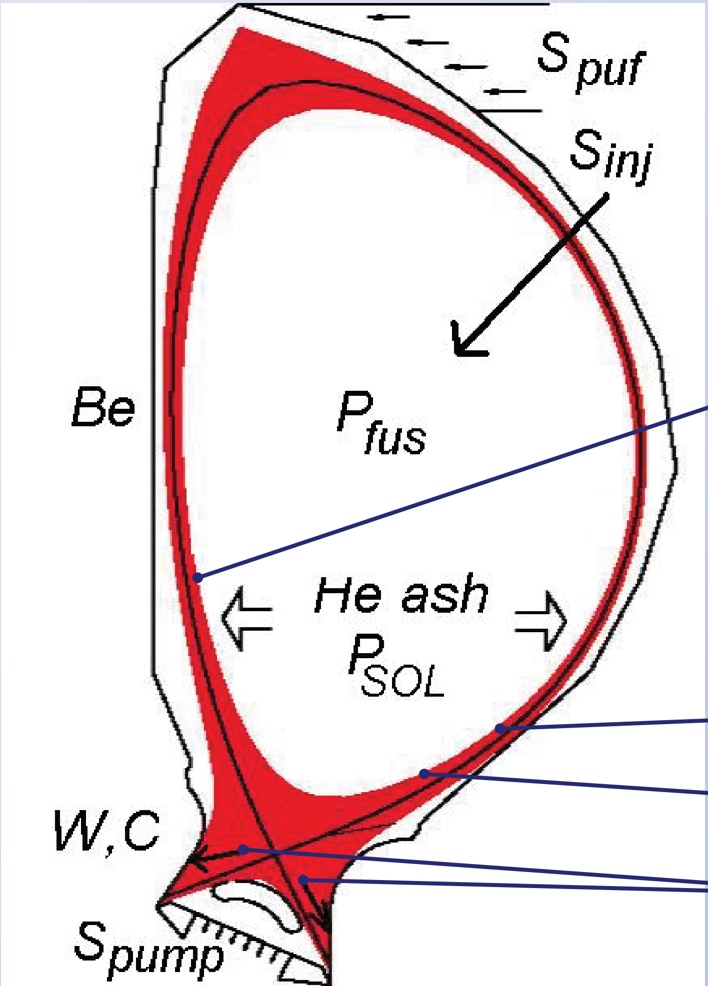



2 main control parameters: blob size / mean free path; recycling time scales
Penetration depth or neutrals may either increase or decrease (!)

# The ITER divertor design challenge

(computational engineering today, despite of incomplete knowledge in many contributing edge plasma issues)

Provide sufficient convection without accumulating tritium and with sufficiently long divertor lifetime (availability).




$P_{fus} \approx$ **540-600 MW**

$\Rightarrow$ **He flux 2 · 10$^{20}$s$^{-1}$**

$\Rightarrow$ $P_{SOL}$**≈86-120 MW**

$n_s$ **≈(2-4)·10$^{19}$ m$^{-3}$**

$S_{inj}$ **≤ 10·10$^{22}$ s$^{-1}$**

$S_{pump}$ **≤ 200 Pa·m$^{-3}$/s**

!

$Z_{eff}$ **≤1.6**

$C_{He}$ **≤6%**

$q_{pk}$ **≤10 MW/m$^2$**

?

# Compare: space flight re-entry problems
# e.g. Space Shuttle

1-2 eV plasma temperature

**~10 MW/m², for some minutes**

**10 MW/m² stationary: perhaps tolerable, but not trivial**

## Computational Science Workflow
## "Waterfall Model" (1960-th...)
## (the dream of code development managers)

**1) Requirement (e.g.: integrated fusion edge code for ITER)**

**2) Planning and design**

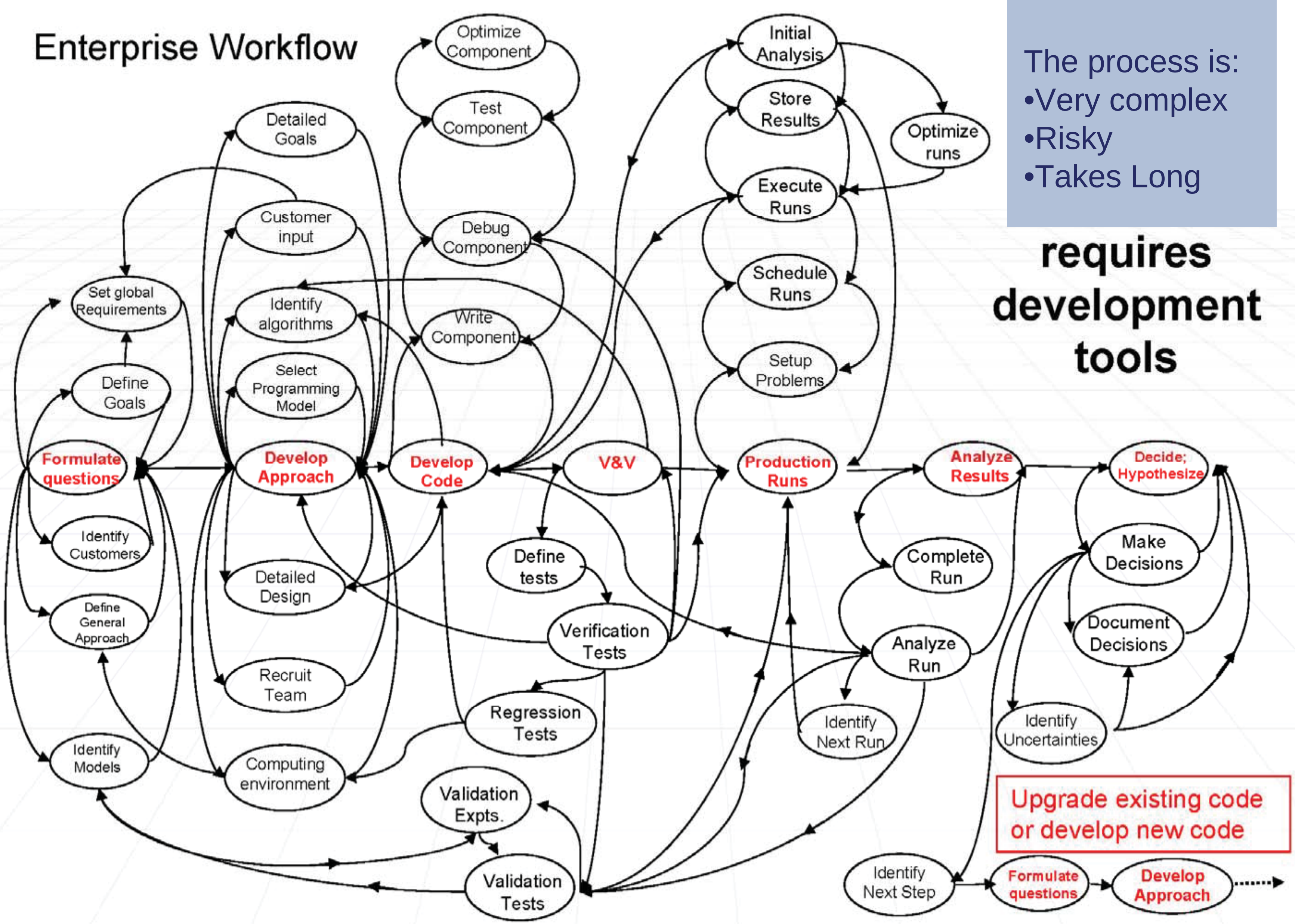
**3) Code (Programming)**

**4) Test**

**5) Run**

Computational edge plasma Science and Engineering is moving from "few effects" codes developed by small teams (1-3 scientists) to "many effect codes" codes developed by larger teams (10-20 or more).

# The reality in large scale code development projects




The process is:
- Very complex
- Risky
- Takes Long

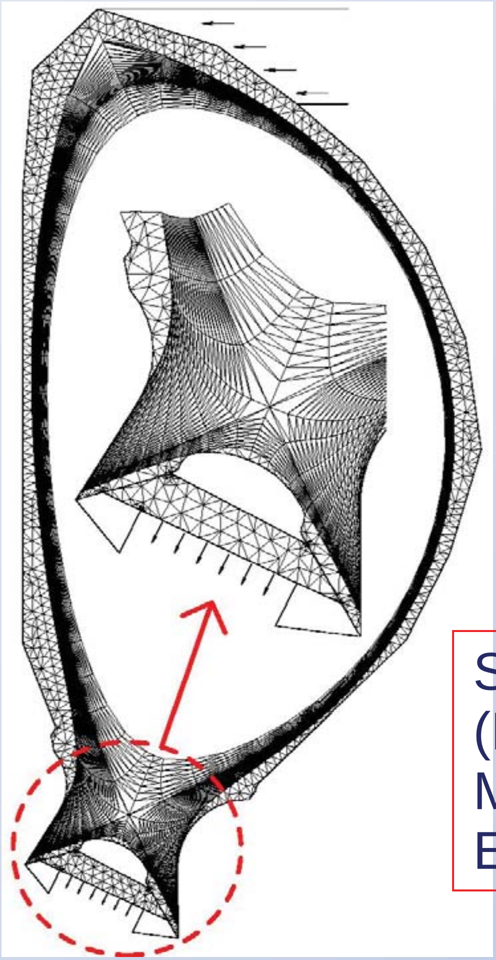
**requires development tools**

## Numerical tool for the edge plasma science: B2-EIRENE code package (FZJ-ITER)

Reiter, D., PPCF **33** 13 (1991)

Reiter, D., M. Baelmans et al., Fusion Science and Technology **47** (2005) 172.

Self-consistent description of the magnetized plasma, and neutral particles produced due to surface and volume recombination and sputtering



Computational Grid

Plasma flow Parameters

**B2**: a 2D multi species ($D^{+}$, $He^{+,++}$, $C^{1+..6+}$,…) plasma fluid code

CR codes: HYDKIN

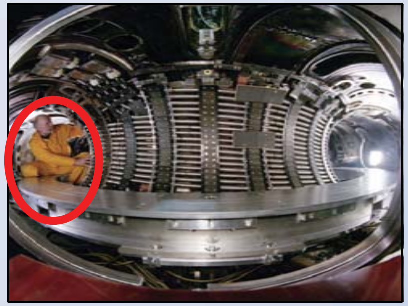
Source terms (Particle, Momentum, Energy)

**EIRENE:** a Monte-Carlo neutral particle, trace ion and radiation transport code.

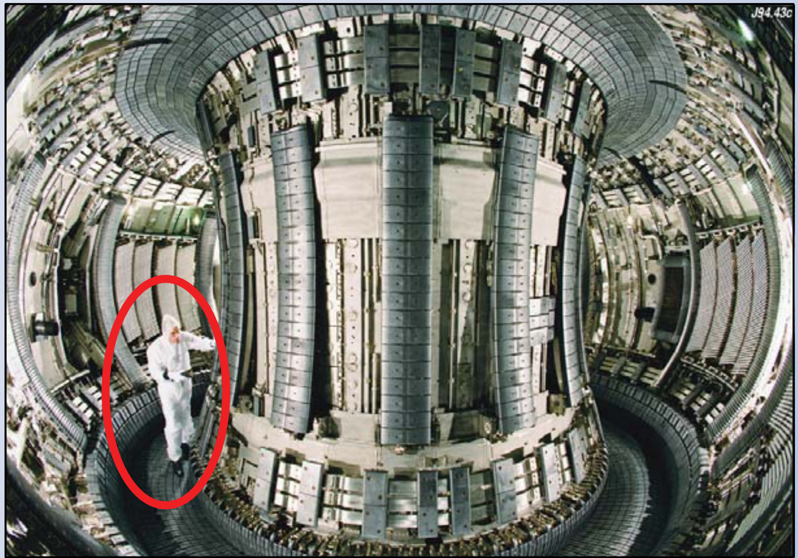
see www.eirene.de

# Fusion devices

TEXTOR (R=1.75 m), Jülich, GER

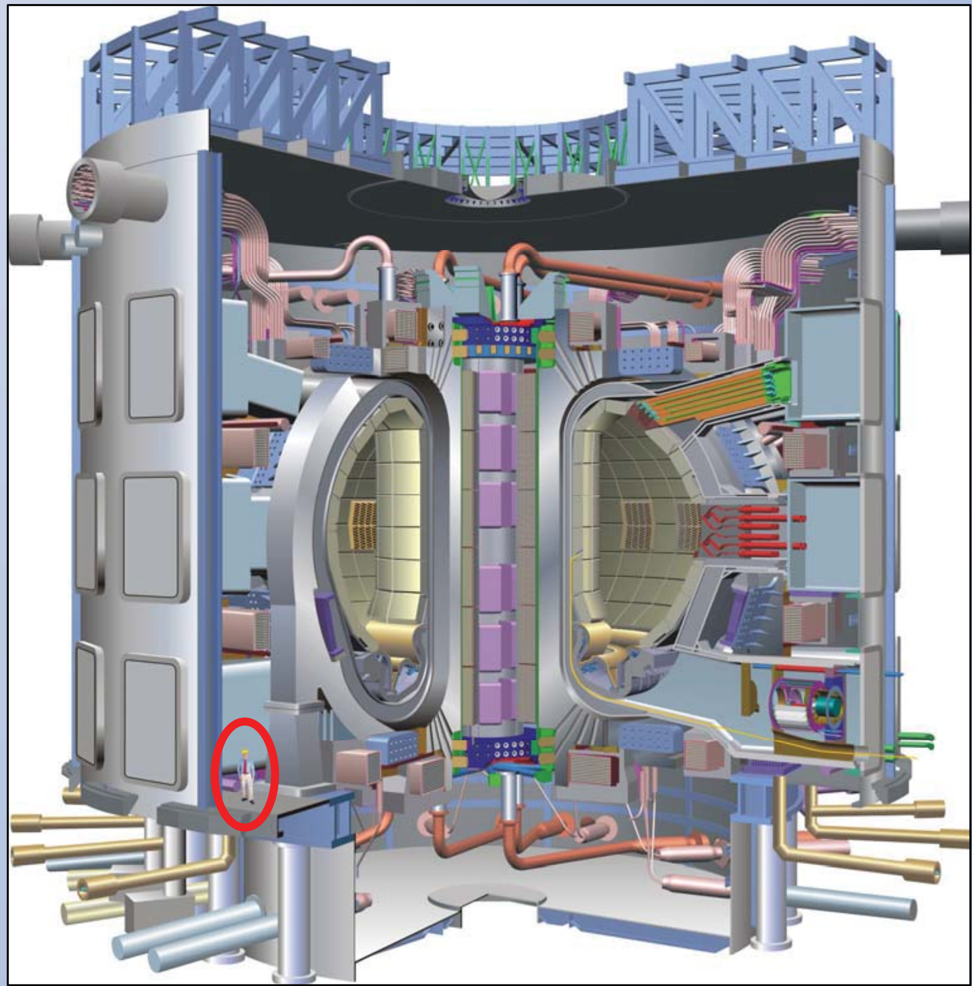


JET (R=2.96 m), Oxford, UK




joint: EU

ITER (R=6.2 m), Cadarache, FRA



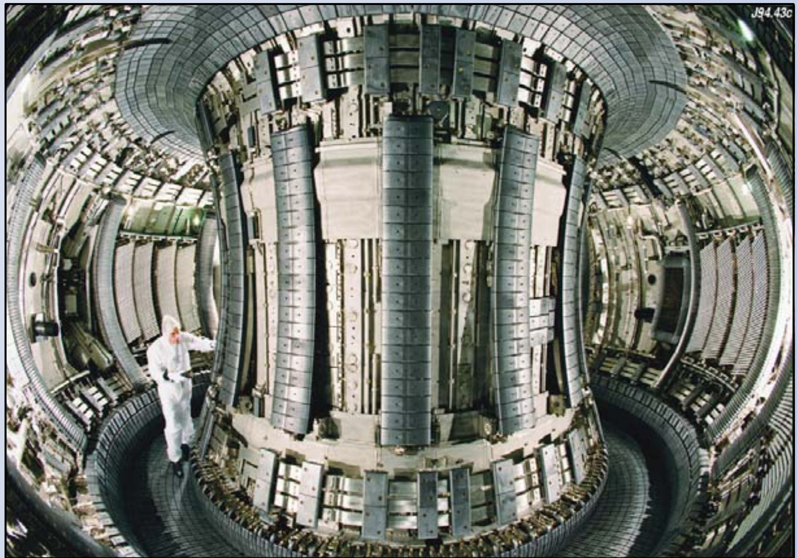
joint: world-wide

# Fusion devices: typical edge transport code runtime

TEXTOR (R=1.75 m), Jülich, GER

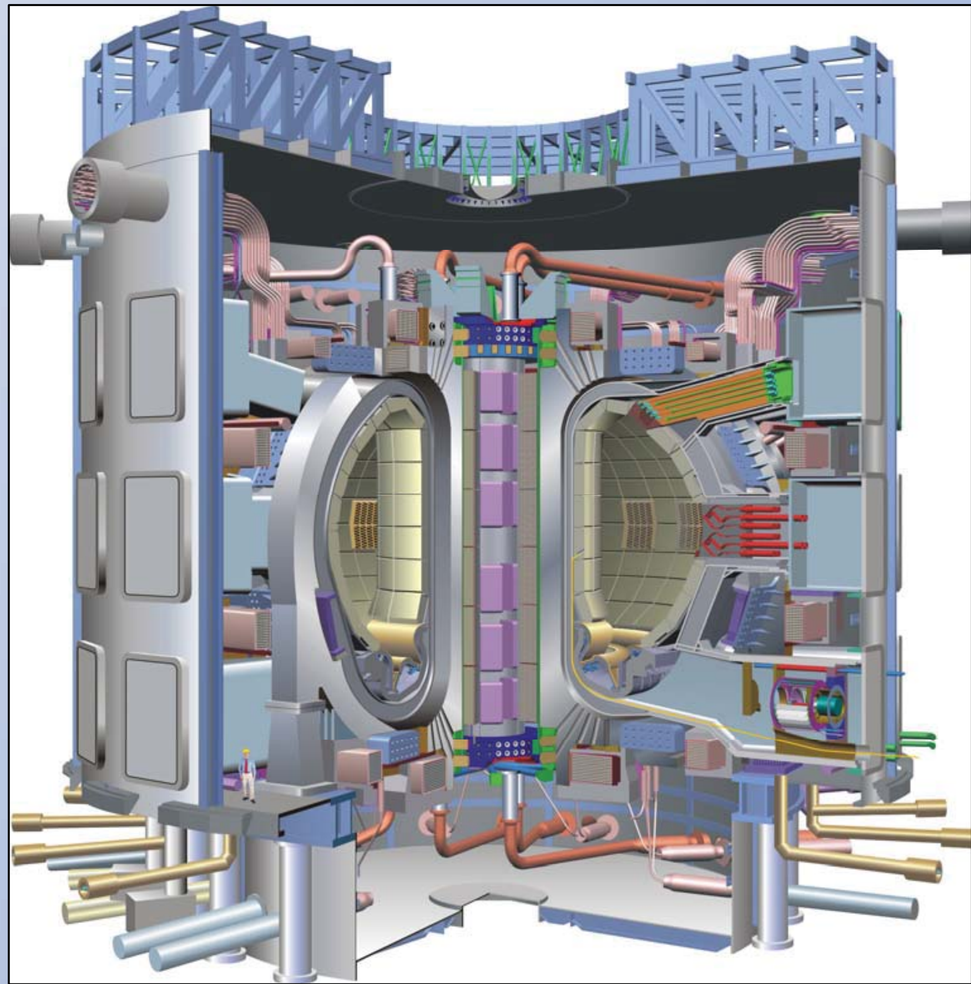
1 day

JET (R=2.96 m), Oxford, UK




joint: EU 1-2 weeks

ITER (R=6.2 m), Cadarache, FRA



joint: world-wide 3 months

Why become edge transport codes so slow
for ITER sized machines?
(for same model, same equations, same grid size)

Because of more important
plasma chemistry
(increased non-linearity,
non-locality, in sources).

Advection - diffusion → reaction - diffusion

# Fluid equations for charged particles

(Very strong, non-local, highly non-linear sources, + Monte Carlo noise)

## Continuity equation for ions and electrons

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

## Momentum balance for ions and electrons

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

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

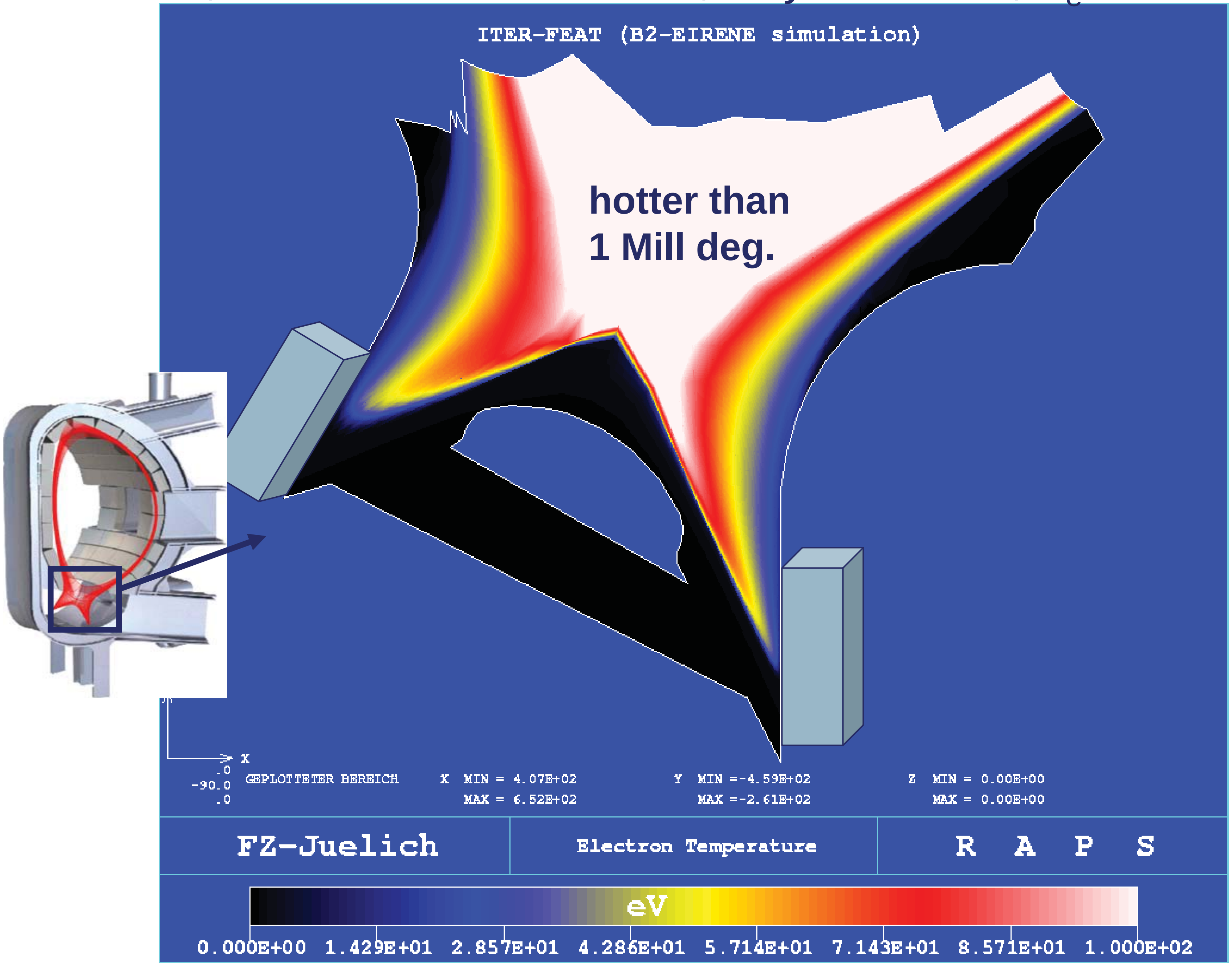
## Energy balances for ions and electrons

$$\frac{\partial}{\partial t}\left( \frac{3}{2} n_i T_i + \frac{m_i n_i}{2} \vec{V}_i^{\,2} \right) + \vec{\nabla} \cdot \left[ \left( \frac{5}{2} n_i T_i + \frac{m_i n_i}{2} \vec{V}_i^{\,2} \right) \vec{V}_i + \overleftrightarrow{\Pi}_i \cdot \vec{V}_i + \vec{q}_i \right] = \left( e n_i Z_i \vec{E} - \vec{R} \right) \cdot \vec{V}_i - Q_{ei} + S_E^i$$

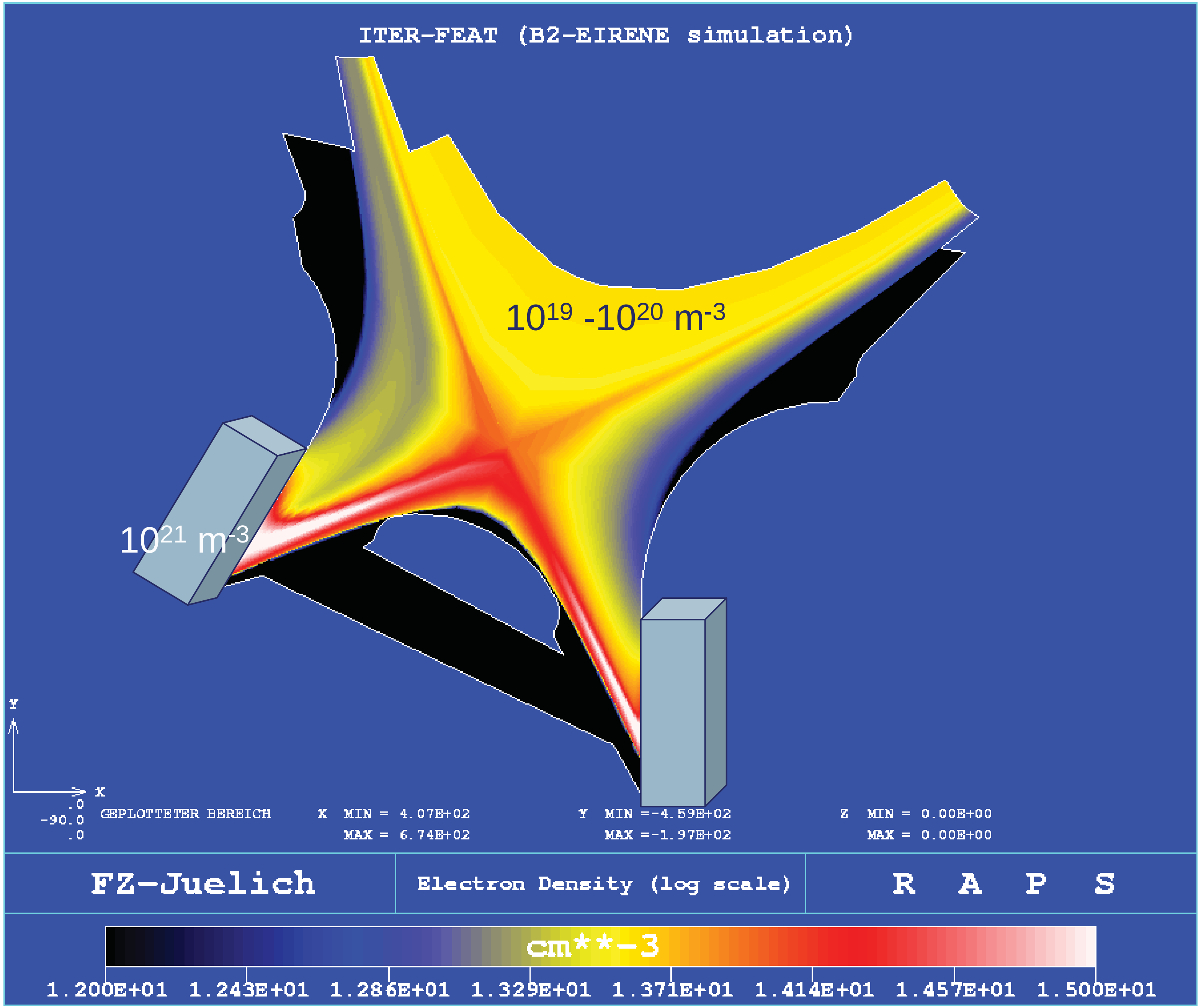
$$\frac{\partial}{\partial t}\left( \frac{3}{2} n_e T_e \right) + \vec{\nabla} \cdot \left( \frac{5}{2} n_e T_e \vec{V}_e + \vec{q}_e \right) = -e n_e \vec{E} \cdot \vec{V}_e + \vec{R} \cdot \vec{V}_i + Q_{ei} + S_E^e$$

System of PDGL's with locally dominating sources:
"diffusion-reaction-equations" rather than pure CFD

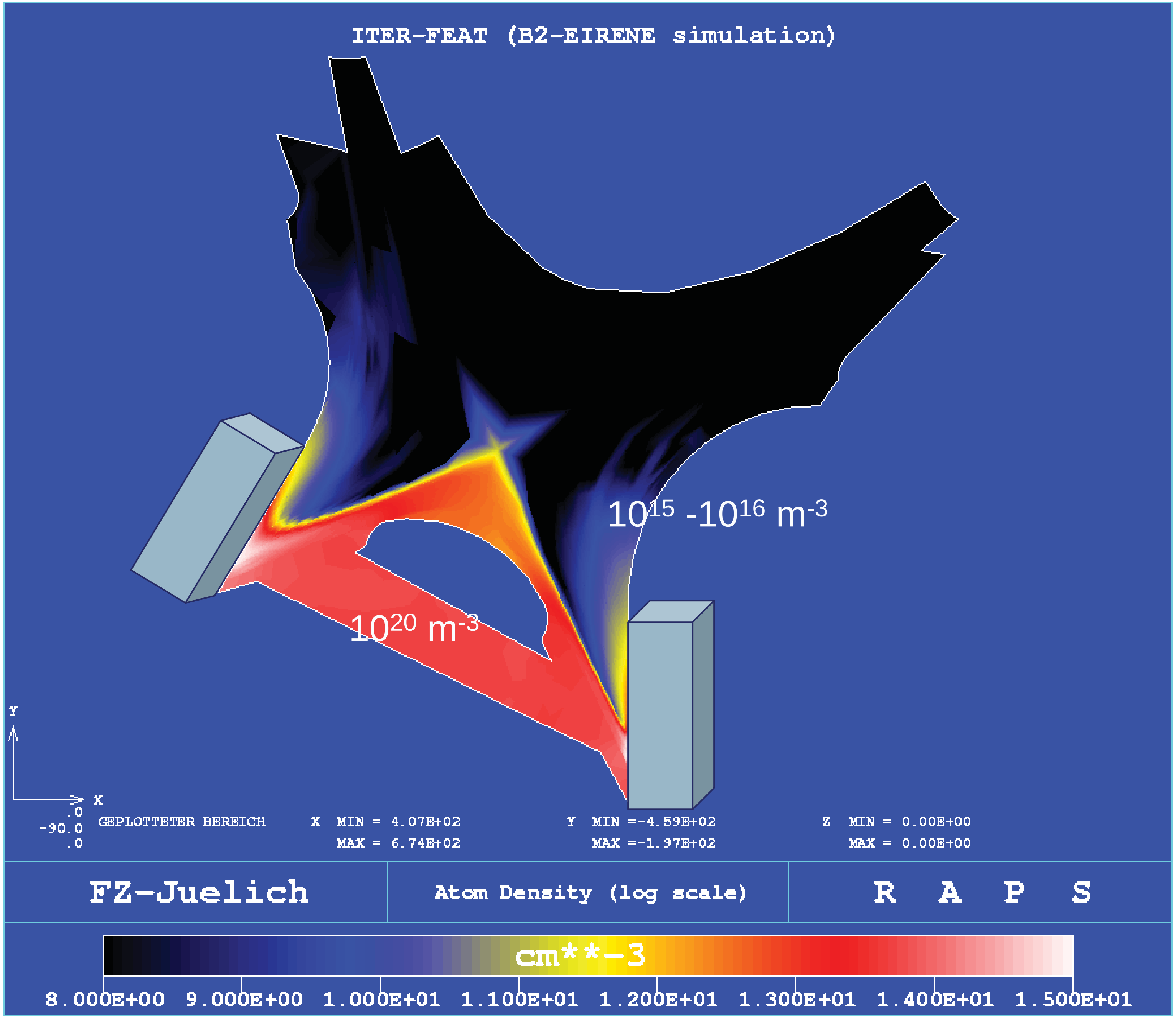
# ITER, B2-EIRENE simulation, fully detached, $T_e$ field



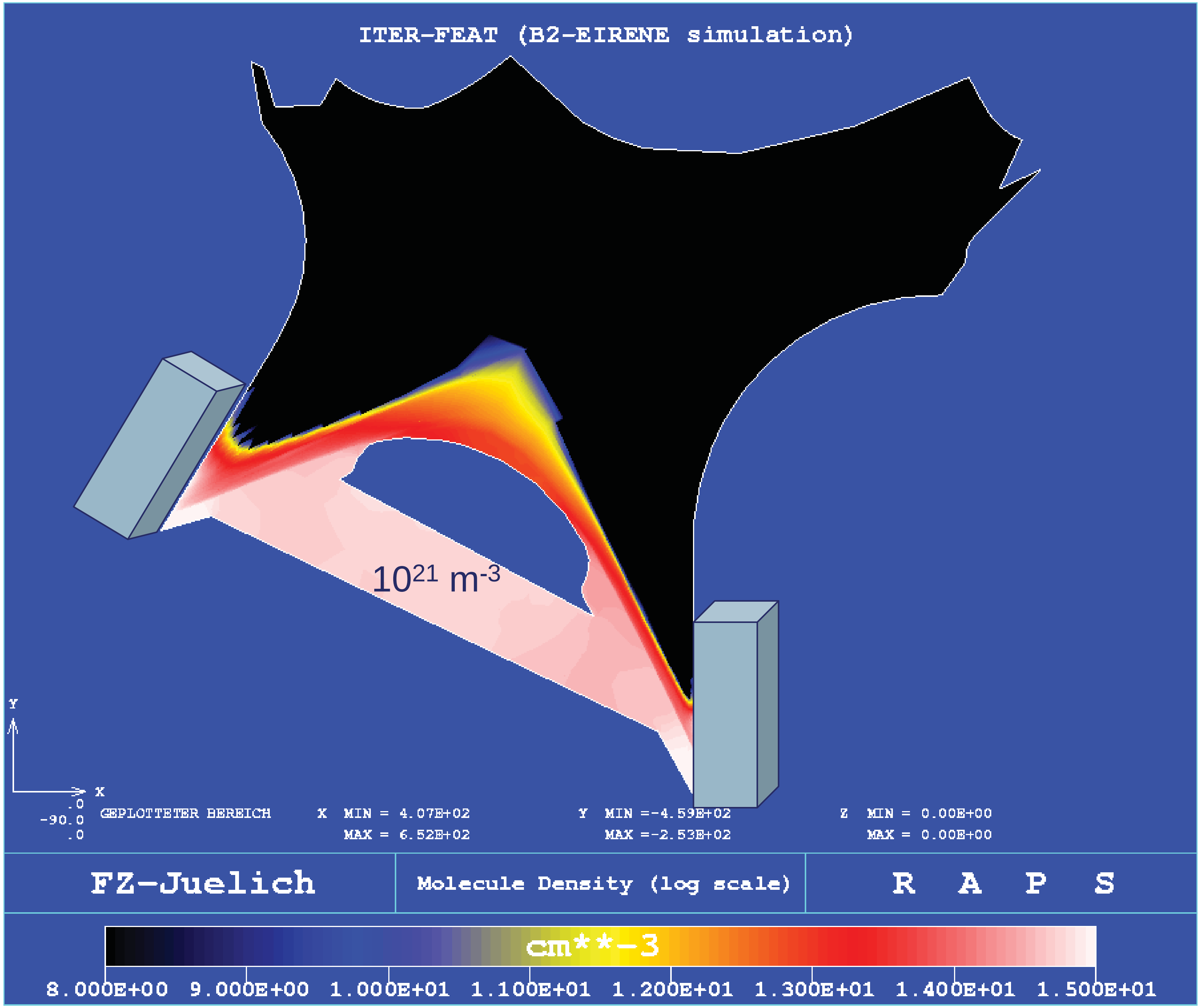
# ITER, B2-EIRENE simulation, detached, $n_e$ field



# ITER, B2-EIRENE simulation, detached, $n_A$ field

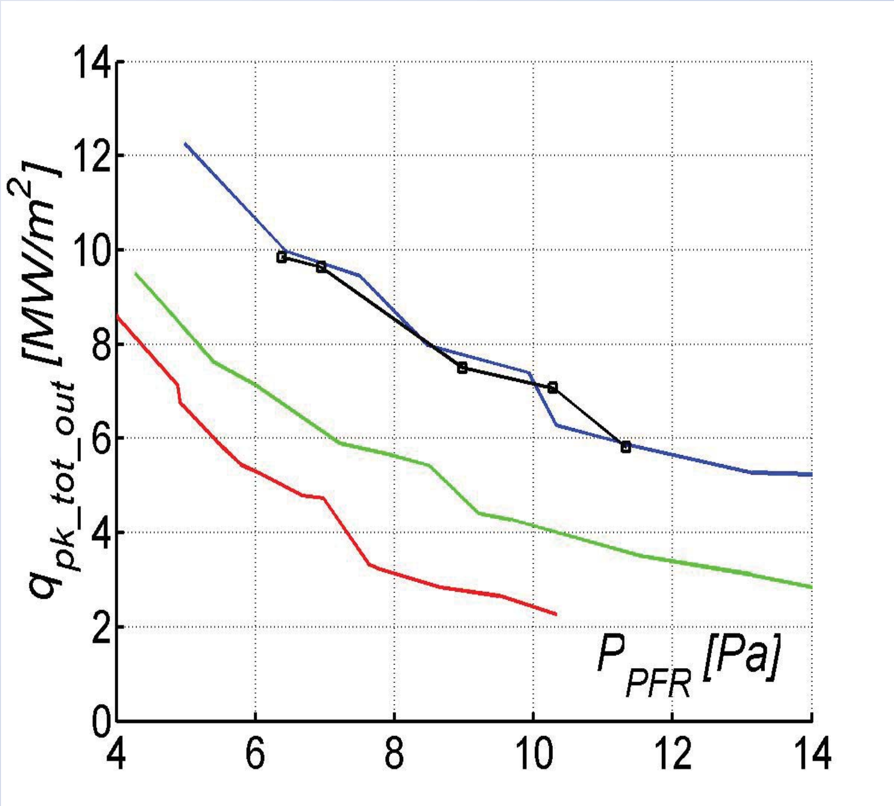


# ITER, B2-EIRENE simulation, detached, $n_{H2}$ field

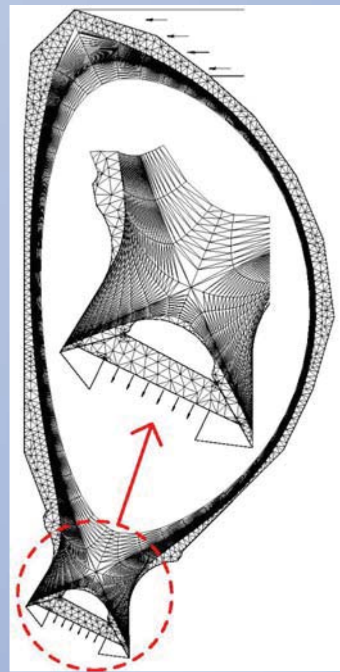


# Consequences for ITER design (B2-EIRENE): shift towards higher divertor gas pressure to maintain a given peak heat flux (Kotov et al., CPP, July 2006)

**ITER divertor engineering parameter:**
**target heat flux vs. divertor gas pressure**



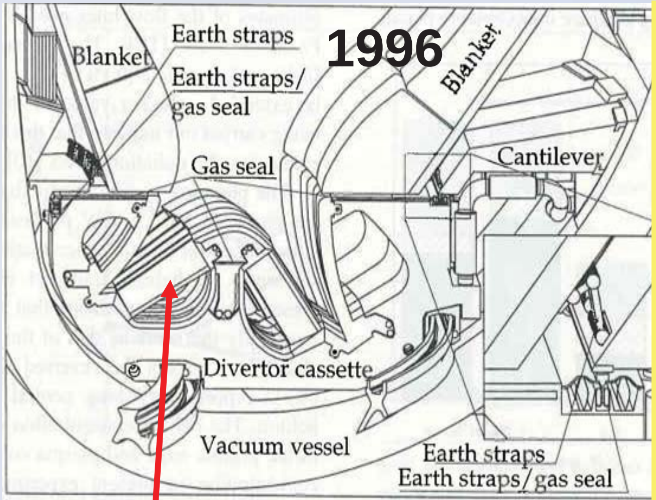

**— 1996**
**(ITER physics basis1999)**
**— 2003, neutral - neutral collisions**
**— ….+ molecular kinetics ($D_2(v)+D^+$, MAR)**
**— 2005, + photon opacity**



**$P_{PFR}$**: average neutral pressure in Private Flux Region

ITER design review 2007-2009:
“Dome“ re-design now ongoing

# Evolution of ITER divertor design




**2001: FEAT**

**no "wings"**

**dome**

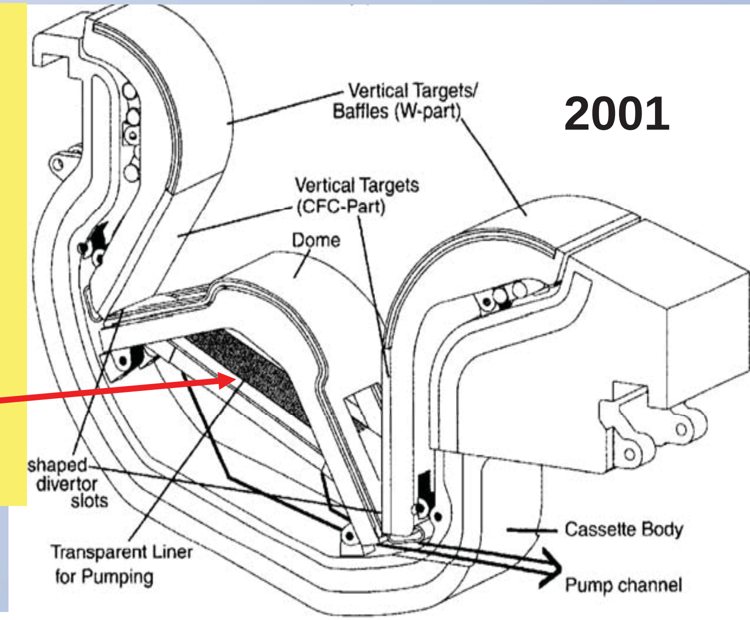
**to prevent neutrals reaching X-point**

**baffles**

**to confine neutrals**

**grill**

**to catch carbon**




**1996: big ITER**

**"wings"**

**to brake the gas**

**("momentum removal")**

**dome**

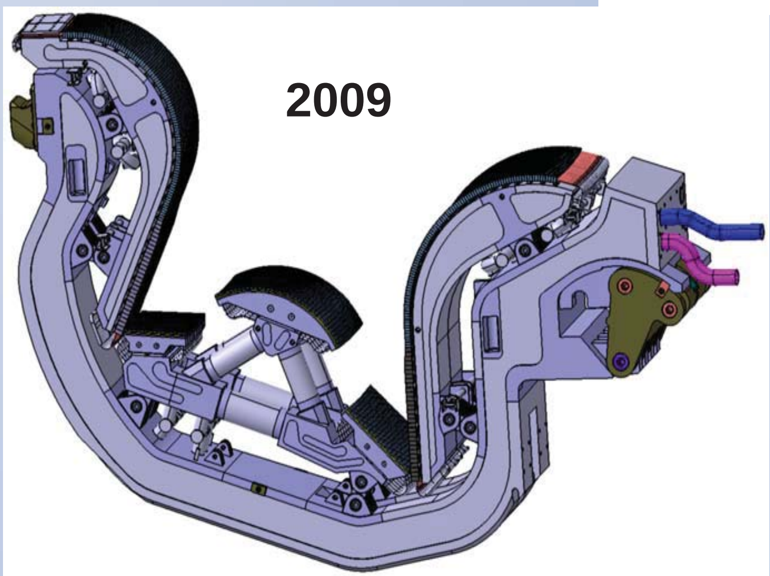
**to support wings**

**baffles**

**to confine neutrals**

**sealing**

**between cassettes**




**2009: final design**

**no "wings"**

**dome**

**to compress neutrals**

**baffles**

**to support targets**

**no sealing**

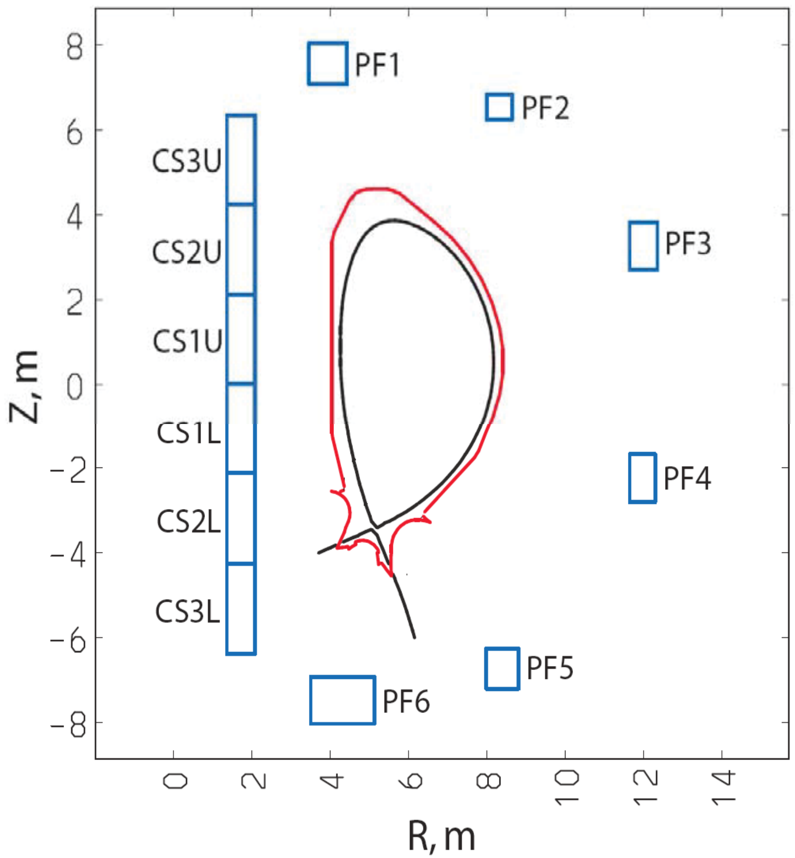
Courtesy: A.K. Kukushkin,

"15 years B2-EIRENE comp. engineering". Fus.Sci.Tech. to appear, 2011

# 2007: ITER design review: ALARM….

The ITER design review found that PF coil set would not support range of operating space for 15 MA, $Q_{DT}$ = 10 inductive scenario goals to be met when more realistic assumptions used

- excessive V-s consumption during $I_p$ ramp-up → restrictions on flattop time
- peaked current profiles during ramp-up → instability
- broader current profiles due to H-mode pedestal → PF6 coil current and field limits exceeded
- central solenoid separation forces restricting operational space



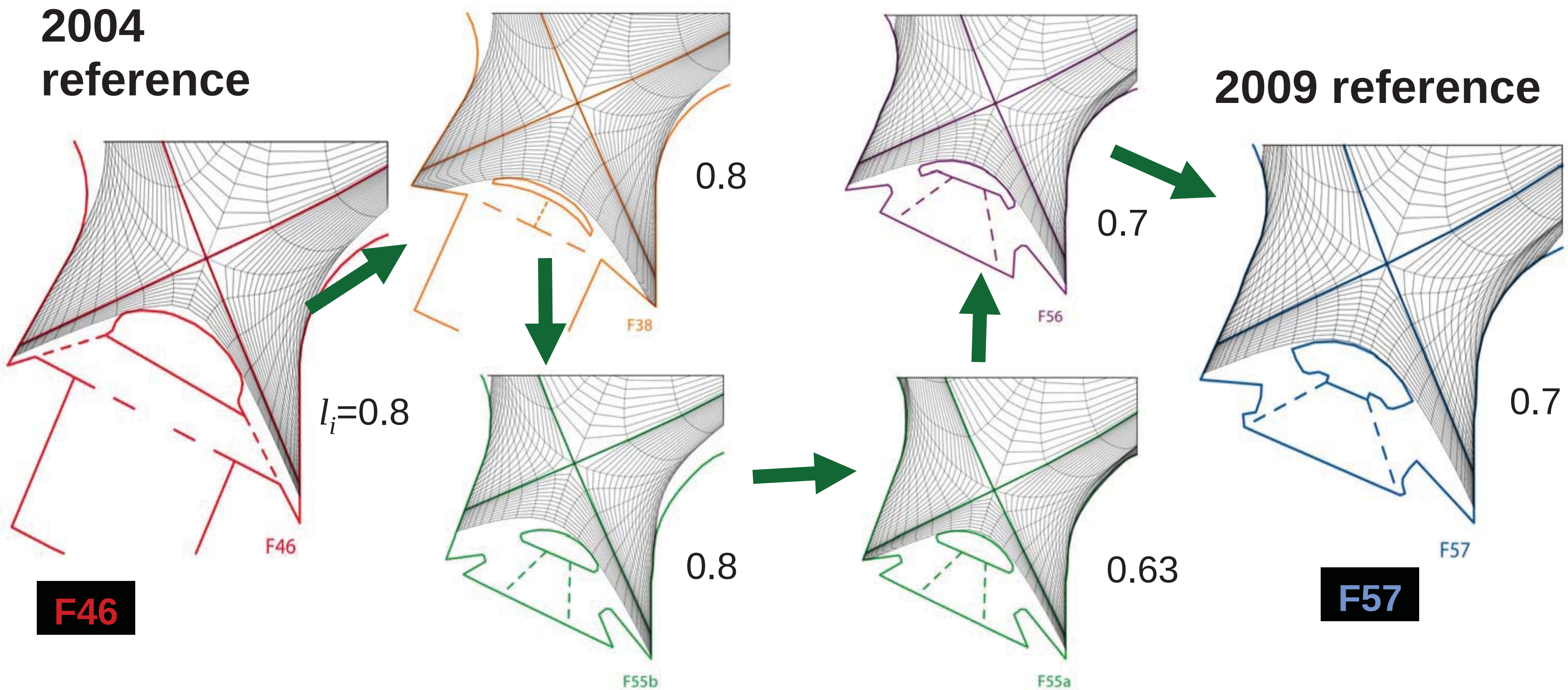

- divertor dome and slot clearances of 2007 design too small for nominal operating points and during disturbance transients

**→ Modification of PF system → Change in equilibrium**

# The geneology of ITER divertors
# 2007-2009: New reference design

B2-EIRENE: main ITER edge plasma design tool

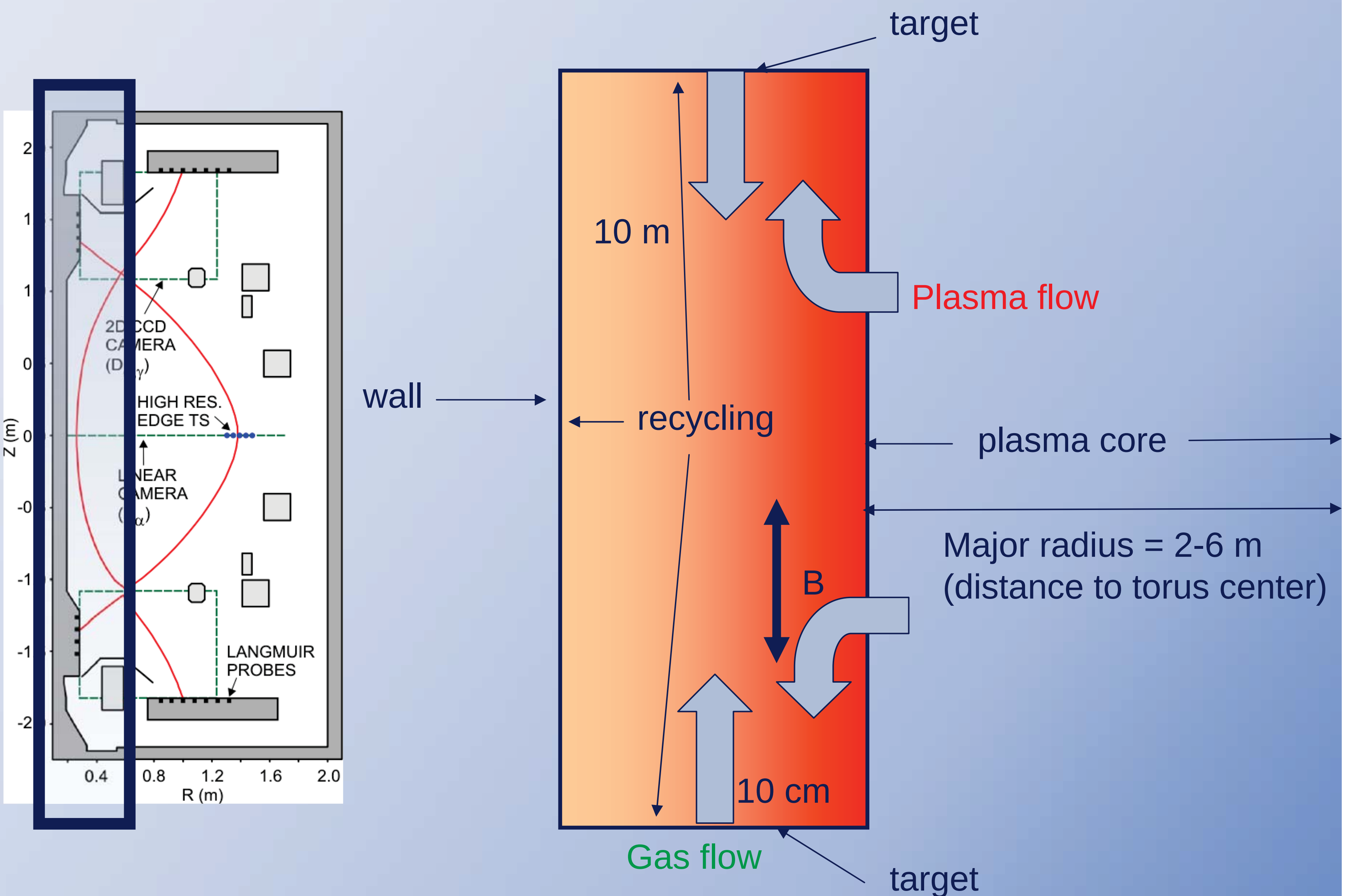
Kukushkin A., Lisgo, S. et al. *(ITER IO)*
Kotov. V., Reiter D. et al., *(FZ-J)*
Pacher G. et al. (*INRS-EMT, Varennes, Québec, Canada*)




Calculations slow → so use the previously studied variants to see the progression

Extend parallelization of EIRENE to B2-EIRENE (2008), + HPC-FF, ….

# A simple model, to illustrate the numerical challenge



**The often hidden challenge: code convergence, iterating on noise ??,…..**

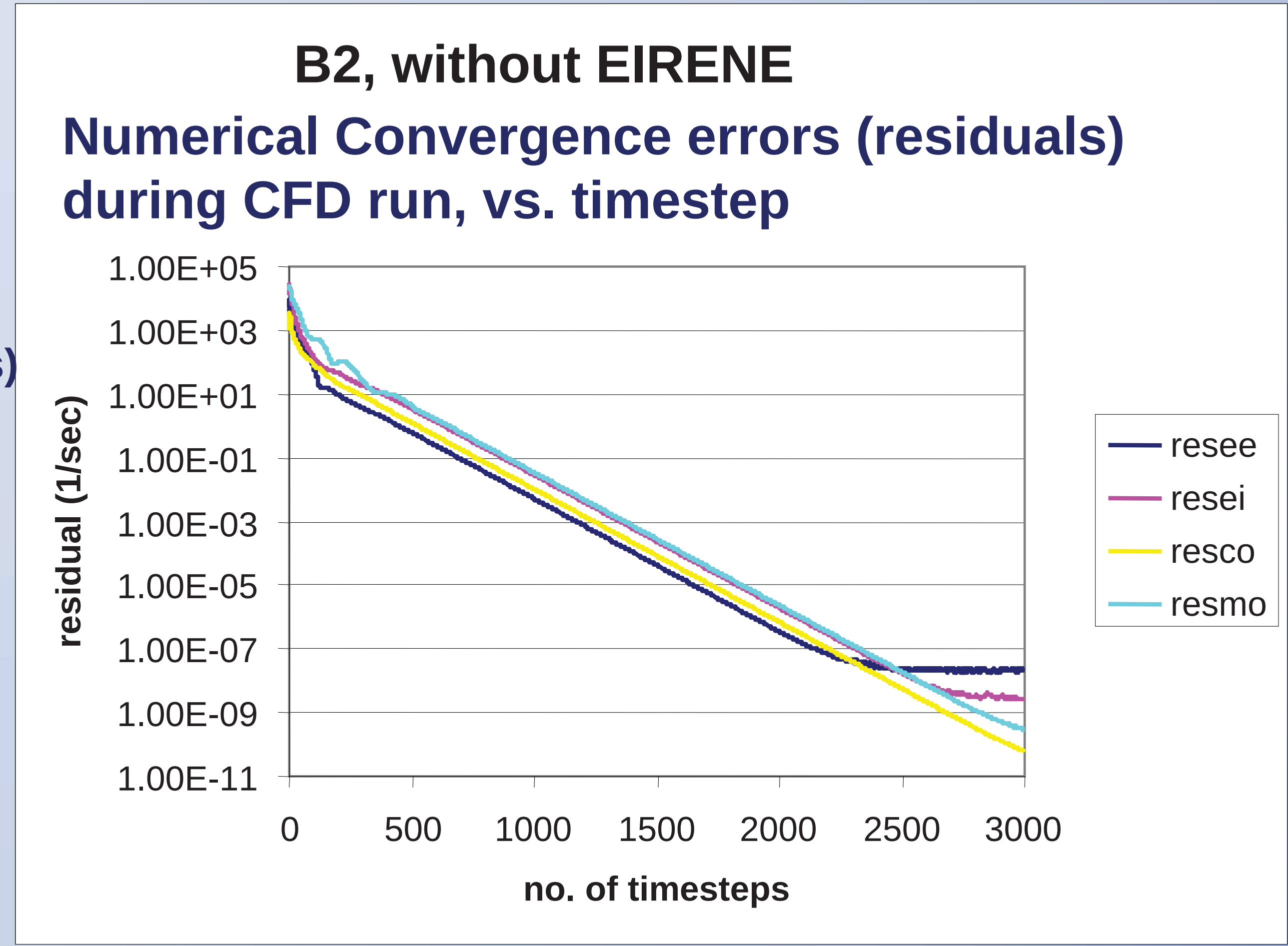
## Code performance: Plasma Flow alone, B2, serial

**Part. Balance ($D^+$)**

**En. Bal ($D^+$)**

**En. Bal. (electrons)**

**Moment. Balance (Navier Stokes)**

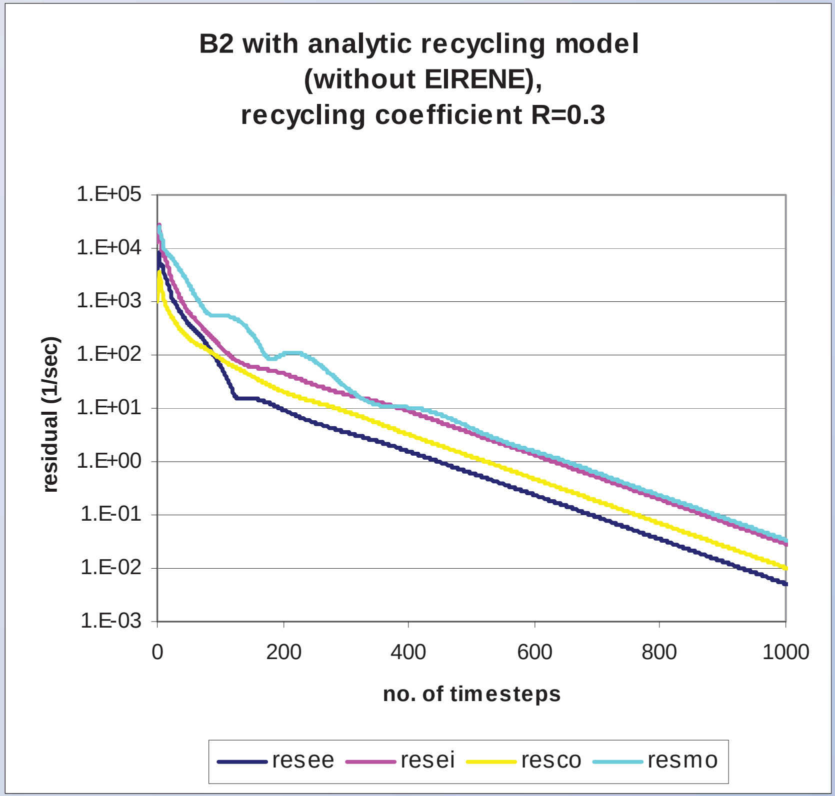



**Expected uncritical behavior, errors reduced exponentially to machine precision.**

# convergence behaviour of the coupled B2-EIRENE codesystem (1)

## Numerical Convergence errors (residuals) during CFD run, vs. timestep

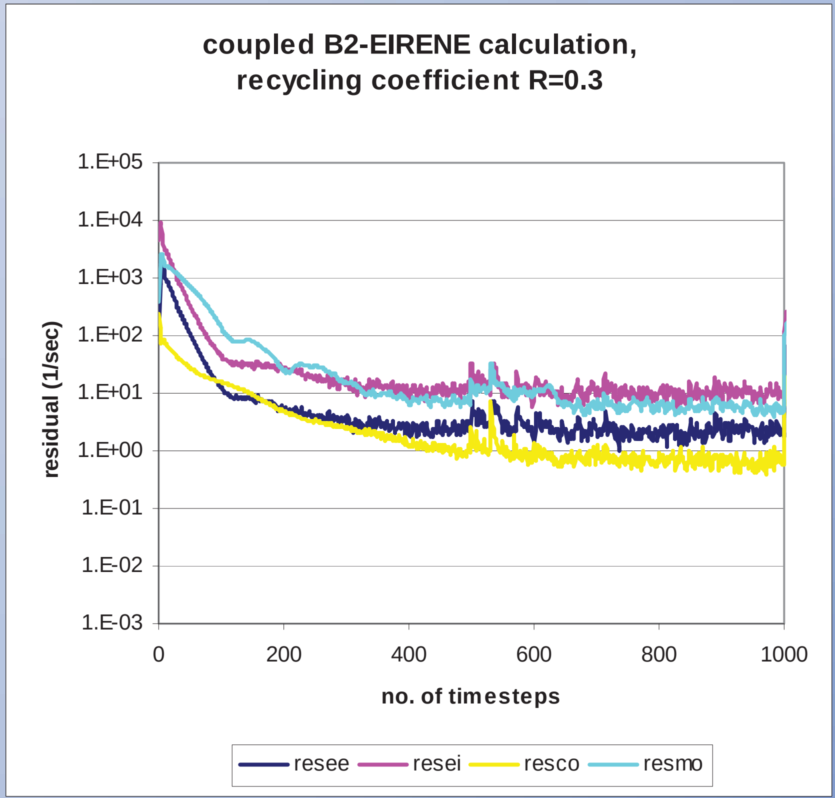
B2, R=0.3




This is what we want

(Analytic recycling model=
unrealistically simplified Boltzmann eq.)

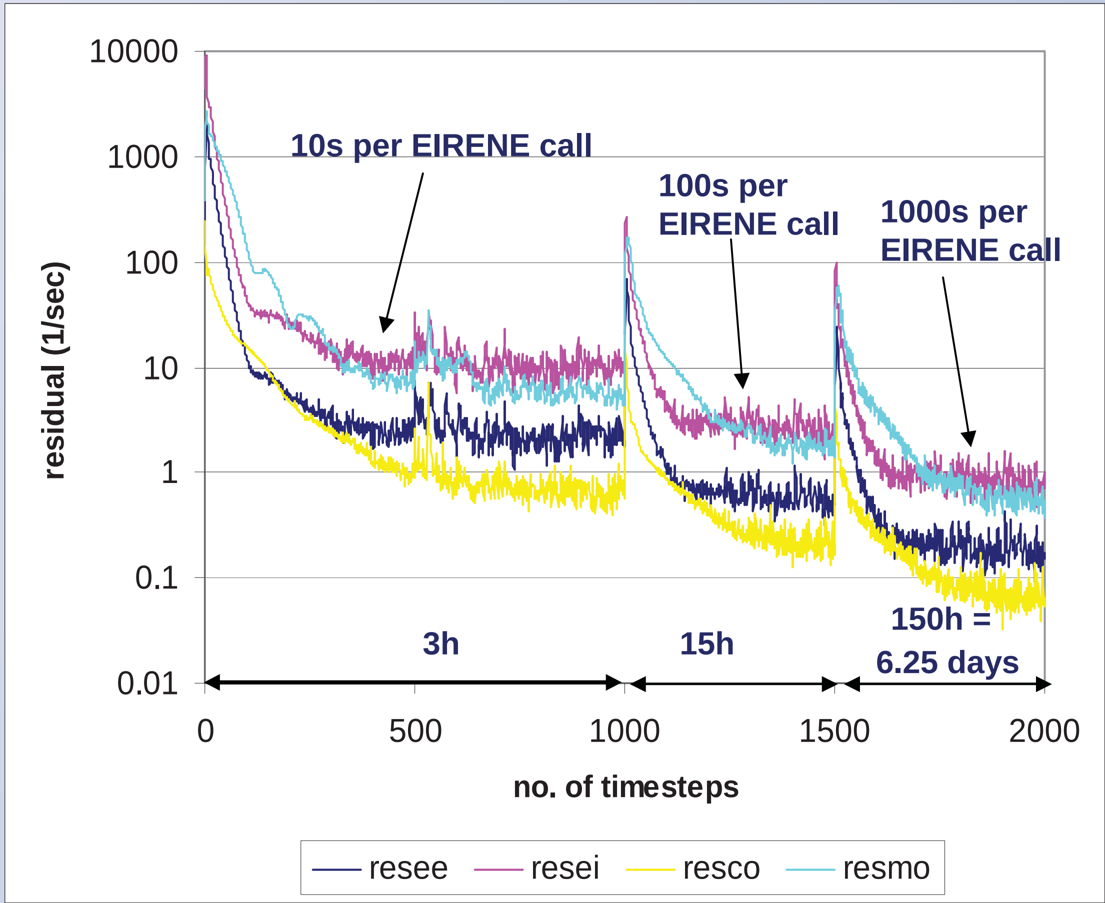
B2-EIRENE, R=0.3




And this is what we get

(full Boltzmann eq., Monte Carlo)

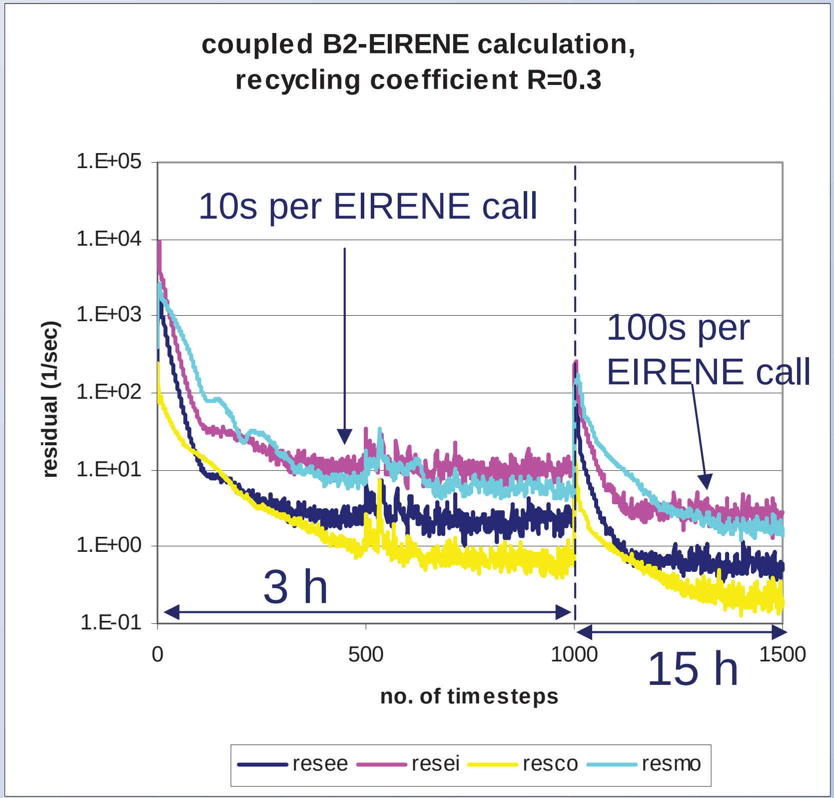
Code performance: serial, B2-EIRENE, ITER test case, Linux PC 3.4 GHz (typical for all “micro macro models” in computational science)

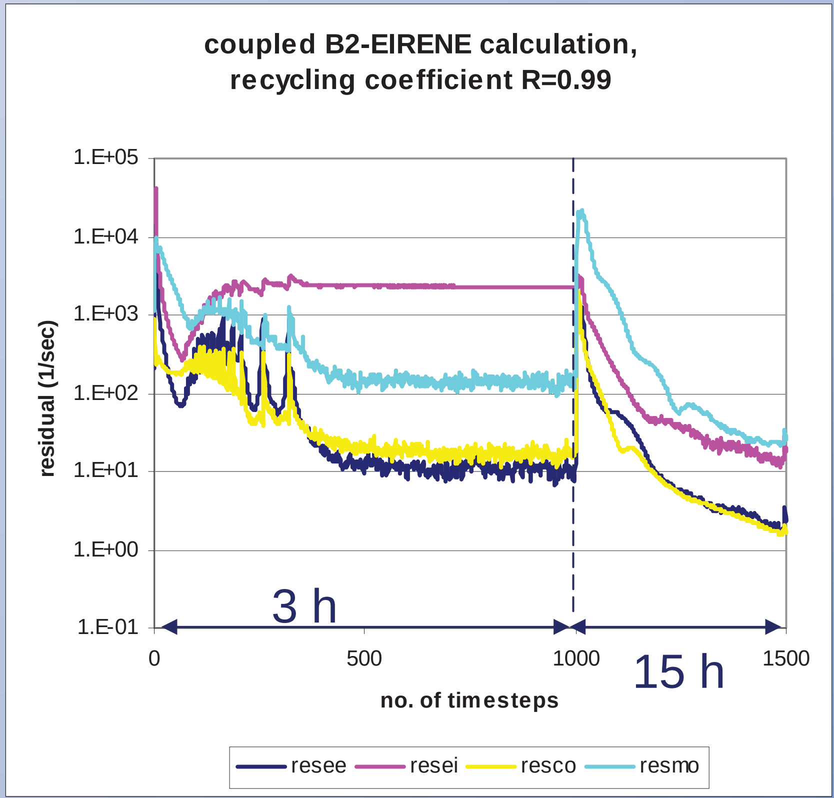



**Convergence limited by statistical Monte Carlo noise.**
**In order to reduce error by factor 10, runtime (or number of processors) has to be increased by factor 100**

What is a measure for: Performance ? Convergence ?
→ Comp. Sci + appl. Math.

# convergence behaviour of the coupled B2-EIRENE codesystem (2)



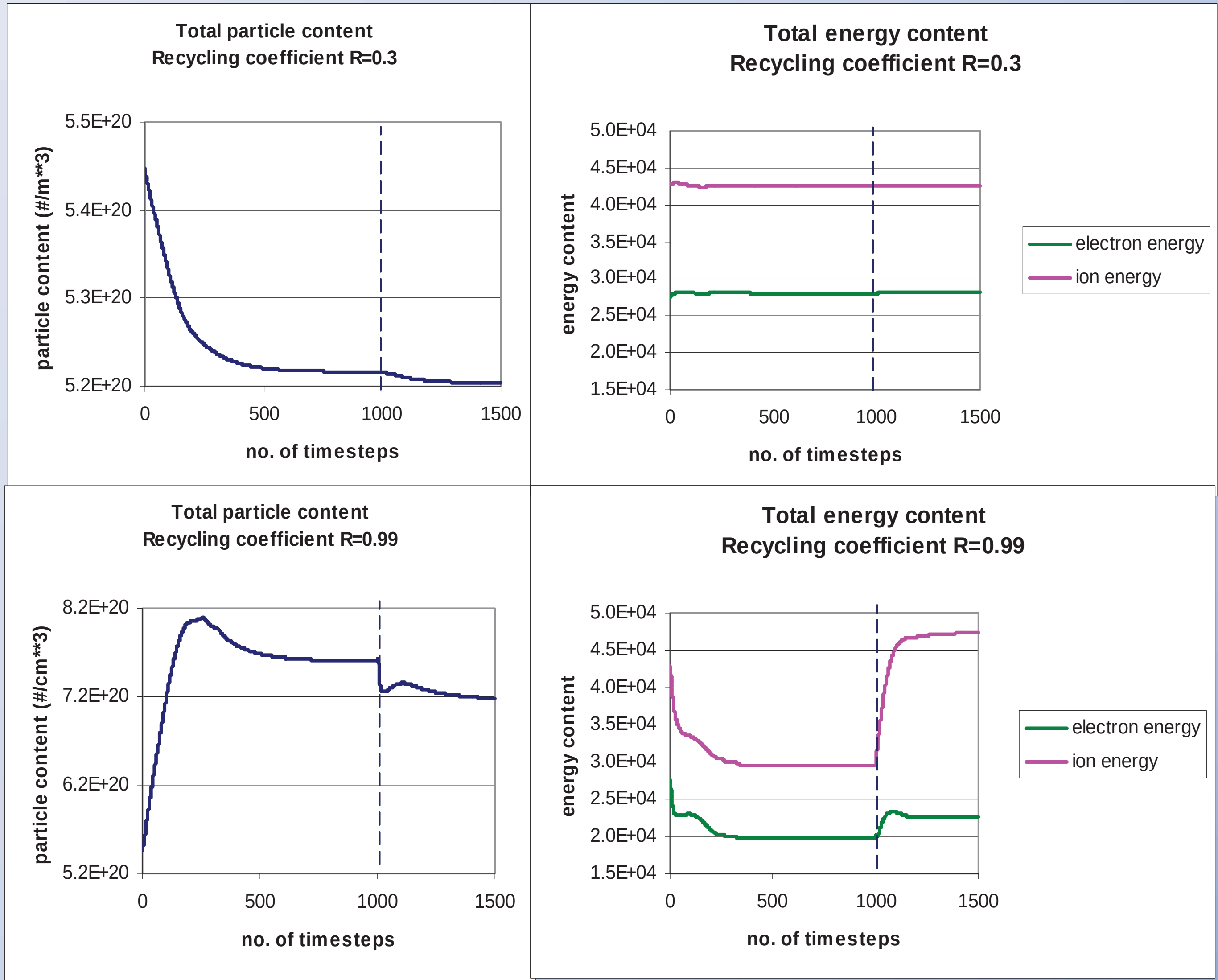




low recycling

high recycling

Convergence in given CPU-time depends
on level of recycling (= vacuum pumping speed)

# convergence behaviour of the coupled B2-EIRENE codesystem (3)




low recycling
R=0.3

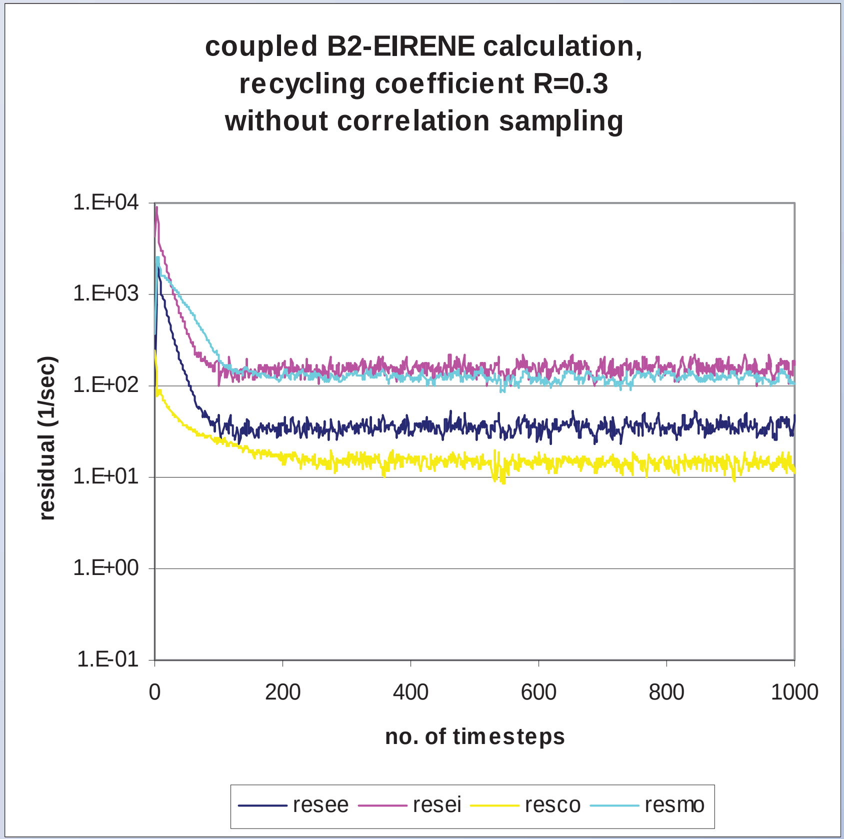
high recycling

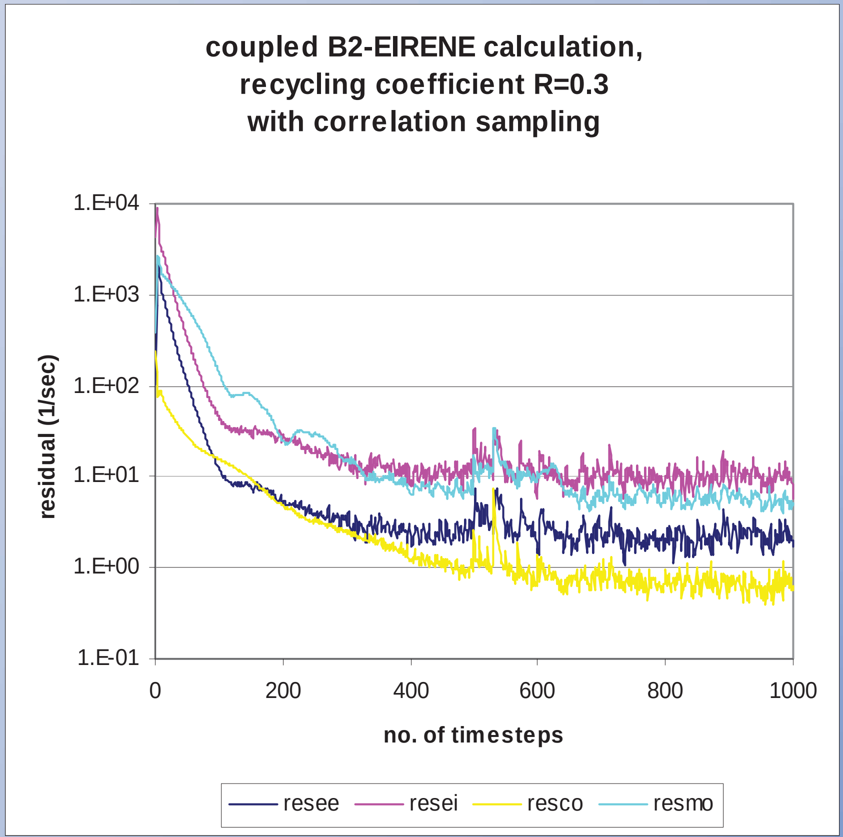
R=0.99

"Is is enough to see one lion to know you are in a desert"

# Correlation sampling and convergence of B2-EIRENE

## Here: correlation produced by simple manipulation of random number generator




Without correlation sampling cpu time has to be increased by a factor 100 to reach the same convergence level !

How much correlation ? Damping of noise, without freezing error from early iterations.

# Recent Progress and Challenges

The experimental experience:

to stir a liquid

Creating turbulent (chaotic) flow
can largely increase heat transfer
(avoid local overheating)

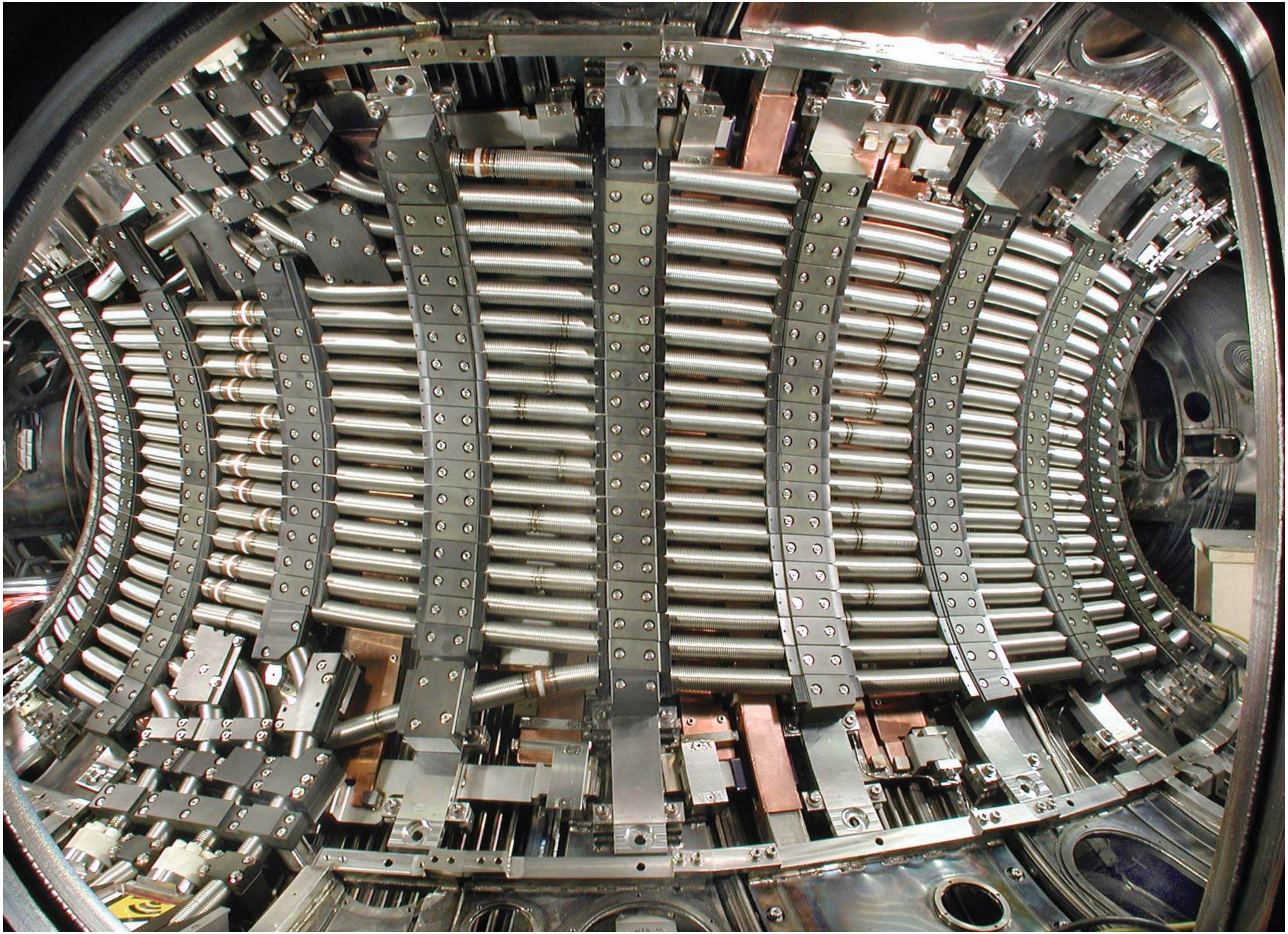
The theory:

"passive scalar transport in chaotic force fields"

Not yet understood on a quantitative level
very active modern research field of
•theoretical physics
•large scale numerical computing.

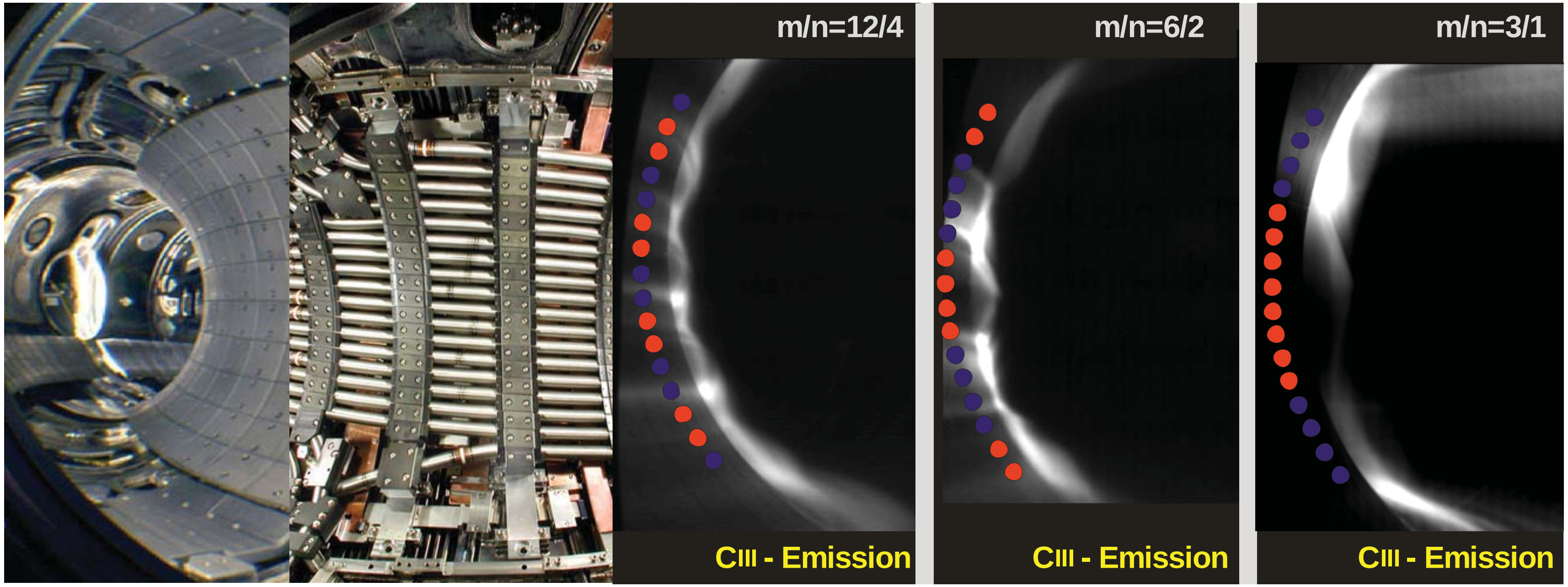
## Avoid excessive heat loads by stirring (magnetically) the plasma?

## TEXTOR-DED: Dynamic Ergodic Divertor



# Dynamic Ergodic Divertor (DED) in TEXTOR

flexible tool to study the impact of resonant magnetic perturbations on transport, stability and structure formation (helical divertor)




**16 coils mounted at the HFS:**

- covered with graphite tiles
- helical set-up
- resonant on q=3 surface

**resonant perturbation:**

- m/n = 12/4, 6/2, 3/1 base mode
- different penetration depth
- $B_{DED}/B_{\theta}$ ~ 10%

**different operation modes:**

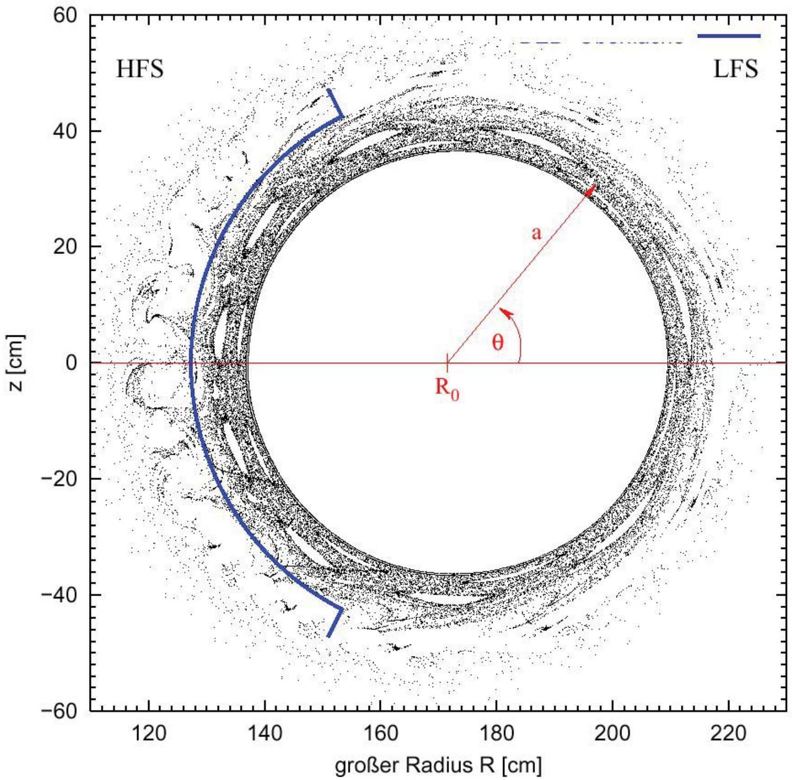
DC operation

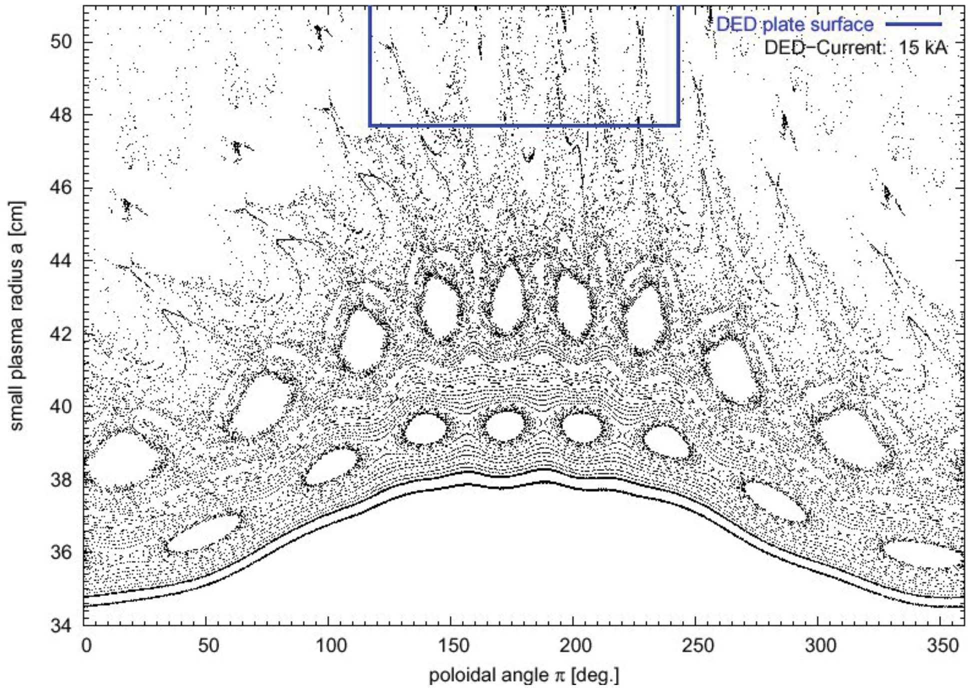
AC operation [1-10kHz]

*slow strike point sweeps*

# Field line tracing- 3D plasma fluid –neutral gas kinetic modeling

Partially ergodic 3D magnetic field topology
→ 3D edge codes→ also Monte Carlo for plasma flow fields (EMC3)

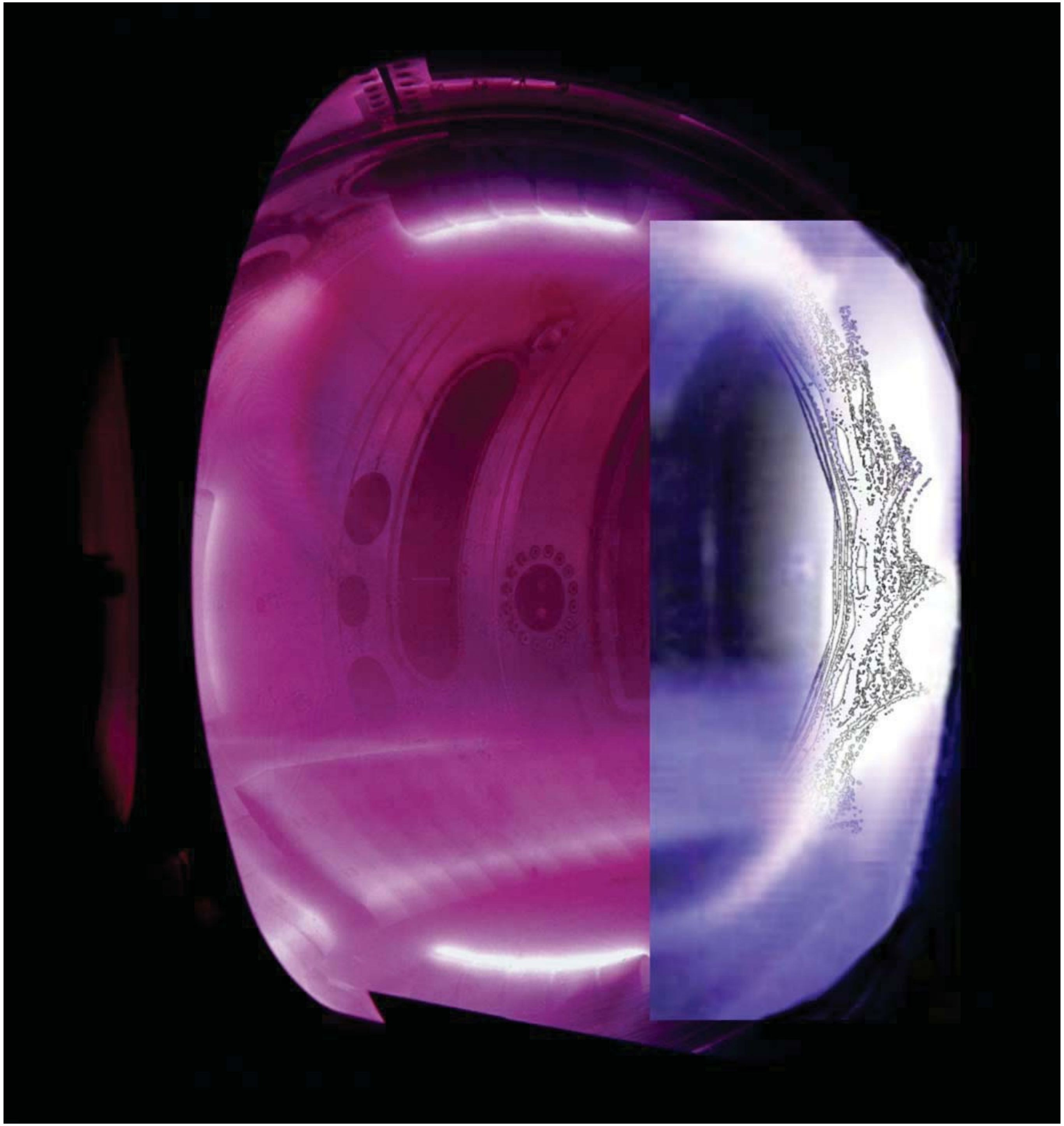



TEXTOR-DED B-Field (R-Z) TEXTOR-DED B-Field (r-θ)

D.Harting, D.Reiter, JUEL-4173, May 2005

Trilateral Euregio Cluster
TEC



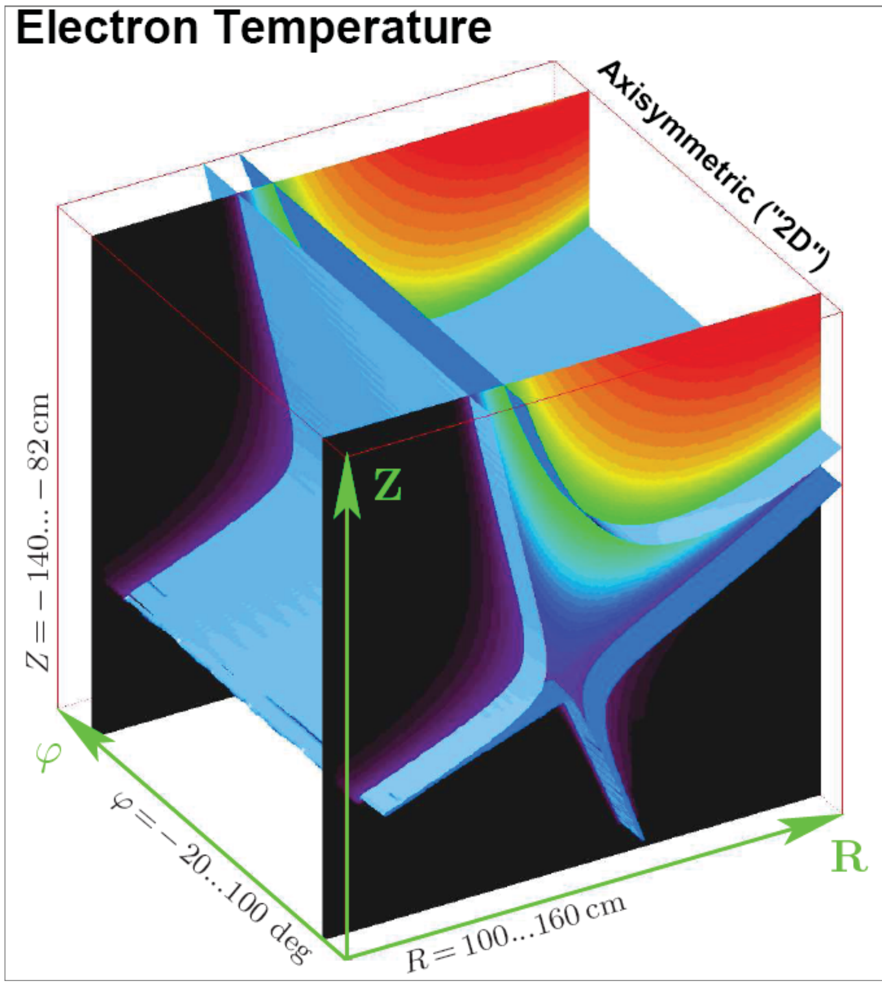
# “Particle” methods: also well established in fluid dynamics

- Lagrangian method ← Eulerian (grid based) method
- Advantages:
- + concentrate “particle” in the interesting region
- + Convective transport essentially without numerical dissipation in arbitrarily complex geometry
- Disadvantages:
- - Non-convective terms (collisions, diffusion)
- Solution: Monte Carlo fluid (random walk model)
- in Fusion: this is the concept of E3D and EMC3-EIRENE codes (IPP Greifswald)
- - looses accuracy in region of interfacial boundaries

# EMC3-EIRENE:

## FZJ: mainly tokamak applications (RMPs)

## Example: DIII-D ELM mitigation scenarios




Goal: quantify PSI, when RMPs are applied in ITER

# Towards fully 3D CFD:
# The EMC3-EIRENE code (IPP Greifswald – FZ-Juelich)

JÜLICH
FORSCHUNGSZENTRUM

(initially developed for stellarator applications W7AS, W7X, LHD) was advanced to a more flexible grid structure to allow divertor tokamak + RMP applications.

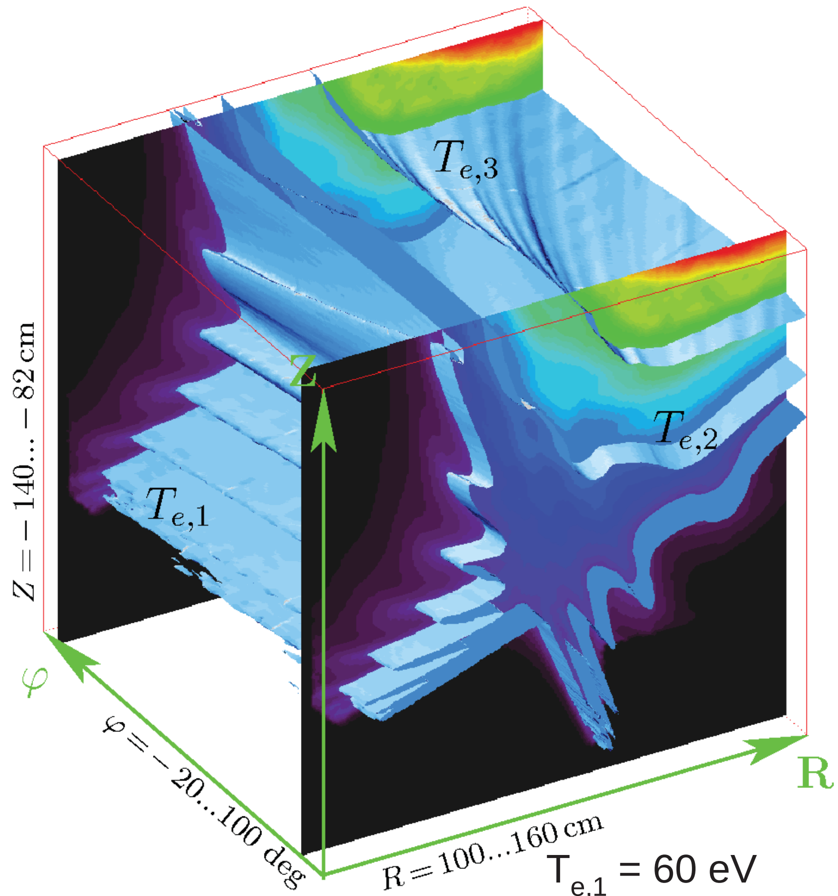
- first self-consistent 3D plasma and neutral gas transport simulations for poloidal divertor tokamak configurations with RMPs.

- Simulation results for ITER similar shape plasmas at DIII-D show a strong 3D spatial modulation of plasma parameter, e.g. in $T_e$.

- EMC3-EIRENE code verification (by benchmarks with 2D tokamak edge codes) and validation (TEXTOR, DIII-D, JET, LHD experiments) ongoing

- EMC3-EIRENE is currently being prepared for contractual ITER RMP design studies (jointly by FZJ and IPP, 2010…)

Electron Temperature, DIII-D, with RMPs

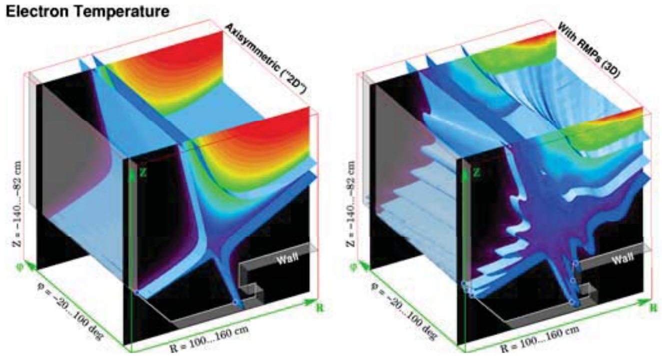



$T_{e,1}$ = 60 eV
$T_{e,2}$ = 120 eV
$T_{e,3}$ = 200 eV

# ITER contractual edge modelling

## Goal: quantify PWI, when RMPs are applied in ITER

(EMC3-EIRENE 3D tokamak edge transport application)




*F4E-GRT-055 (PMS-PE)* ,

FZJ-IPP-CEA

(since July 2010)

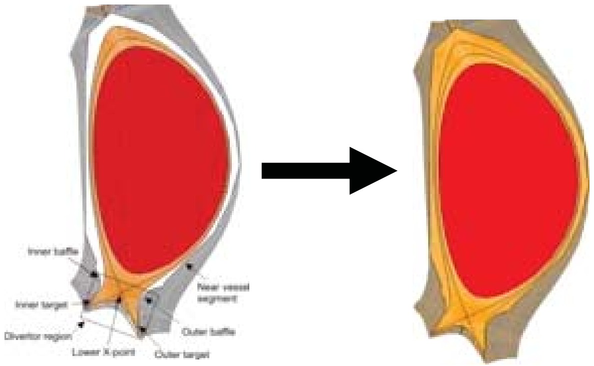
---

## Goal: diagnostic mirror lifetime assessment

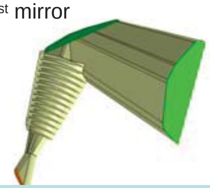
(closing the gap between SOL and wall in B2-EIRENE)

*ITER.CT.09.4300000034*

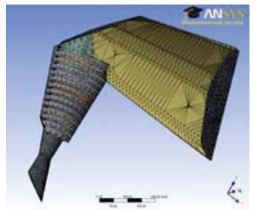
FZJ (since Oct. 2009)



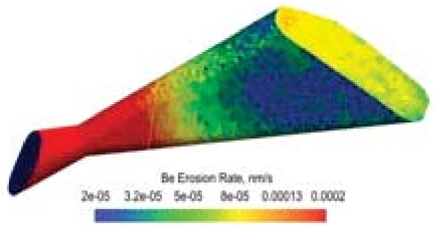

1st mirror



CXRS port plug, CATIA design



EIRENE code model via ANSIS interface (mirror lifetime assessment)




Be erosion rate in CXRS port plug

---

SOLPS4.x (ITER, FZJ) vs. SOLPS 5.y (IPP)

*F4E-OPE-258*

FZJ, Univ. St. Petersburg, (Dec. 2010)

# Conclusions/Outlook

**Similar to previous steps: progress to ITER is based mainly on experimental and empirical extrapolation**

**guided by theory and aided by modelling**

**Present goal:**

**include all of edge physics that we are sure must be operative (opacity, A&M physics, surface processes, drifts…, even while our capability to confirm these directly remains limited.**

**Codes = bookkeeping tools**

**Present upgrading:**

**- low temperature plasma chemistry**

**- consistent wall models**

**- drifts and electrical currents in the edge**

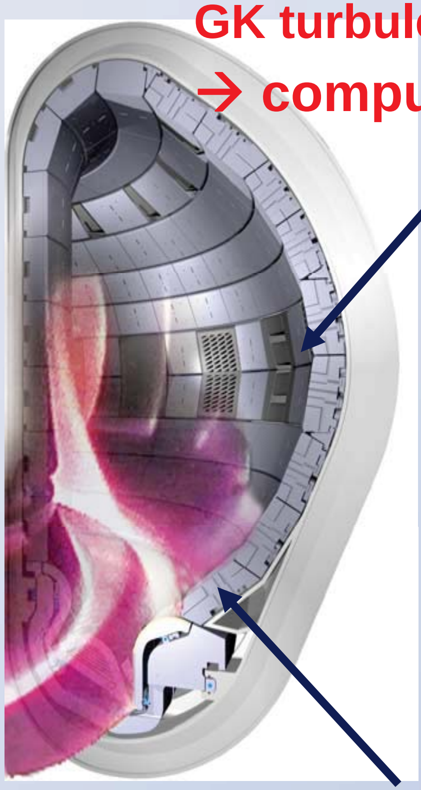
**- 2D → 3D**

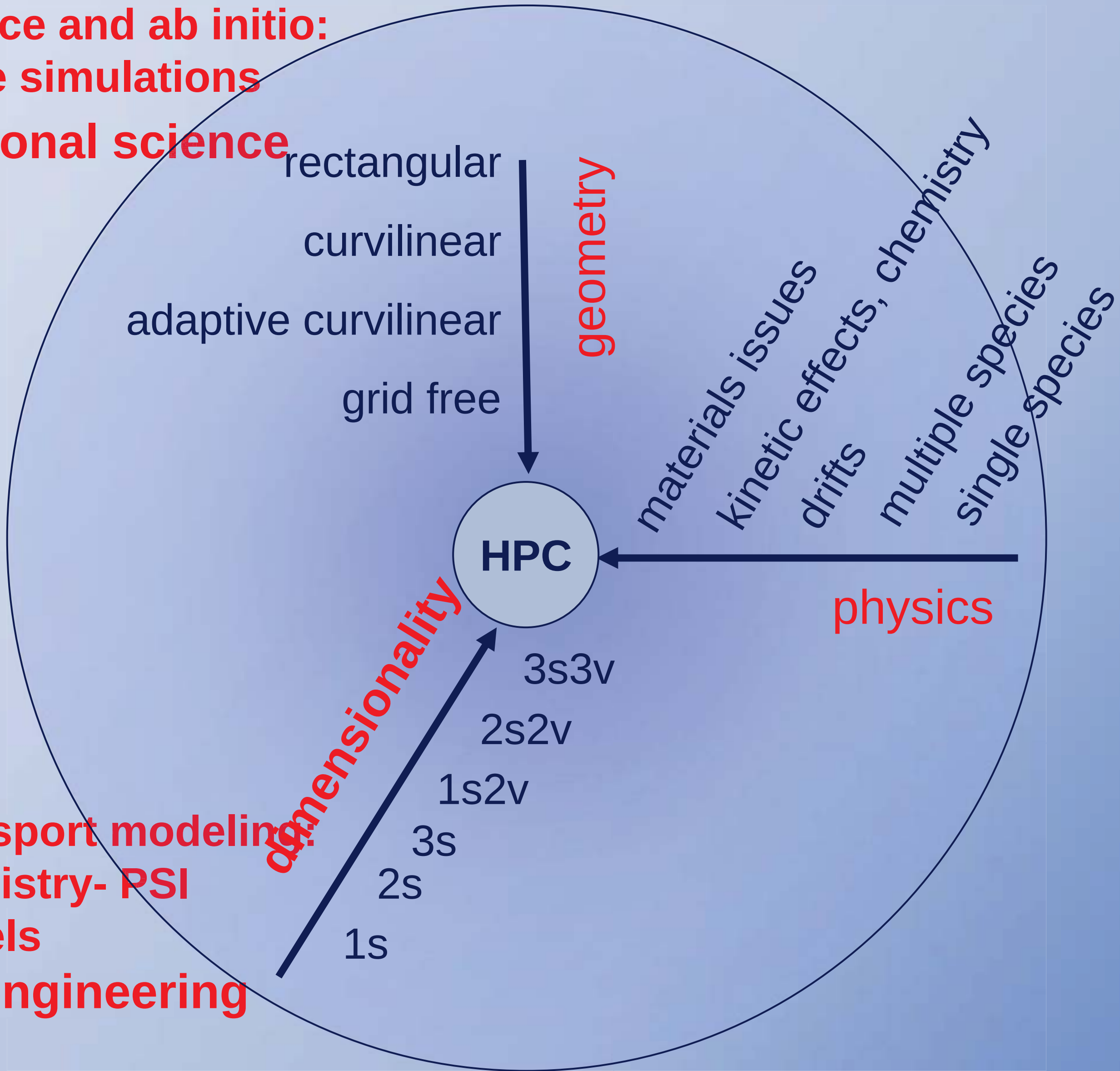
**- coupling to first principle edge turbulence codes**

**- code integration: Core- ETB – Edge (ELM modelling)**

# Integrated edge plasma simulation: “From the barrier to the target”

**Fluid turbulence and ab initio:**
**GK turbulence simulations**
**→ computational science**






**Integrated edge transport modeling:**
**fluid - kinetic – chemistry- PSI**
**“micro-macro” models**
**→ computational engineering already now**

# Summary: Edge Theory and Modelling

**Where are we? A reality check**

**Compare with aircraft aerodynamics**

Things in Common:

- Both use fluid models/codes as primary analysis tool
- In both cases one can get fairly far with 2D (ITER design) but in the end: 3D is needed
- Both involve a powerful controlling fluid-solid interaction/interface
- Both involve turbulence in an important way
- Both are applied sciences:
  What, Why, How (how can we make this application work?)

# Compare with aircraft aerodynamics

The differences:

- Aero: involves 2 states of matter.
  Edge Plasma : minimum 3, sometimes all 4
- Aero: no B or E fields, no currents, Maxw. Eq. play no role.
  Edge Plasma: Maxwells eqs. are as important as fluid eqs.
- Sub-sonic aero: largely incompressible flow.
  Edge Plasma : fluid is compressible
- Aero: one fluid.
  Edge Plasma: many fluids (electrons, ions, impurities, neutrals, photons…)
- Aero: no exchange of matter.
  Edge plasma: the exchanges are dominating

## Compare with aircraft aerodynamics

The differences, cont.:

- Aero: some unsteady effects,
  Edge Plasma: extremely powerful effects (bursts): ELMs…

- Aero: 2D flow field can be studied in small, cheep, wind tunnels, done 1000‘s of times over 100 years
  Edge Plasma: needs 2D (3D) fluid field for all fluids, around the entire edge (when? cost?)

# Summary: Edge Theory and Modelling

**Where are we? A reality check**

Computational aircraft aerodynamics is still an active field of research.

**Edge plasma: orders of magnitude more complex, orders of magnitude less R&D**

If computational edge plasma science would be "largely in hand",

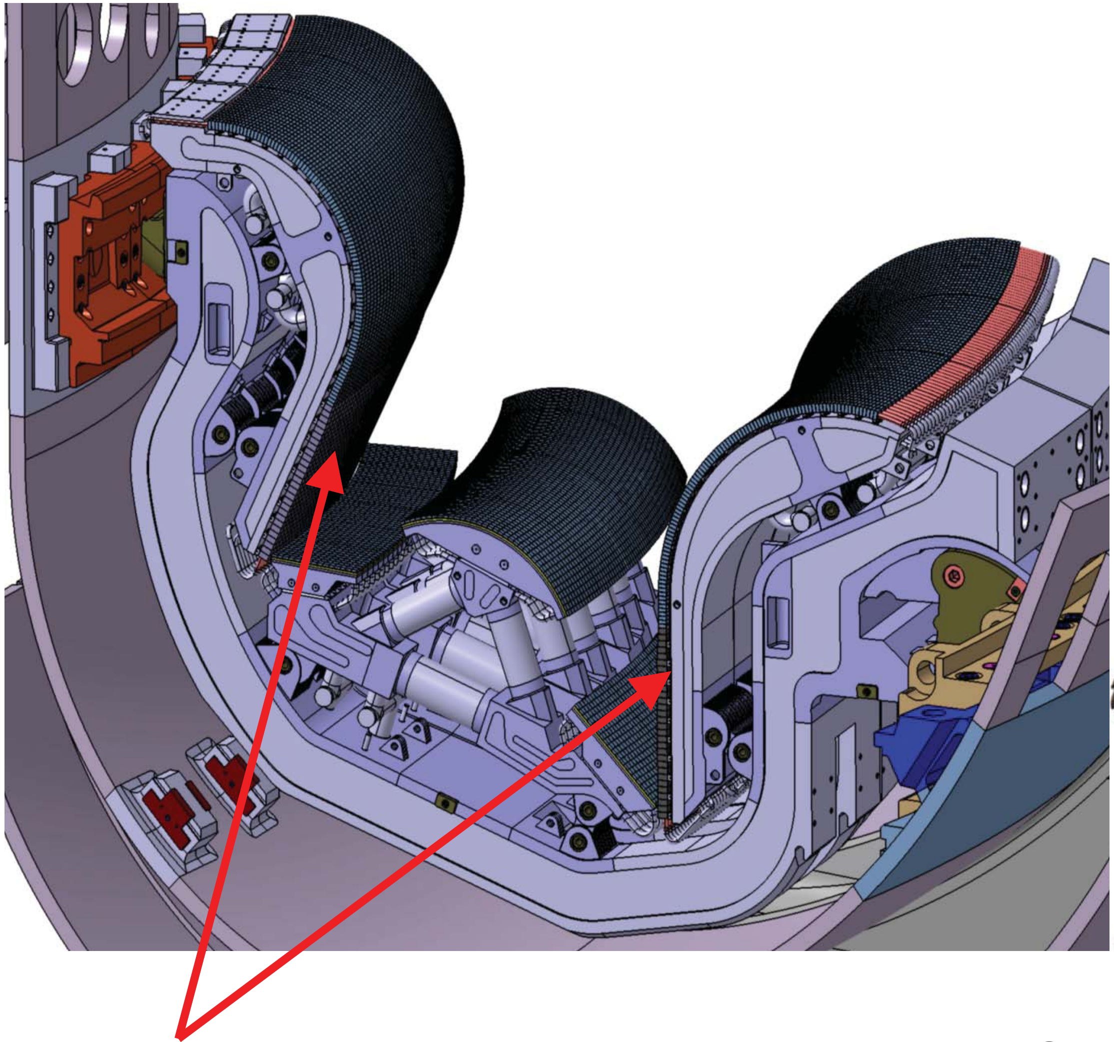
**it would be a miracle.**

A major computational edge plasma science effort is needed, in order to avoid major code failures in the ITER design and operation

# The End


# ENERGY MATTERS

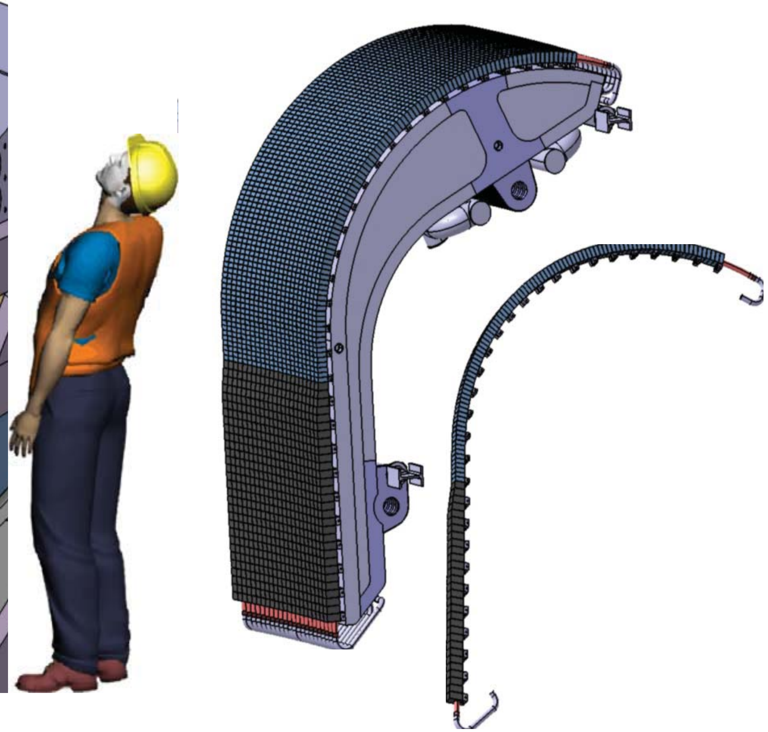
# The divertor



54 units

Total weight: ~470 tonnes

Actively water cooled



Heat flux density = 10 $MW/m^2$!