



TRILATERAL
EUREGIO CLUSTER



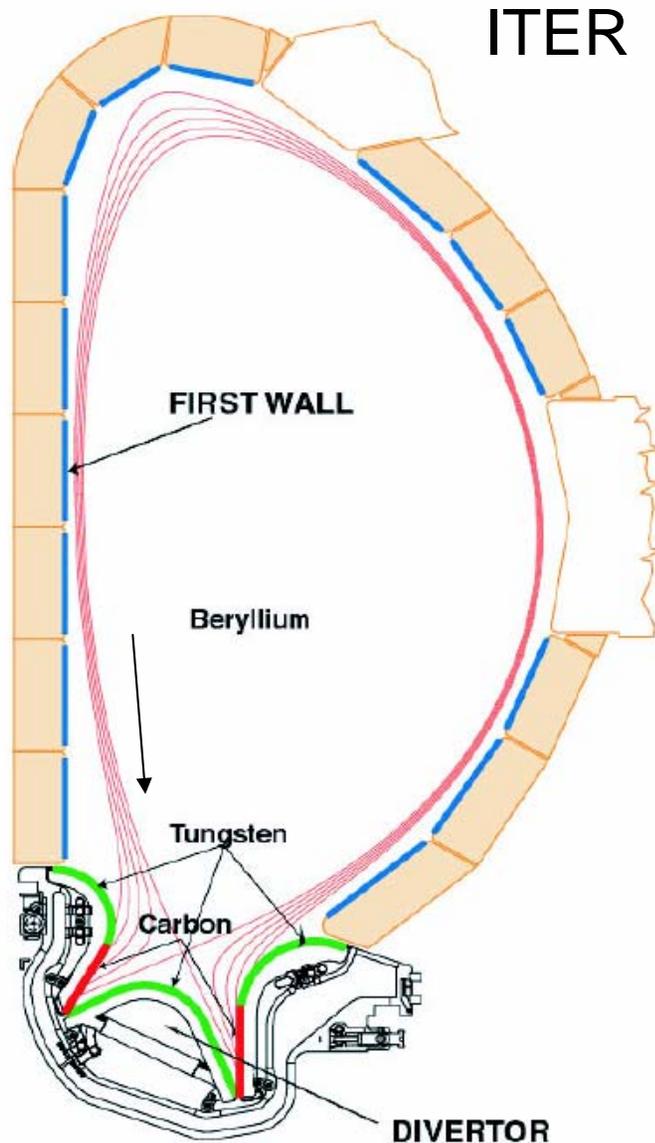
Usage of ADAS data in the Monte Carlo codes for particle transport simulations in plasma (*on example of ERO code*)

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Special thanks for contributions from A.Kirschner, D.Reiter, R.Ding and D.Matveev

Motivation: plasma-surface interaction (**PSI**) in fusion devices



700 m² beryllium first wall

- low Z
- oxygen getter

100 m² tungsten baffles, dome

- high Z
- low sputtering

50 m² graphite CFC target plates

- no melting

Erosion of wall materials, transport and re-deposition →

- Lifetime & tritium retention
- Material mixing effects

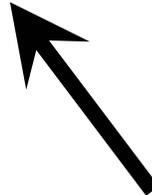
*Plasma-surface interaction in divertor can determine the **ITER availability** . . .*

Code development:

- *PSI & transport*
- *material mixing*
- *castellated surfaces*
- *atomic data, ADAS*

Benchmarking:

- *PISCES-B (with beryllium)*
- *TEXTOR*
- *JET, ASDEX-UG, ...*

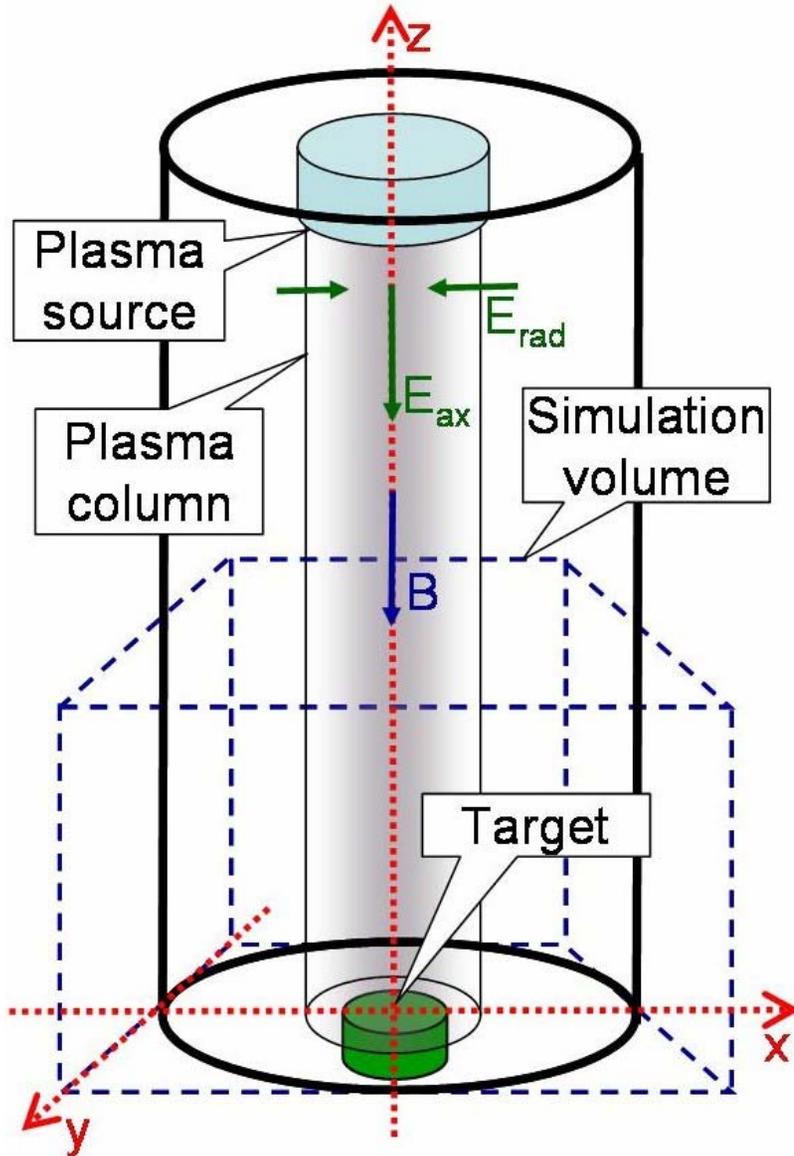


Estimations for ITER:

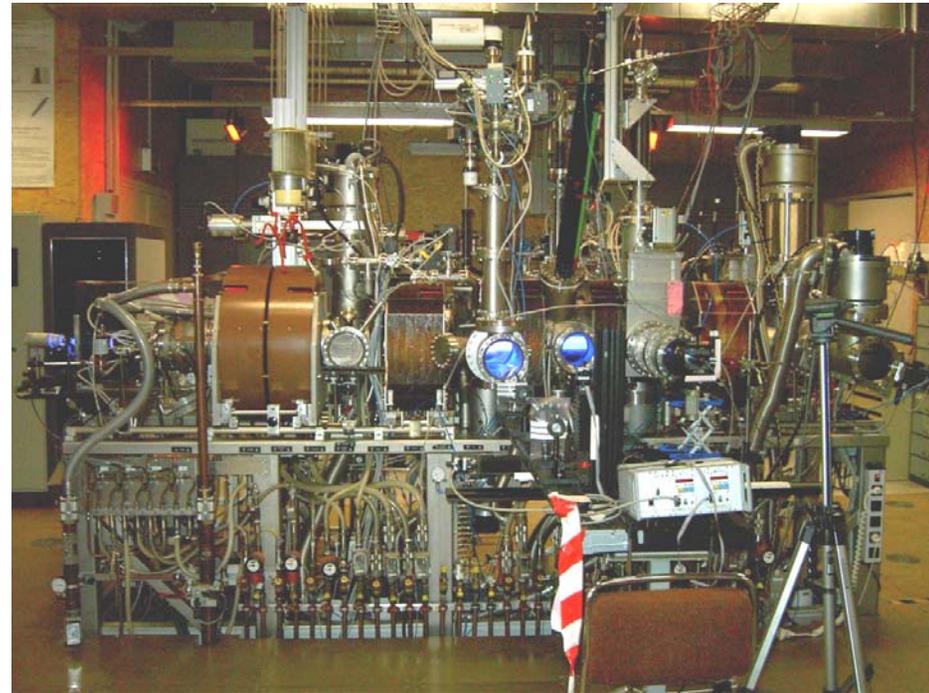
- *tritium retention*
- *target & limiter lifetime*
- *impurities into plasma*

Coupling with other codes:

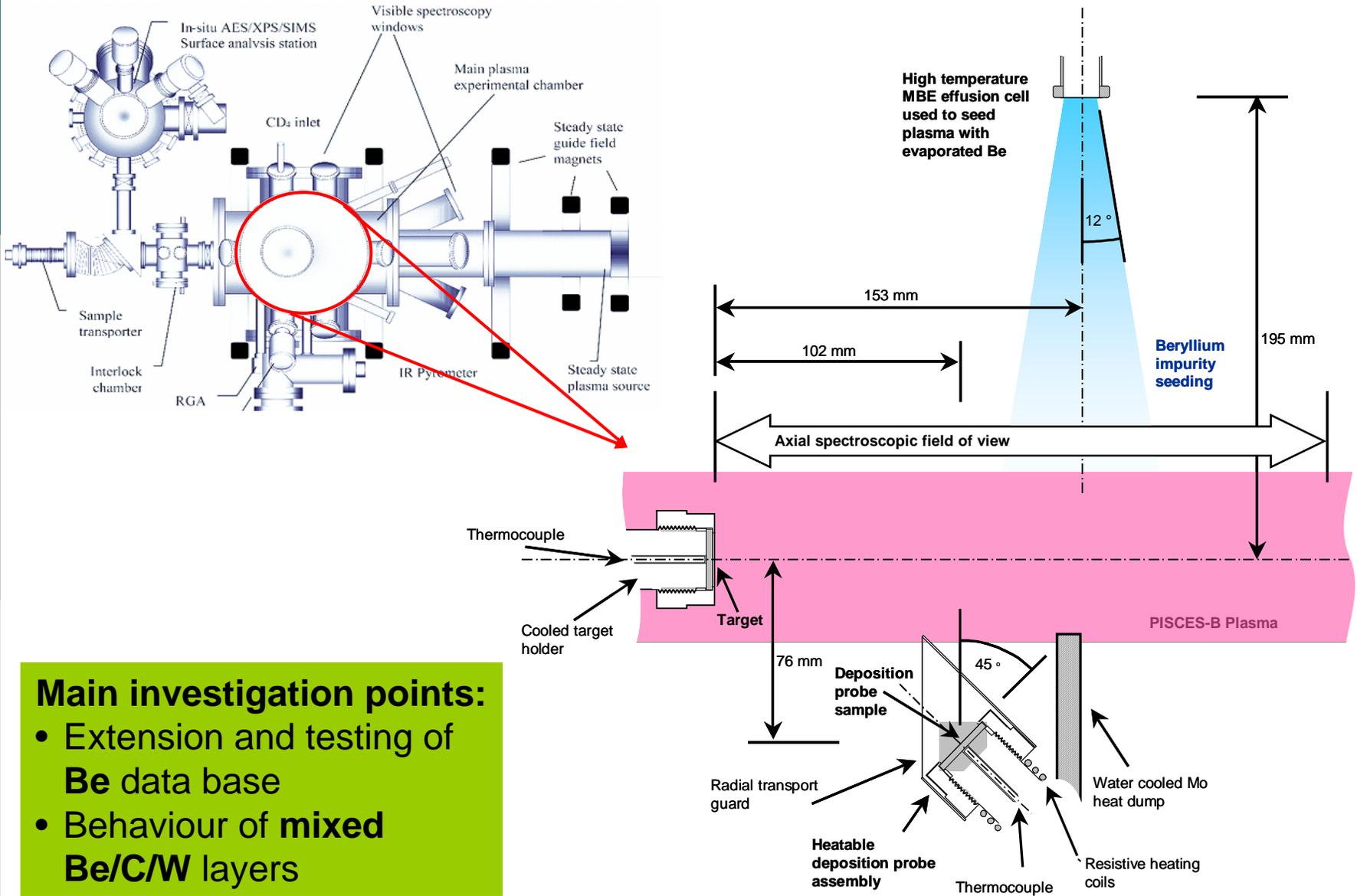
- *plasma parameters from: e.g. B2-Eirene, Edge-2D*
- *surface mixing: TriDyn, MolDyn*



- Less complicated geometry than a tokamak
- Continues operation
- Plasma conditions relevant for ITER divertor



PSI-2 facility (Berlin). Planned to be transferred to FZ Jülich in 2009.





- **Monte-Carlo (MC) method**
 - Error estimation
 - Random generators
- **Edge plasma and PSI simulations**
 - B2-EIRENE code (SOLPS)
 - ERO code
 - ERO light emission model
 - ERO – PSI modelling (TRIM, TRIDYN, MolDyn)
 - Elastic collisions
 - HYDKIN database
- **ERO – examples of application**
 - Hydrocarbon injection at TEXTOR (D/XB)
 - Test limiters – W and C
 - Be spectroscopy patterns at PISCES-B
 - ITER predictions (divertor plates lifetime, tritium retention)
- **Technical issues (ERO) – parallelization, benchmarking**



Monte Carlo basics

For numeric calculation of κ -dimensional integral error (“guaranteed error”) can be estimated as

$$\delta \sim dA \cdot N^{-1/\kappa}$$

$$\delta < 0.01dA \Rightarrow N \geq 100^{\kappa}$$

Already by $\kappa=5$ really challenging number! . .

Monte-Carlo approach – let’s use mathematical expectation!

$$M(s_i) = \int_G f(P) dP = I(f), \quad s_i = f(P_i)$$

$$S_N(f) = \frac{1}{N} \sum_{j=1}^N s_j \Rightarrow M(S_N) = I(f), \quad D(S_N(f)) = \frac{1}{N} D(f)$$

Chebyshev inequality:

$$\delta \sim |S_N(f) - I(f)| \leq \sqrt{\frac{D(f)}{\eta N}} \Leftrightarrow P = 1 - \eta$$

$$\eta = 0.01 \Rightarrow \delta \sim 10 \sqrt{D(f) / N}$$

Any pair of s_i independent from each other!

$$D(\overline{S_N}) \leq D(S_N) = D(f)$$

More precise estimation is based on central limit theorem:

$$\frac{|S_N(f) - I(f)|}{\sqrt{D(f)/N}} \sim \rho(y) = \frac{1}{2\pi} \int_{-\infty}^y \exp\left(-\frac{t^2}{2}\right) dt$$

All s_i are fully independent!

$$|S_N(f) - I(f)| \leq \sqrt{D(f)/N} \sim \rho_0(y) = 1 - \frac{1}{2\pi} \int_y^{\infty} \exp\left(-\frac{t^2}{2}\right) dt$$

$$|S_N(f) - I(f)| \leq 3\sqrt{D(f)/N} \quad \text{P} = 0.997$$

$$|S_N(f) - I(f)| \leq 5\sqrt{D(f)/N} \quad \text{P} = 0.99999$$

Some demotivation: $D(f)$ should be kept small!..

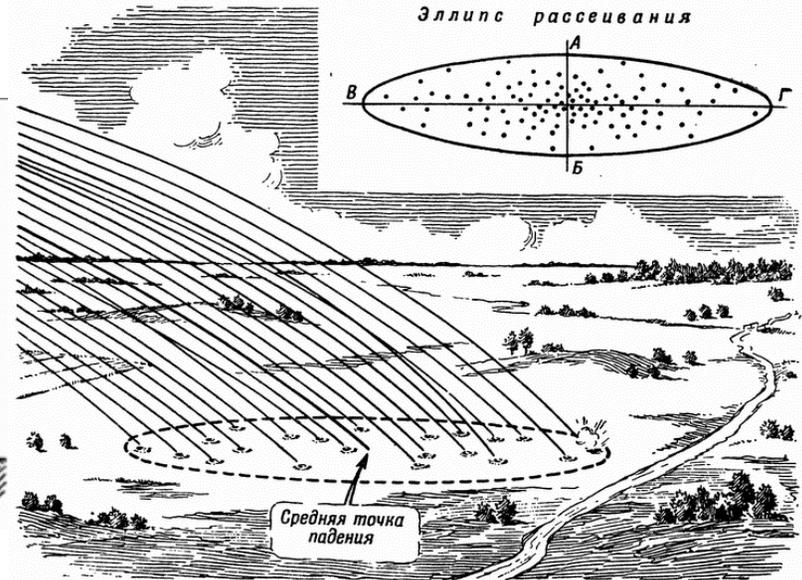
2 main ways to improve performance:

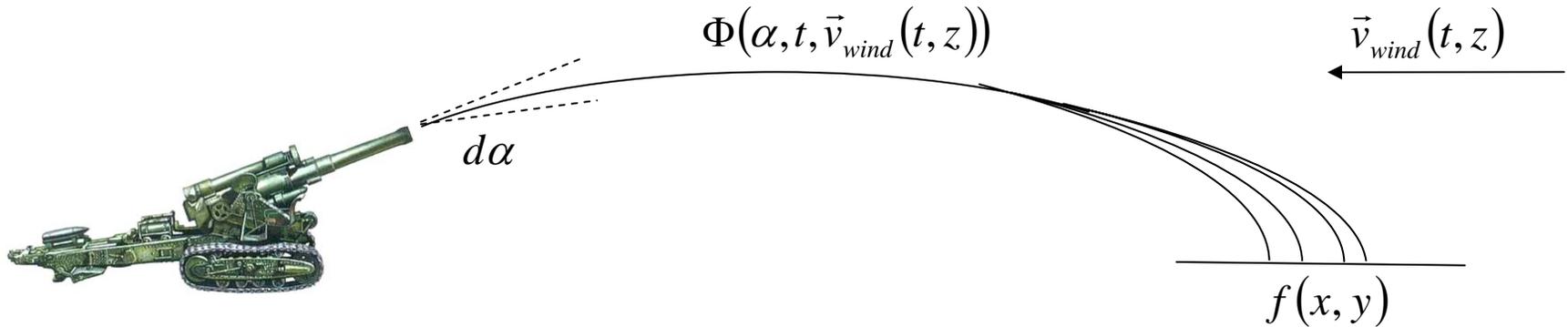
- 1) Choice of integration points distributed as $g(P)$ e.g. such that $f(P)/g(P) = \text{const.}$
- 2) Separate the integration region into sections with various dispersion.

Артиллерия



This problem was solved (with acceptable accuracy!) long before people has learned how to integrate . . .





Determined solution:

$$f(x, y) = \oint \left(\int \Phi(\alpha, t, \vec{v}_{wind}(t, z)) dt \right) \cdot d\alpha$$

α – solid angle!

Monte-Carlo solution:

α – correct distributed arbitrary value

s_i – how many trajectories come to $[x_i \pm dx, y_i \pm dy]$

Typical task – find dispersion.

Determined solution: 2 more integrations by x, y

MC solution: just find dispersion of S_N . . .

Obviously, trajectory of a plasma particle is much more complicated!

Let's assume that on specie can act processes 1, 2, ...

$$\frac{dN}{dt} = \langle v\sigma_1 \rangle n_e \cdot N + \langle v\sigma_2 \rangle n_e \cdot N + \dots$$

$$\beta = n_e (\langle v\sigma_1 \rangle + \langle v\sigma_2 \rangle + \dots)$$

$$\int \frac{dN}{N} = \int \beta dt \Rightarrow -\ln N = \beta t + C$$

$$N_{t=0} = 1 \Rightarrow C = 0$$

$$N = \exp(-\beta t)$$

$$P_{\text{change}} \sim \frac{\Delta N}{N} = \Delta N = 1 - \exp(-\beta \Delta t)$$

$$P < .?. > \xi \in [0,1]$$

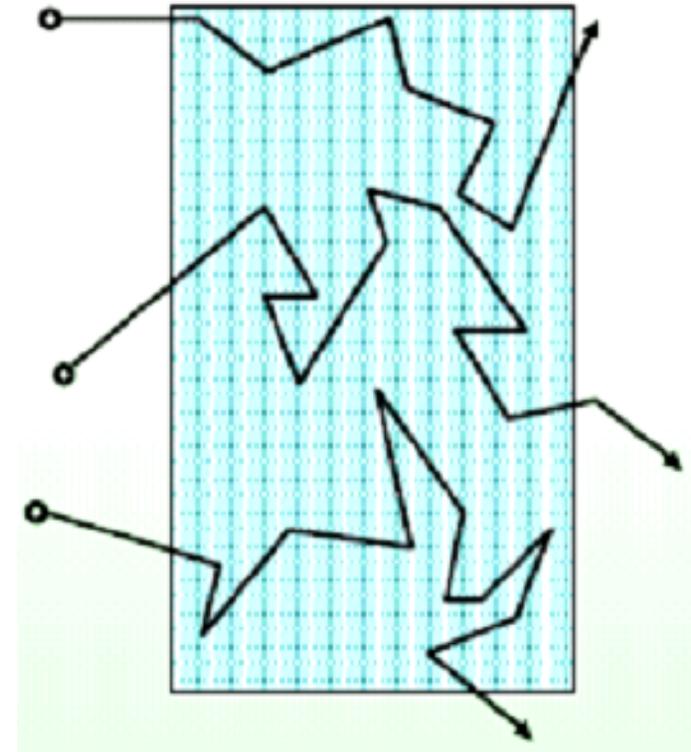
$$P_{\text{no change}} \sim \frac{\Delta N}{N} = \Delta N = \exp(-\beta \Delta t)$$

Monte-Carlo approach: decision is taken based on comparing of probability P with random generated value ξ .

More convenient in this case.

Decision concerning which of processes 1, 2, ... has occurred can be taken based on additional random value ξ_2 .

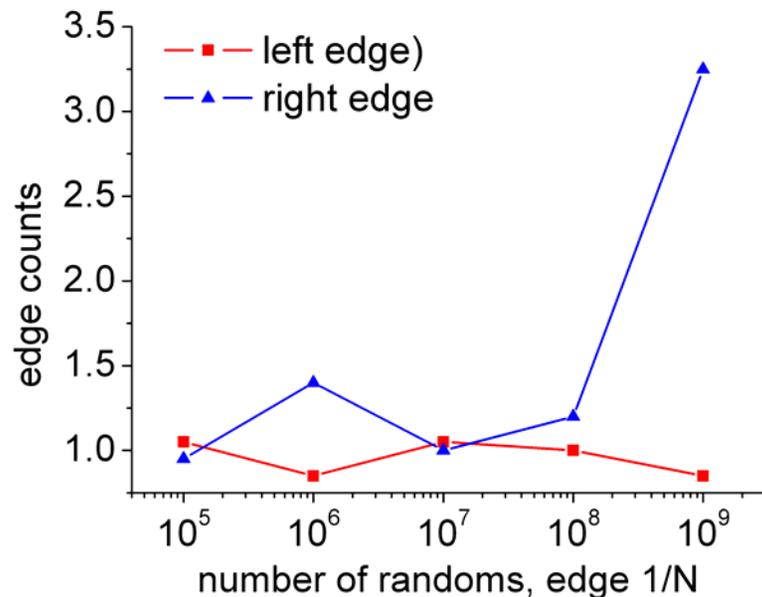
- Calculation error does not depend directly on the problem dimensionality
- Usually the mathematical expressions are relatively simple (free from additional integrations)
- Realisation of many physical processes like particle movement is very natural and straightforward. It is easy to control the reasonability of intermediate results.
- Easy to treat complicated 3D geometries.
- MC method is quite time consuming, however very suitable for parallelisation.



- 1) Generated numbers are fully independent!
 - No or at least very long period.
 - Generated numbers are equally distributed along $[0,1]$
- 2) Generator does not consume too much CPU time
- 3) It is possible to reproduce the generation exactly

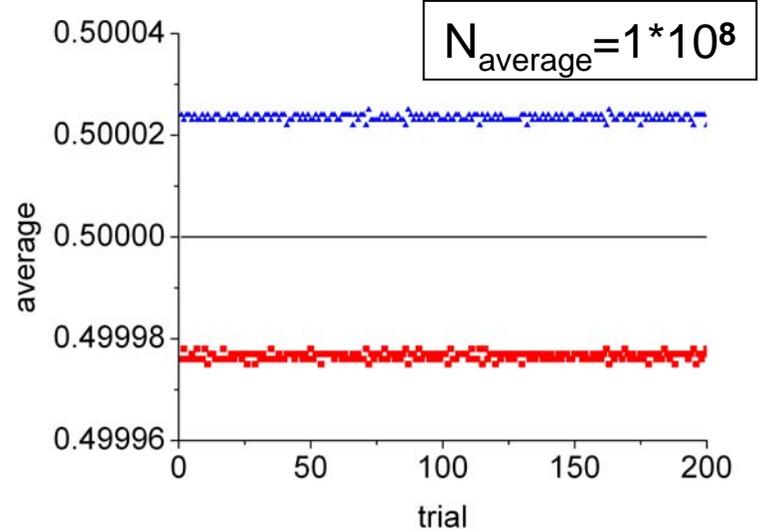
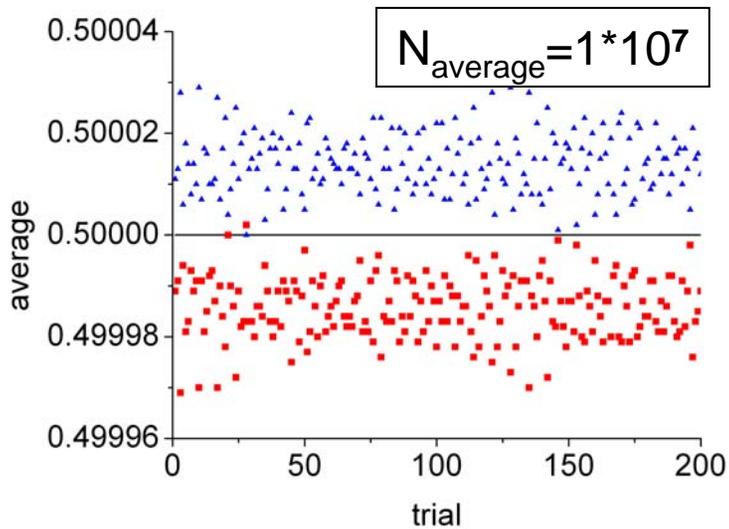
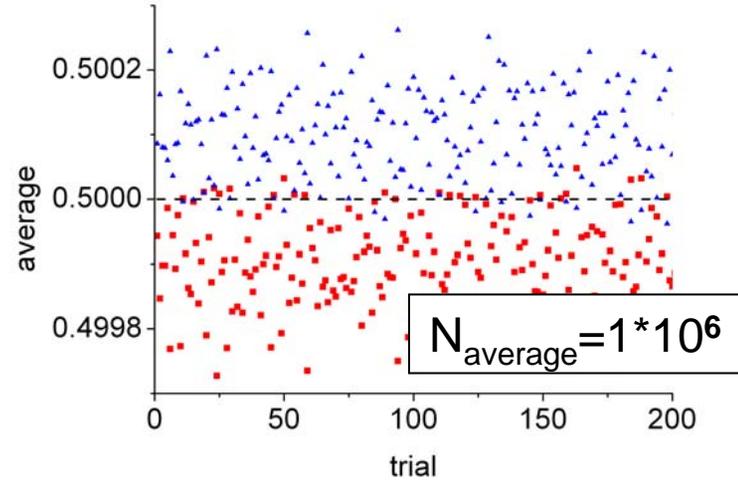
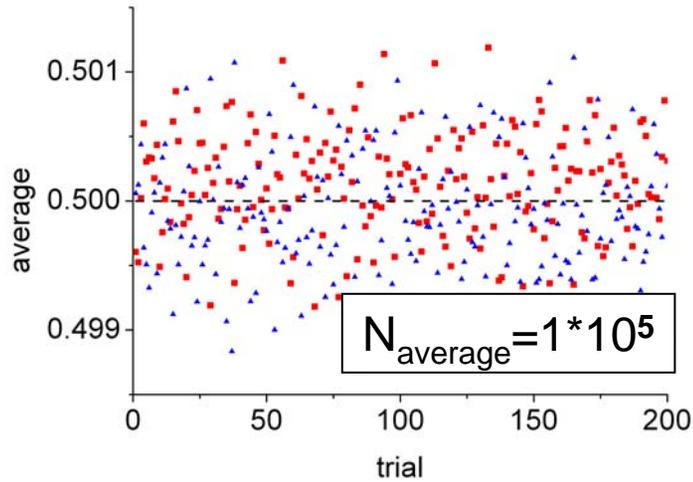
Example

For N uniformly distributed random numbers the average number of hits, $\langle n \rangle$, in the ranges $(0, \varepsilon)$ and $(1-\varepsilon, 1)$ should be equal to $\varepsilon \cdot N$. If we select $\varepsilon = 1/N$, then $\langle n \rangle = 1$.



A specific algorithm must be tested together with the random number generator being used regardless of the tests which the generator has passed . . .

“Not optimal” random generator – combination of 3 recurrent formulas from “Numerical recipes”. Average of **odd (blue)** and **even (red)** numbers.



Plasma simulations, EIRENE and ERO codes

1D core,
STRAHL, ETS

MACROSCOPIC

B2: a 2D multi species (D^+ , He^{++} , $C^{4+..6+}$, ...) plasma fluid code

Plasma flow
Parameters

CR codes:
(HYDKIN)

Source terms
(Particle,
Momentum,
Energy)

EIRENE: a Monte-Carlo neutral particle, trace ion (He^+ , C^+ , C^{++}) and radiation transport code.

see www.eirene.de

MICROSCOPIC

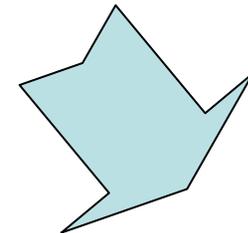
gyro-kinetic,
ERO, PIC

MACROSCOPIC

processed data (integrated, condensed, bundled, ...)

Data as unprocessed as possible

Suit well for **MC** approach



MICROSCOPIC

... , ERO, ...

EIRENE

EIRENE - A Monte Carlo linear transport solver

EIRENE

- Contact
- Manual
- A&M Data
- Surface Data
- Downloads
- Gallery
- Links
- Search
- FAQ

Albert Einstein

"Everything should be made as simple as possible, but not simpler."

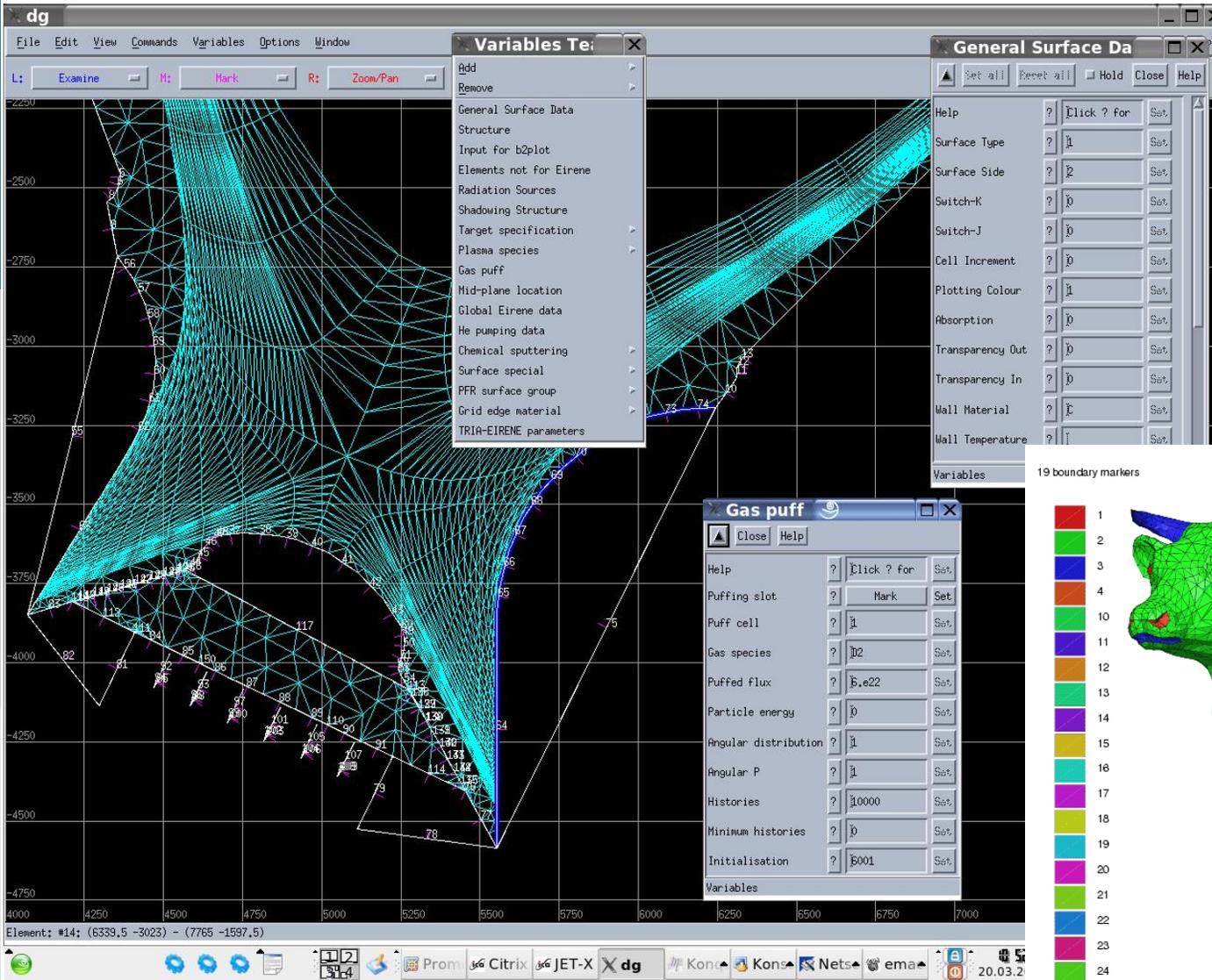


Shaw's Principle:

"Build a system that even a fool can use, and only a fool will want to use it."

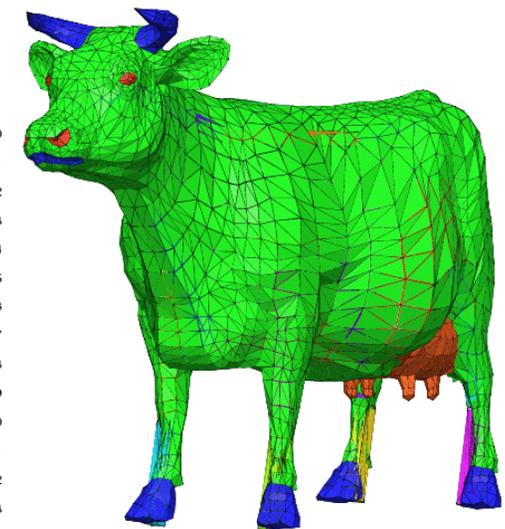
Simulations for **neutral particles!**

Global solution – coupling with B2 or similar codes (B2-EIRENE iterations)

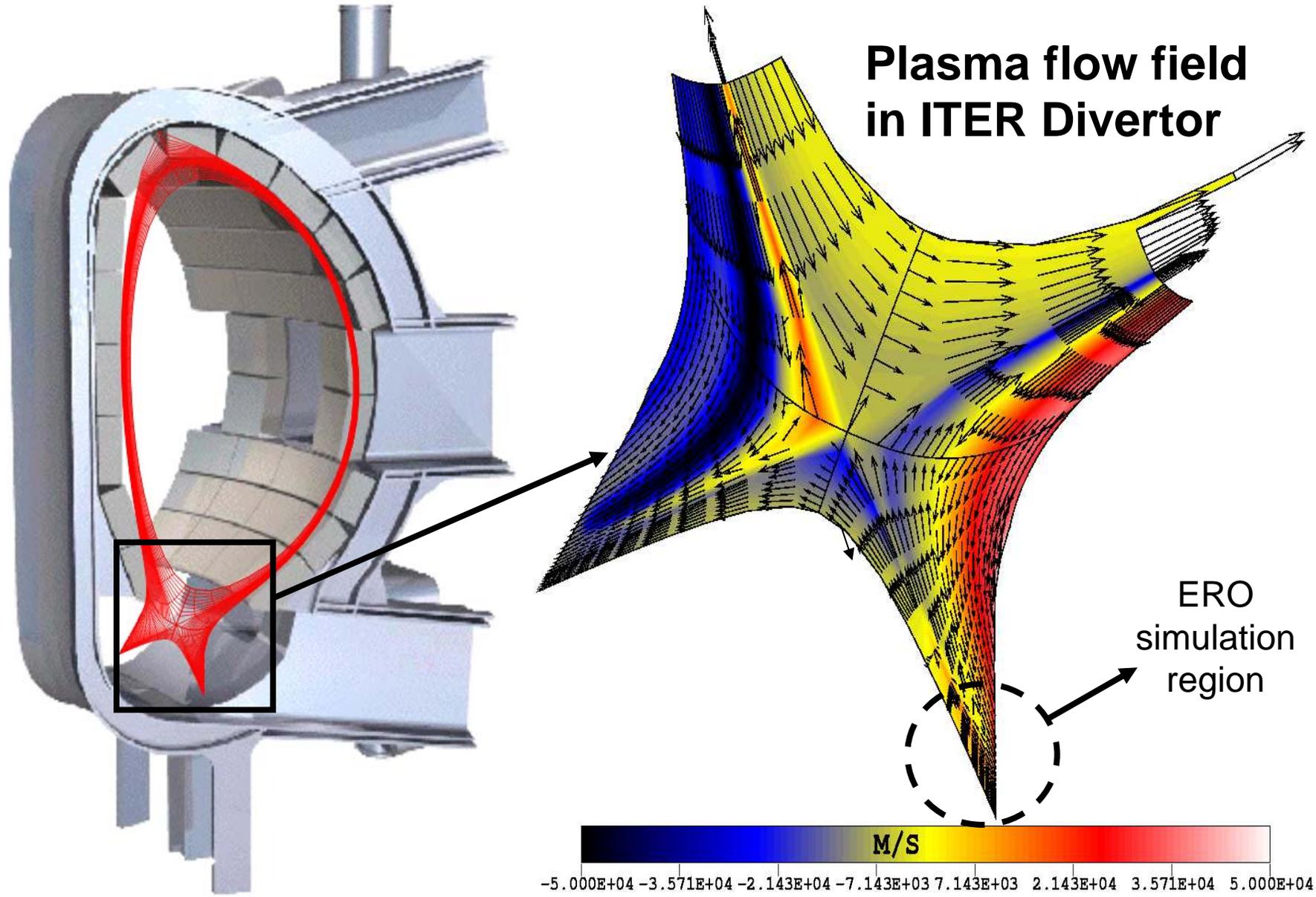


Tetrahedral Mesh
Generator and 3D
Delaunay Triangulator

19 boundary markers



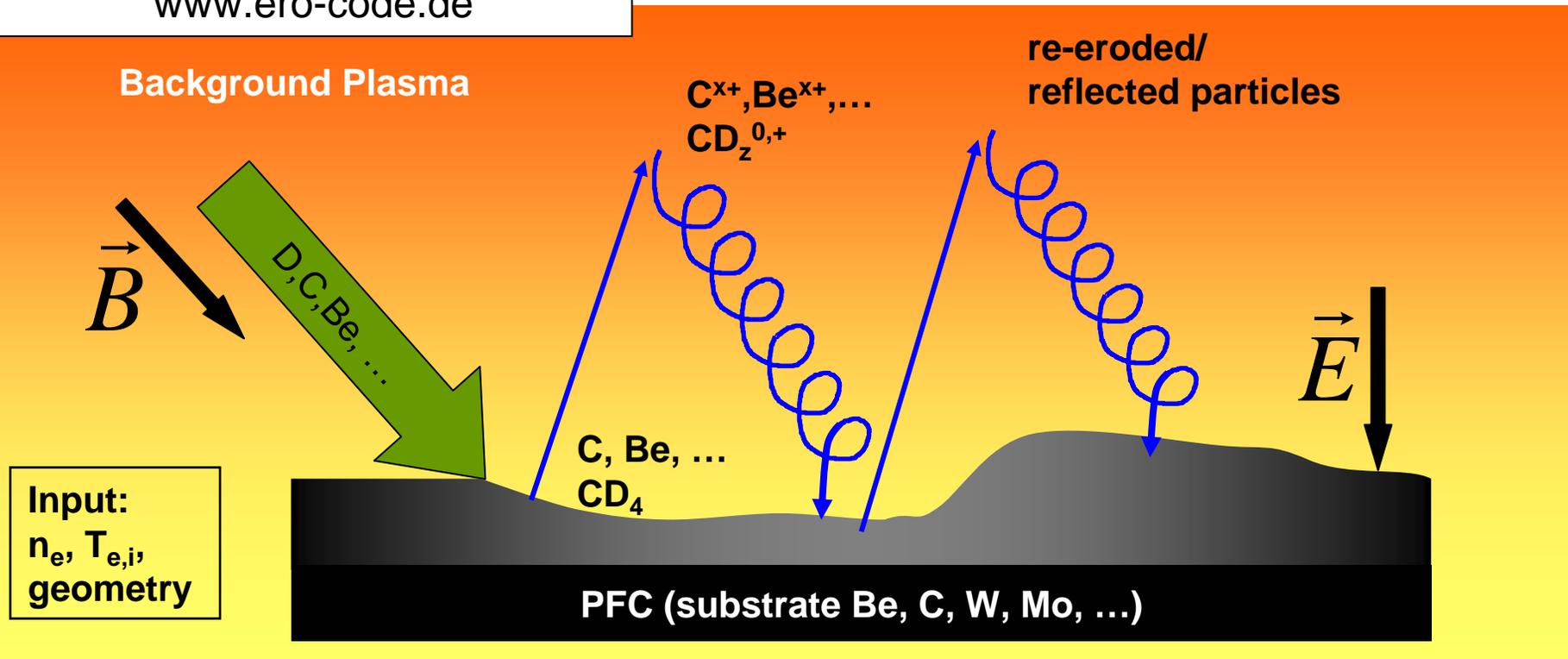
For ITER: 2D GUI, CAD – EIRENE available





ERO code

www.ero-code.de



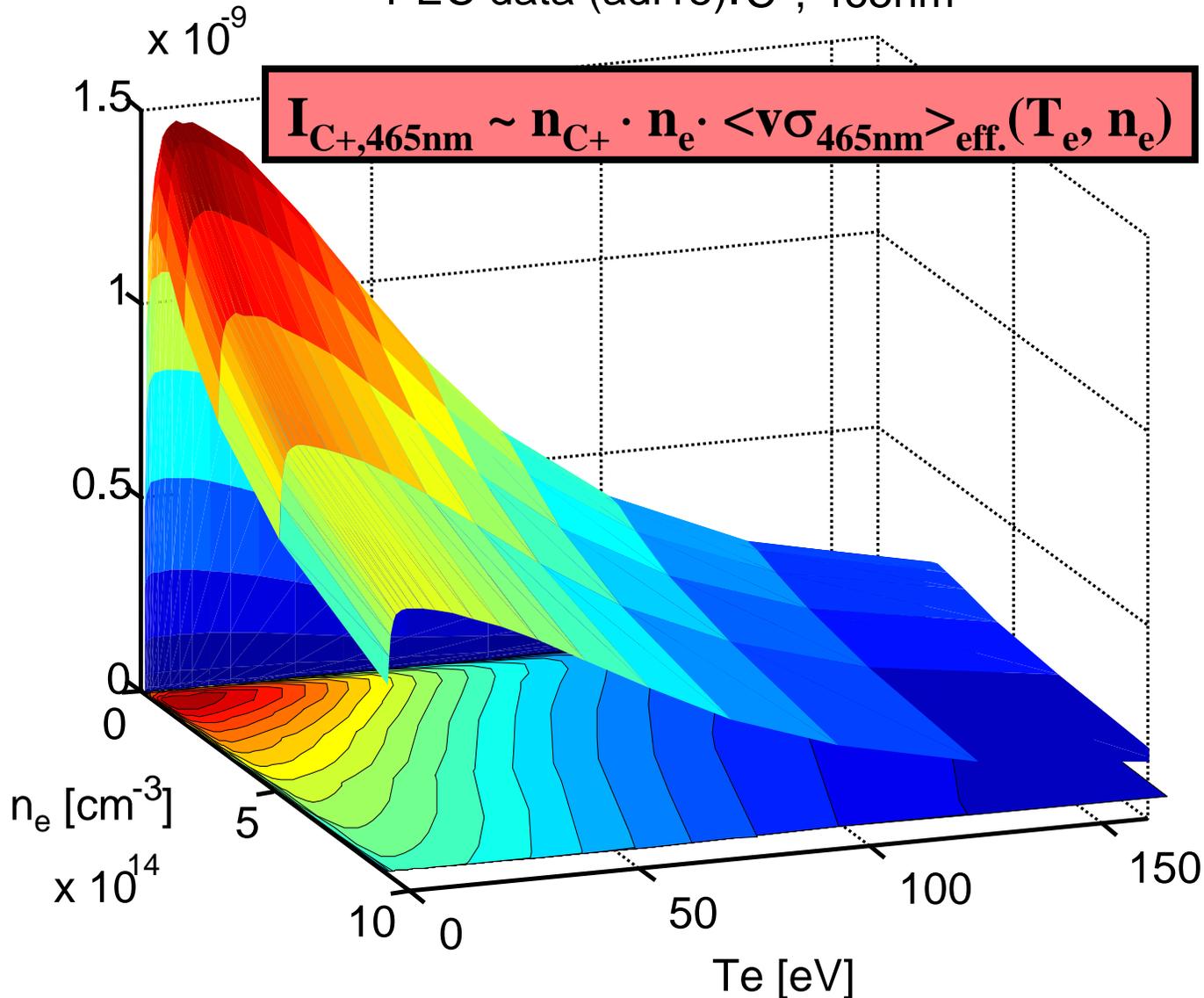
Local transport:

- ✓ ionisation, dissociation
- ✓ friction (Fokker-Planck), thermal force
- ✓ Lorentz force (including $E \times B$ component)
- ✓ cross-field diffusion

Plasma-surface interaction:

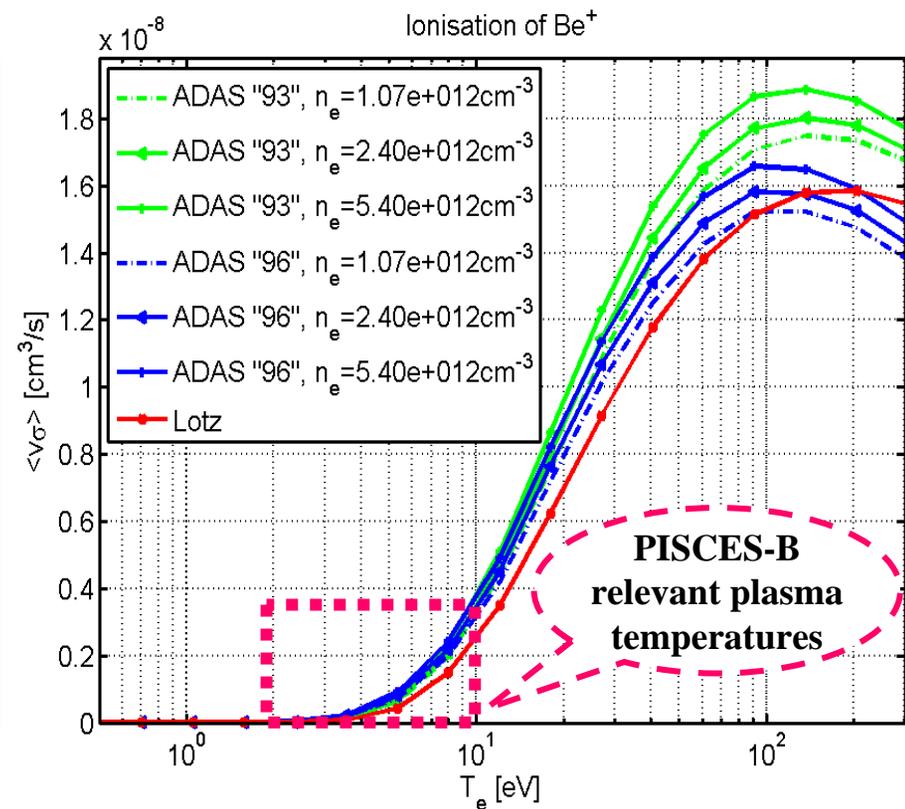
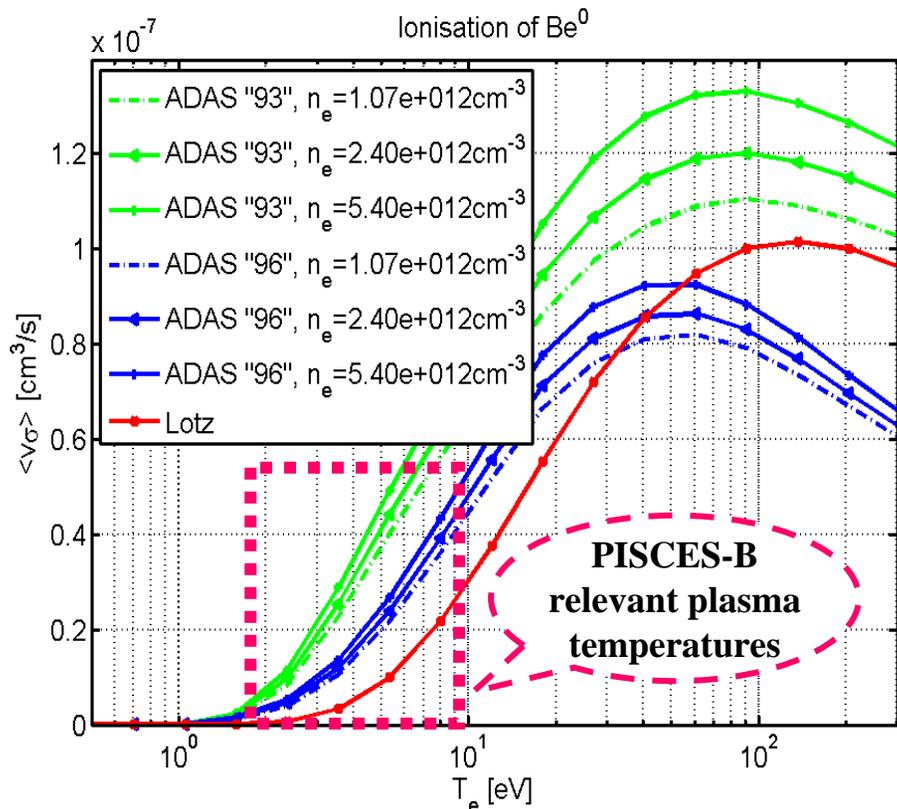
- ✓ physical sputtering/reflection
- ✓ chemical erosion (CD_4)
- ✓ (re-)erosion and (re-)deposition
- ✓ **NEW:** coupling with **TRIDYN**

PEC data (adf15).C+, 465nm



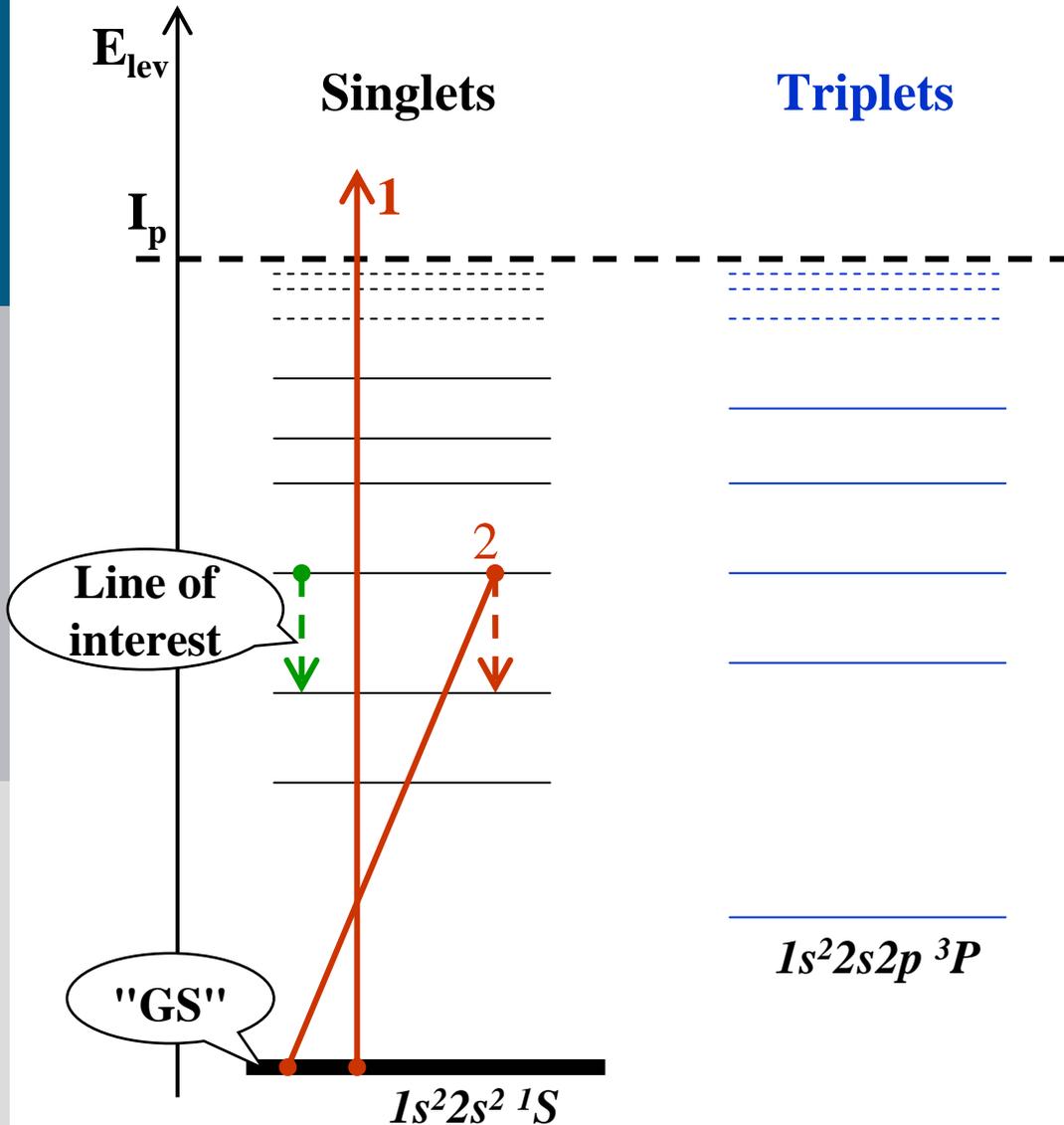
At first, ERO calculates the **3D density distribution** of respective species . . .

This **stationary** approach implies that both excitation and emission acts happen inside the volume cell at hand.



ERO database of **atomic data** is continuously updated according to the respective changes in the **ADAS**.

The **density dependence of effective rates** was shown to be of importance in a number of cases.

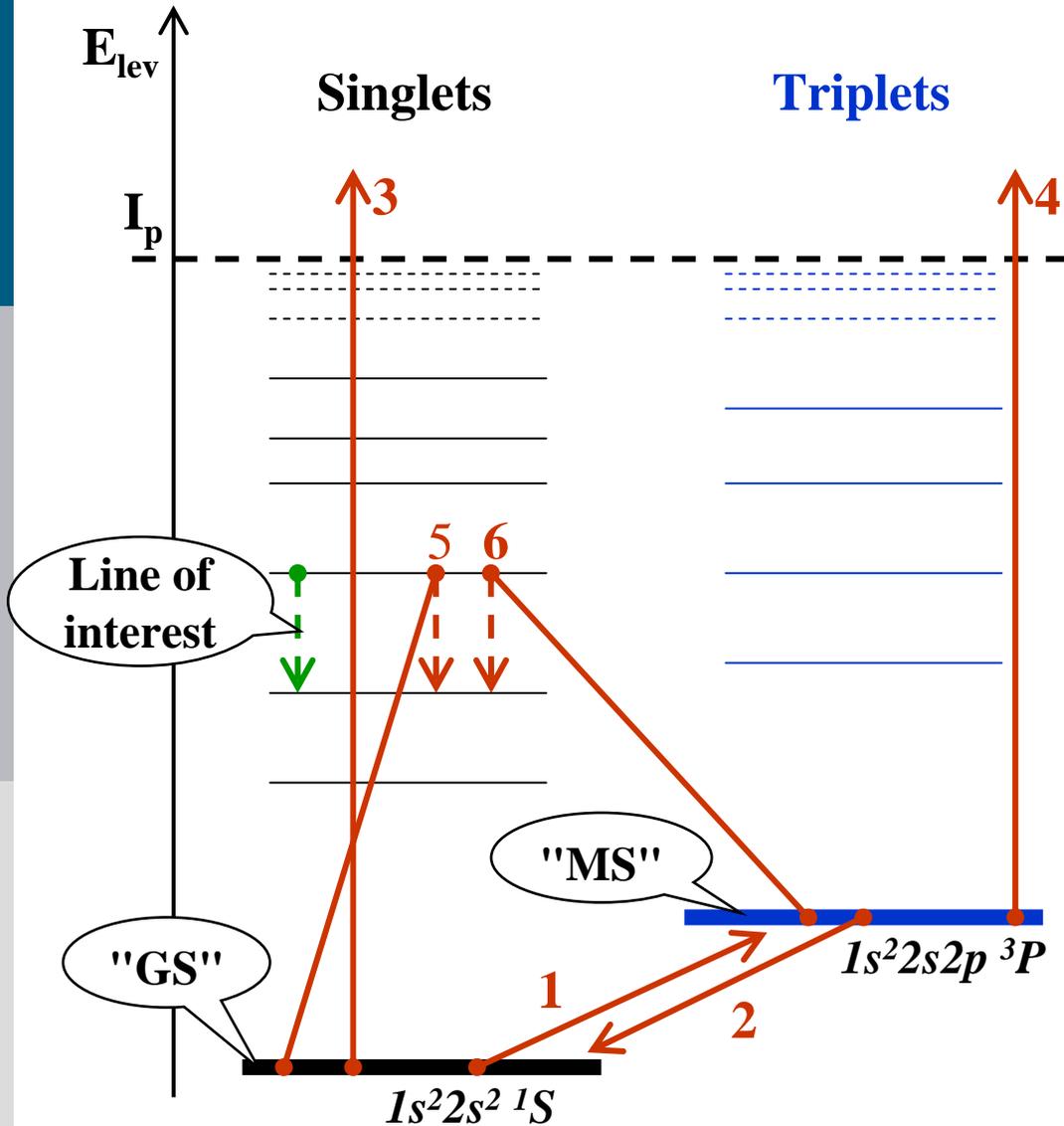


Effective rates:

- 1) $\langle I_z G \rangle$ - ionization from "GS"
- 2) $\langle I G \rangle$ - line intensity, assuming full population of "GS"

One effective PEC (photon efficiency coefficient) for each line + effective ionization

Effective rates represent all possible transitions including cascades, however not the 'slow' evolution of level populations.

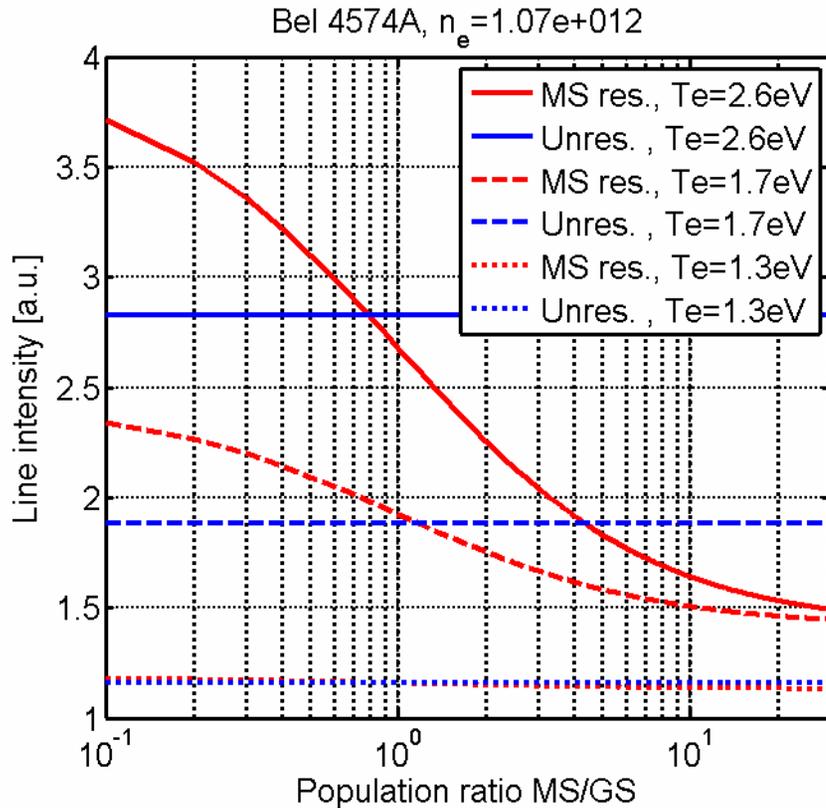


Effective rates:

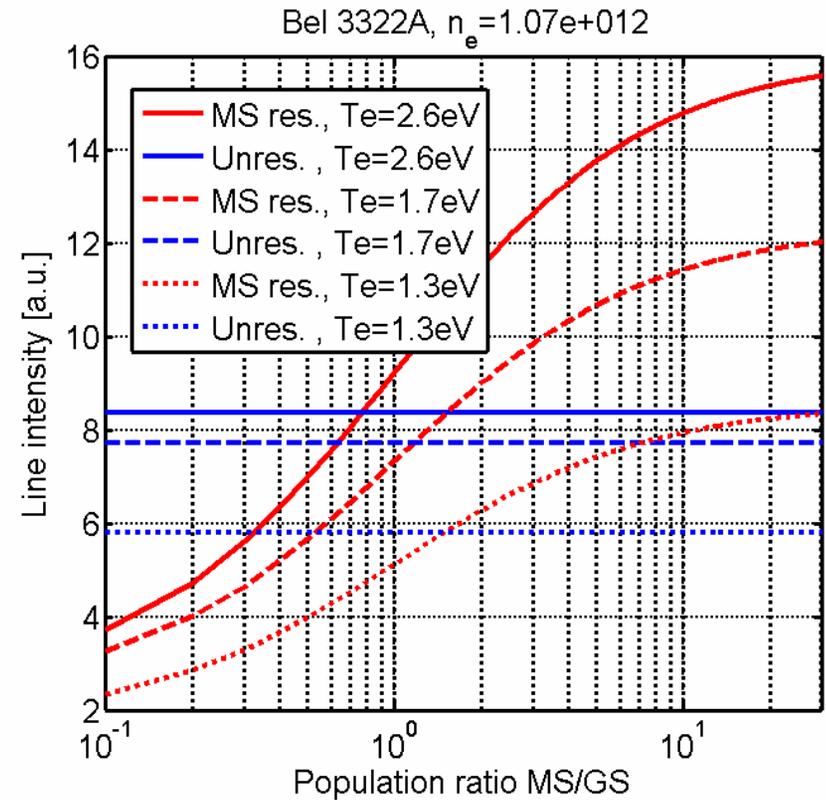
- 1) **<ExGM>** - excitation from "GS" to "MS"
- 2) **<ExMG>** - deexcitation from "MS" to "GS"
- 3) **<IzG>** - ionization from "GS"
- 4) **<IzM>** - ionization from "MS"
- 5) **<IG>** - line intensity, contribution from "GS"
- 6) **<IM>** - line intensity, contribution from "MS"

5, 6 are individual for every line of interest!

Singlet



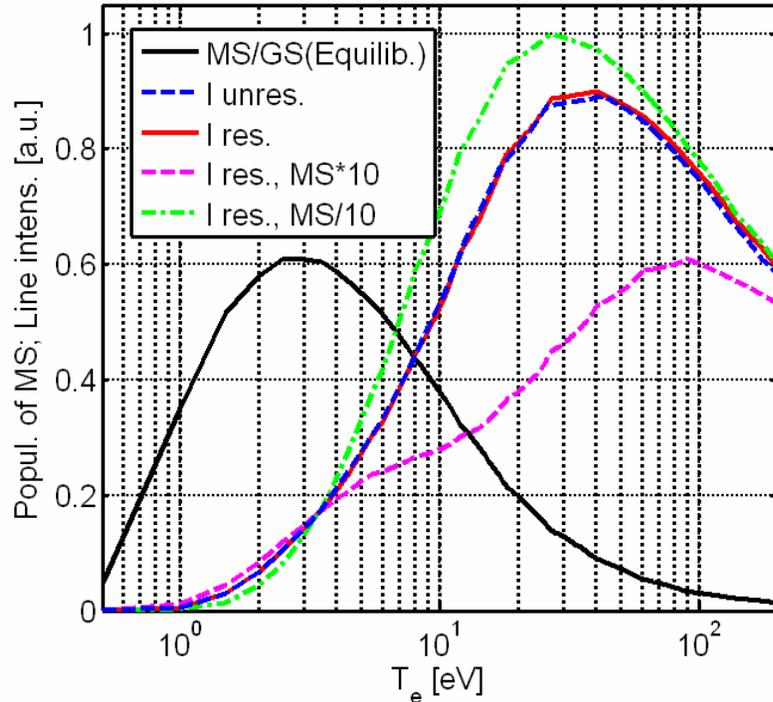
Triplet



$$I \sim N_{GS} \cdot \underbrace{\langle v\sigma \rangle_{GS}(n_e, T_e)}_{\text{Large for singlets}} \cdot n_e + N_{MS} \cdot \underbrace{\langle v\sigma \rangle_{MS}(n_e, T_e)}_{\text{Large for triplets}} \cdot n_e$$

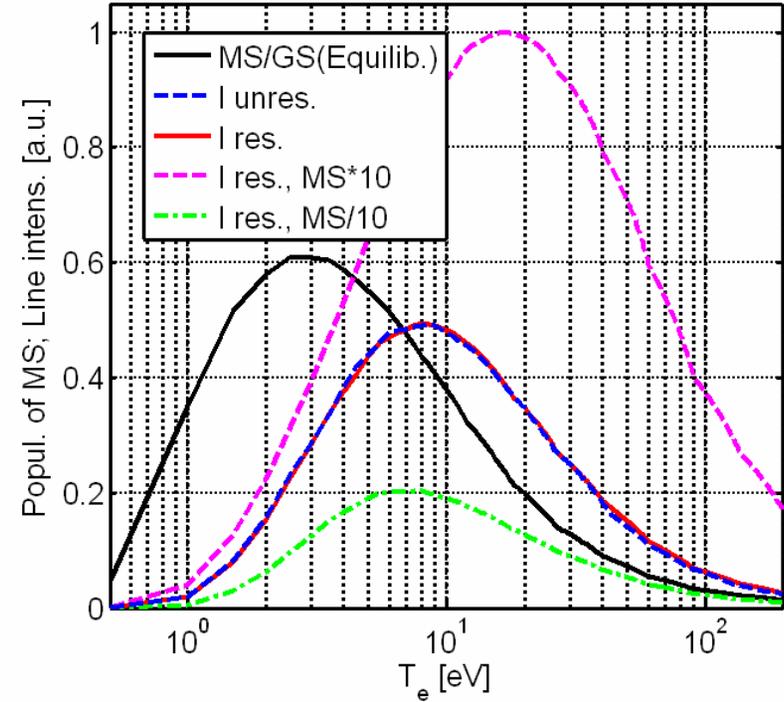
Singlet

ADAS, Bel 4574A, $n_e = 1.00e+012$



Triplet

ADAS, Bel 3322A, $n_e = 1.00e+012$



$$\left\{ \begin{array}{l} \underbrace{0}_{\text{stationary approach}} \equiv \frac{dN_{GS}}{dt} = -\langle ExGM \rangle N_{GS} - \langle IzG \rangle N_{GS} + \langle ExMG \rangle N_{MS} \\ \\ dN_{GS} + N_{MS} = 1 \end{array} \right. \Rightarrow \frac{N_{MS}}{N_{GS}} = \frac{\langle ExMG \rangle}{\langle ExGM \rangle + \langle IzG \rangle}$$

$$\begin{cases} \frac{dN_{GS}}{dt} = -\langle ExGM \rangle N_{GS} - \langle IzG \rangle N_{GS} + \langle ExMG \rangle N_{MS} \\ \frac{dN_{MS}}{dt} = -\langle ExMG \rangle N_{MS} - \langle IzM \rangle N_{MS} + \langle ExGM \rangle N_{GS} \end{cases}$$

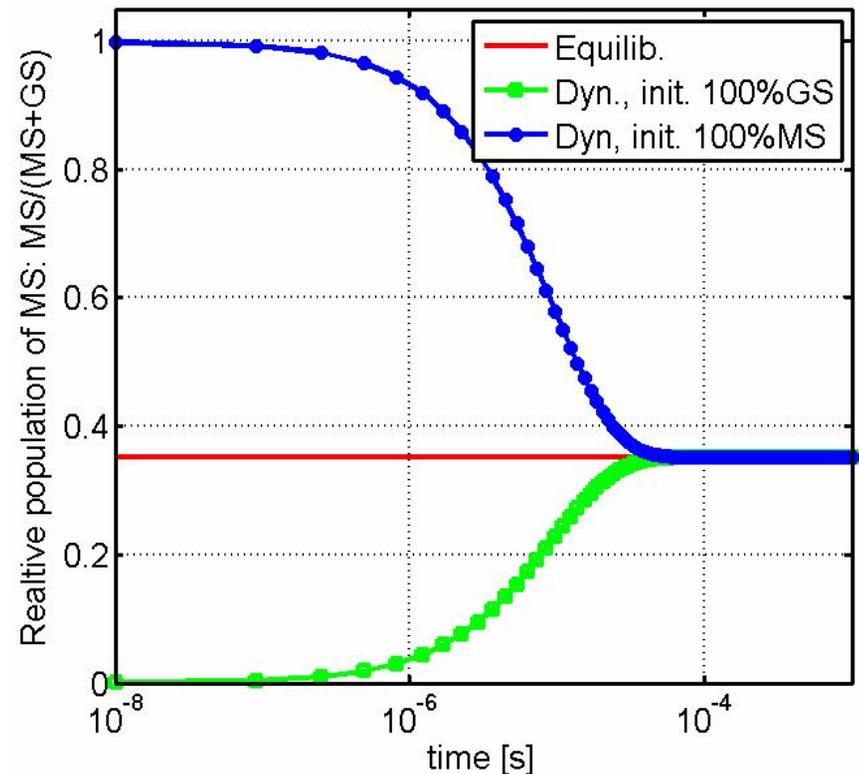
Analytical solution

($C_{1i}, C_{2i}, \lambda_p, \lambda_m$ determined by rates) :

$$dN_i(t) = C_{1i} \exp(-\lambda_p t) + C_{2i} \exp(-\lambda_m t)$$

**Relaxation time between MS and GS
is 10^{-5} - 10^{-4} s**

ADAS; $T_e=1\text{eV}, n_e=2 \cdot 10^{12}\text{cm}^{-3}$



Higher hydrocarbons

(chemical reaction chains and D/XB for CH)

Hydride Collision Databases for Technical Plasmas and Fusion Plasmas

Reviewed Database Series 2002-.....,
FZ-Jülich (R. Janev, D. Reiter),

www.eirene.de

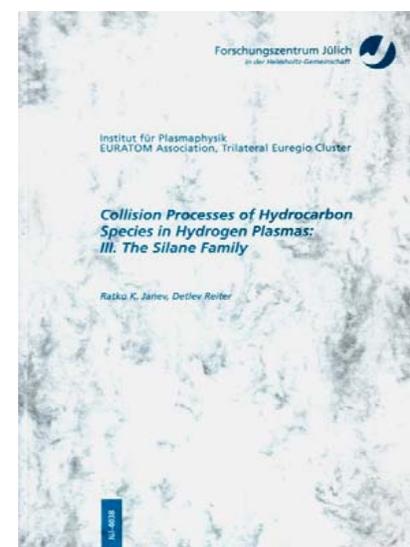
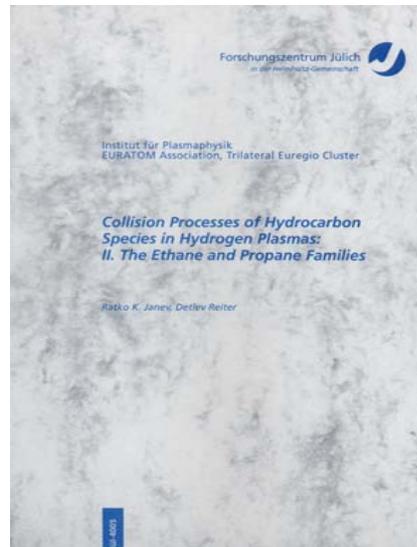
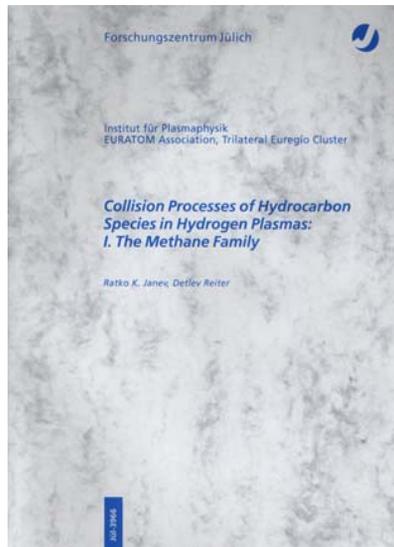
www.hydkin.de

Methane (CH_y)

C_2H_y C_3H_y

Silane (SiH_y)

$\text{p}, \text{H}, \text{H}^-, \text{H}_2, \text{H}_2^+, \text{H}_3^+$



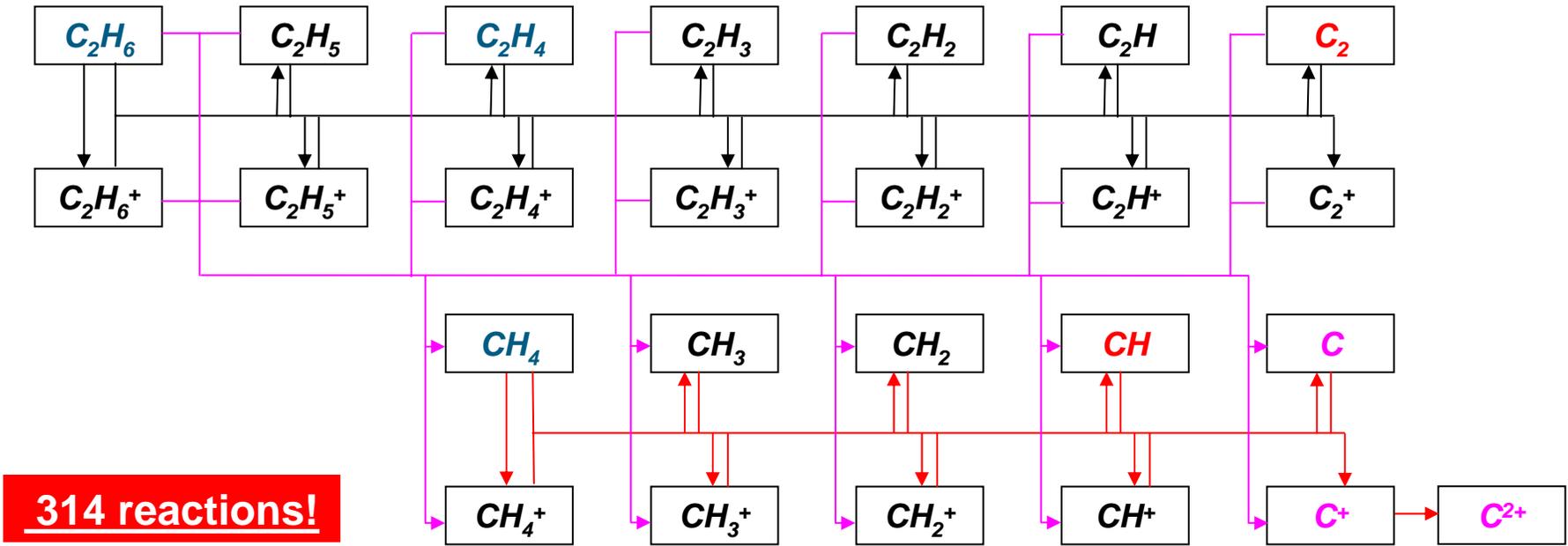
JUEL 3966, Feb 2002
Phys. Plasmas,
Vol 9, 9, (2002) 4071

JUEL 4005, Oct. 2002
Phys. Plasmas,
Vol 11,2, (2004) 780

JUEL 4038, Mar. 2003
Contr. Plas.Phys,
47, 7, (2003) 401-417

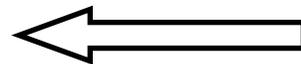
JUEL 4105, Dec. 2003
Encycl. Low. Temp.
PI. 2007 (in russian)

Reaction chains of hydrocarbon molecules (Janev / Reiter)



Emission data

CII, CIII



ADAS

CH A-X, C₂ d-a



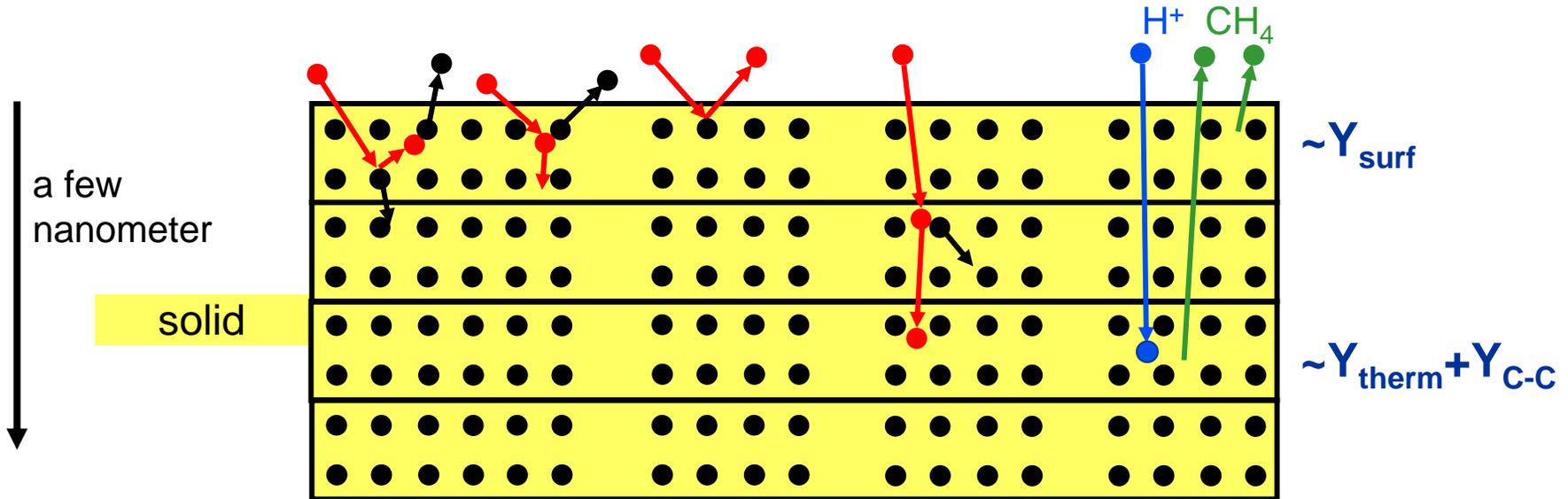
U. Fantz et al. 2005

Probably this is not enough ...

Surface data, PSI part of ERO

Monte-Carlo method: TRIM code (Eckstein et al.)

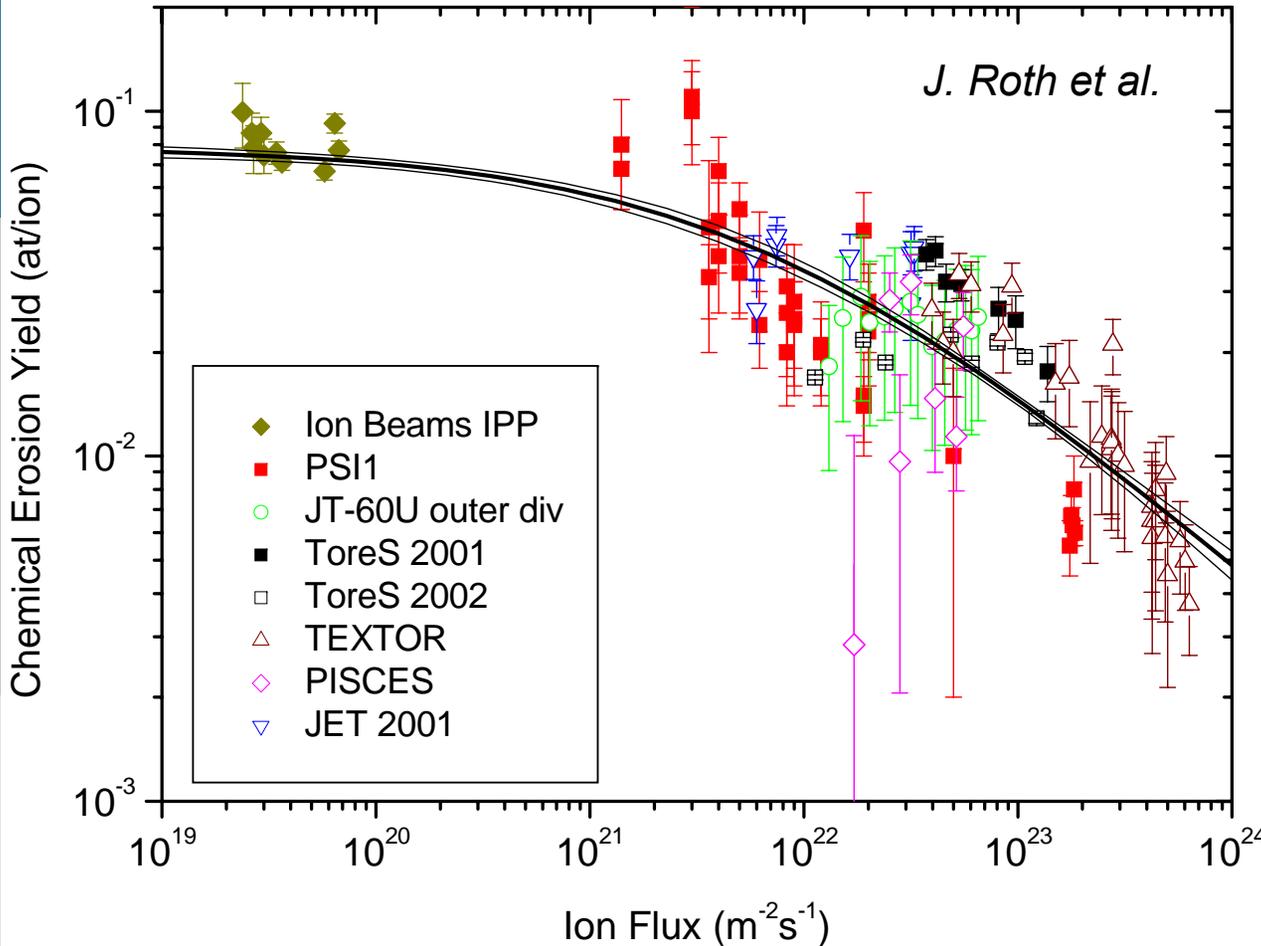
Sputtering Reflection Deposition Chemical Erosion



TRIM : TRansport of Ions in Matter (TriDyn, SDTrimSP)

- using random numbers (e.g. to decide whether collision or not): “Monte-Carlo”
- **binary collisions** between impinging ion and target atoms
(elastic, screened Coulomb-potential) \Rightarrow collision cascades
- inelastic electronic energy loss
- **output: reflection coefficients/ physical erosion yields / concentration-depth profiles / layer growth**

Chemical sputtering yield in dependence on impinging flux



Chemical sputtering decreases with increasing flux

Chemical sputtering depends on surface temperature, contance, morphology, . . .

Flux dependence is predicted by model of thermal reaction cycle.

Elastic collisions

Elastic neutral collisions (ENC):

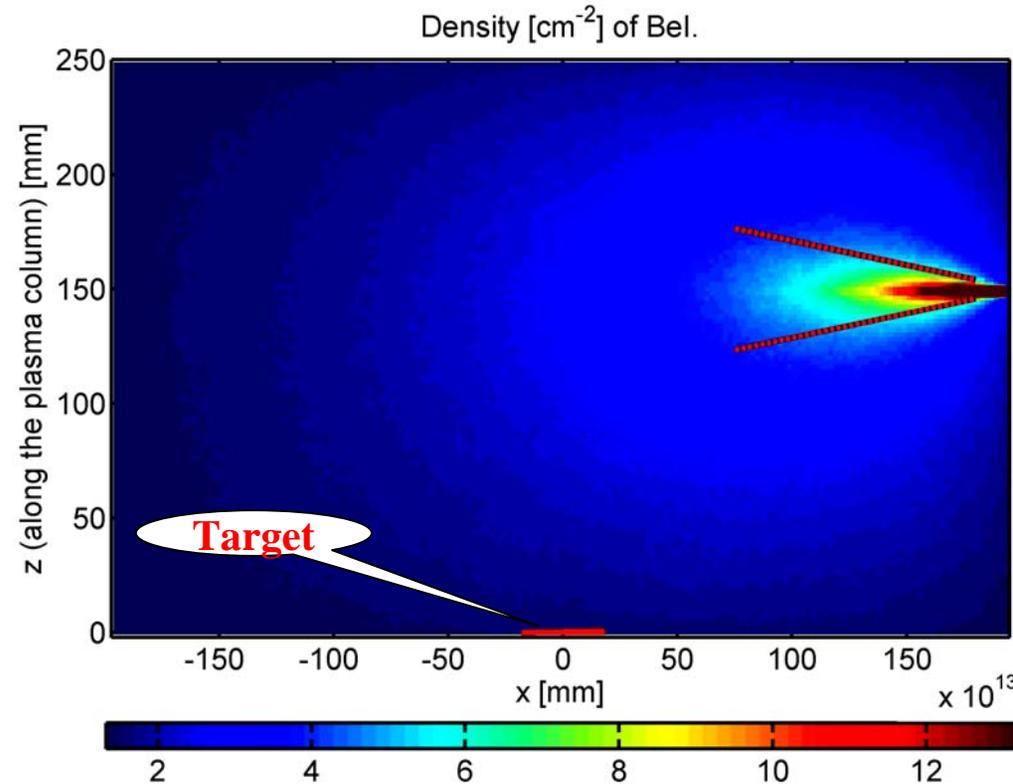
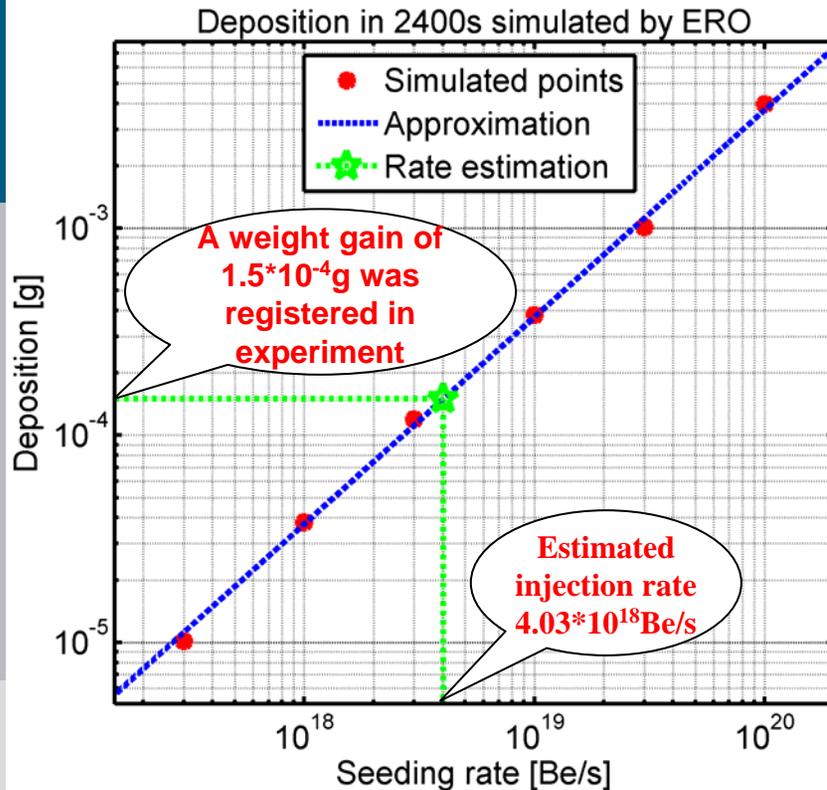
- MC formulation : during time step dt the tracked particle experiences an elastic collision according to a random number ξ , $\xi \in [0,1]$:

$$\xi > \exp(-\langle\sigma v\rangle * n_{ntrl} * dt)$$

- The rates $\langle\sigma v\rangle$ are calculated using the routines by A.Pigarov
- The direction of particles is assumed to be opposite to each other and arbitrary in the center of mass system
- For linear devices $n_{ntrl} = n(D_2)$ is often assumed to be uniform in the volume

- 1) In case of injection simulations ENC lead to broadening of the beam
- 2) ENC lead to an increase of hydrocarbon re-deposition
- 3) For neutral density B2-EIRENE calculations are necessary . . .

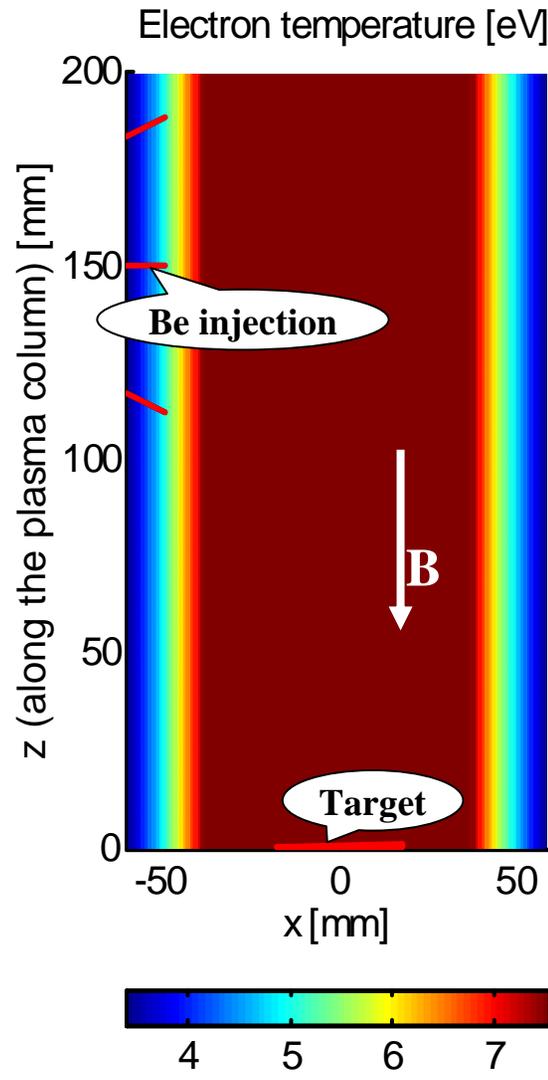
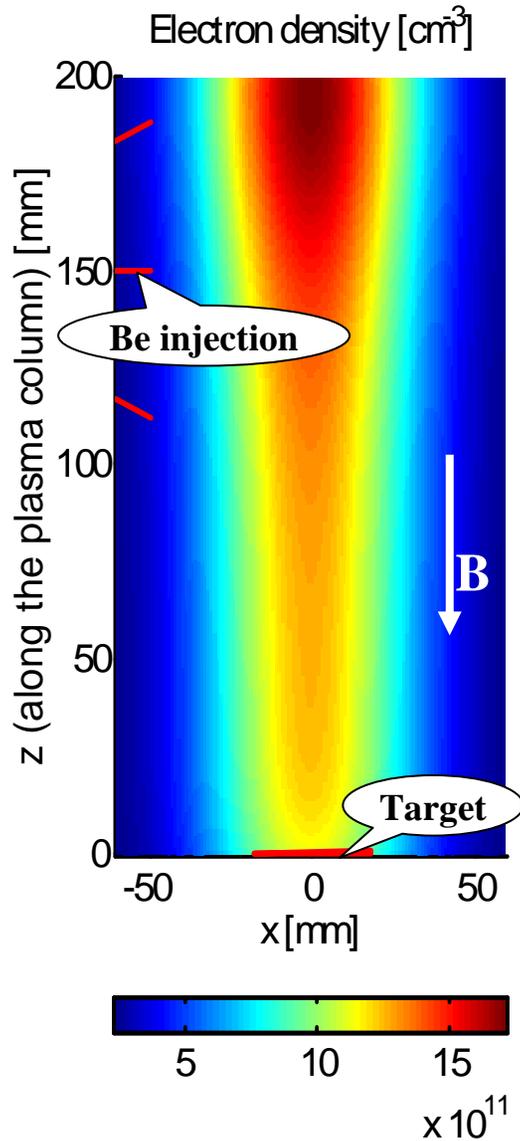
Be injection w/o plasma . . .



2g of Be is spent in more than 10 hours of oven operation.
 This gives a rate of about - $3.7 \cdot 10^{18}$ Be/s.

W/o elastic collision with neutrals there would be no Be at target!

Examples of ERO application



- Plasma column width is about **5cm**
- Vessel radius is about **20cm** filled with neutral gas
- Be comes into the volume from injection or (and) as a result of Be target erosion

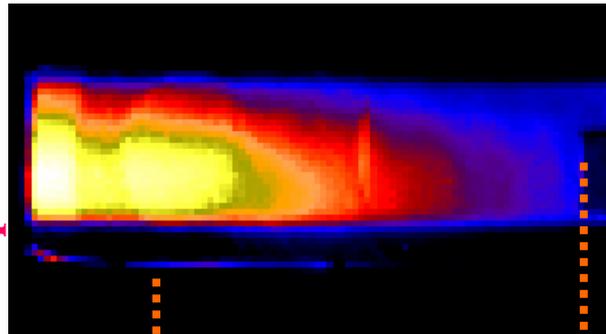
Be, Bell emission is registered:

by 2D camera

"Low density case"
 $(1.2 \cdot 10^{12} \text{cm}^{-3}, T_e = 10.5 \text{eV})$

by spectrometer with a spatial resolution
 (the radial profile position and direction
 can be varied)

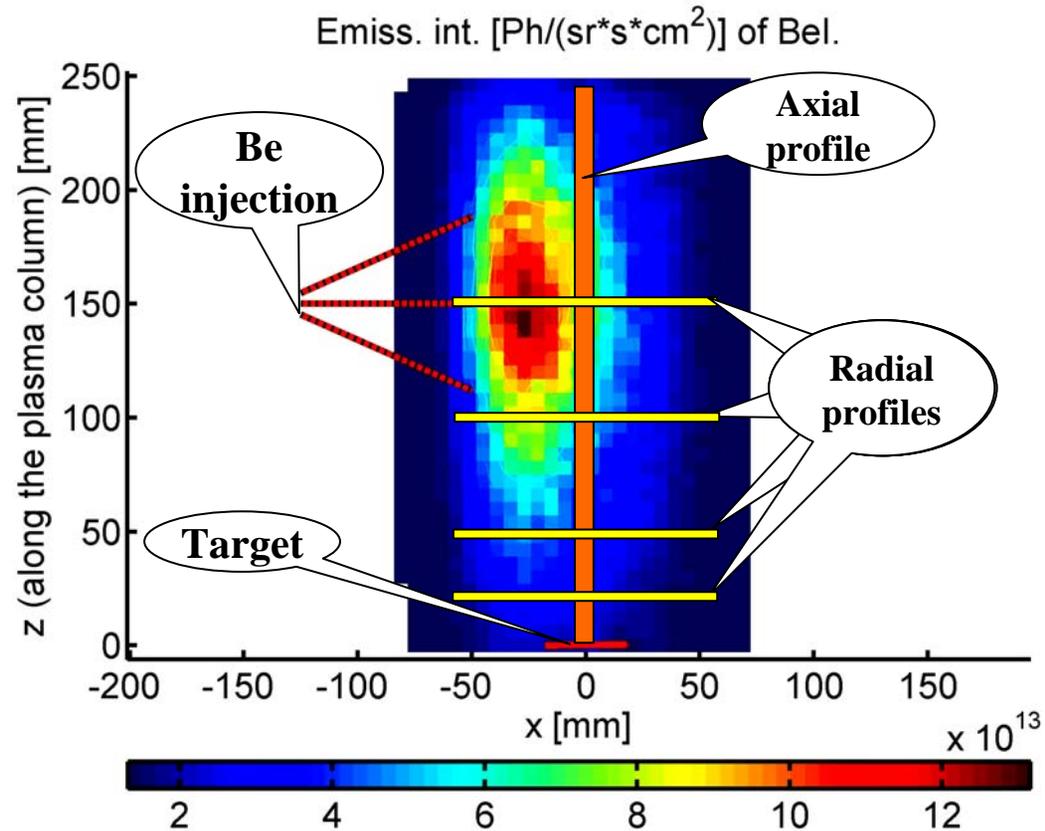
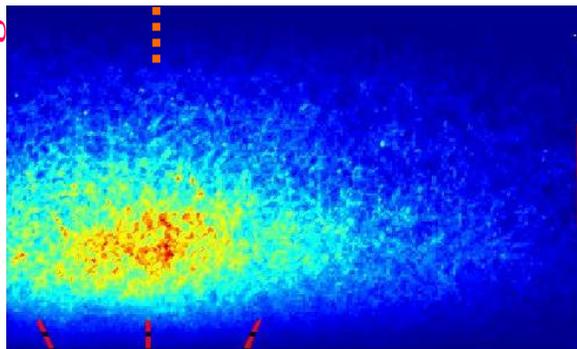
Experiment

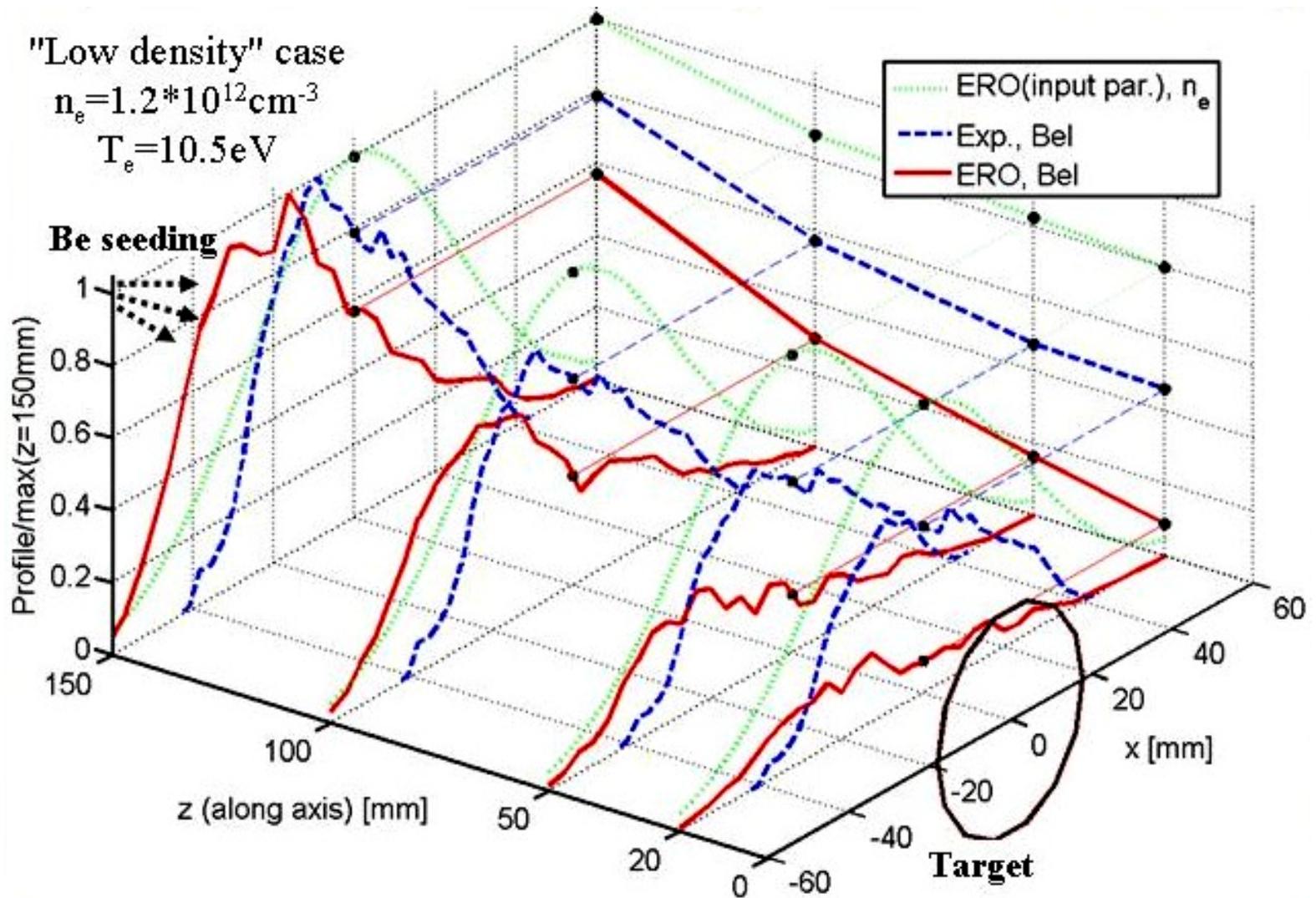


Be injection

Target

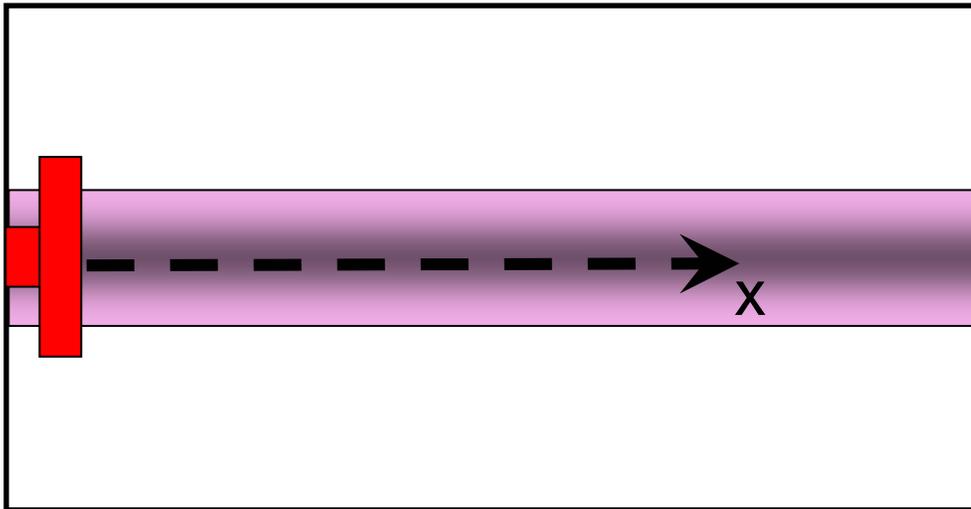
ERO modelling



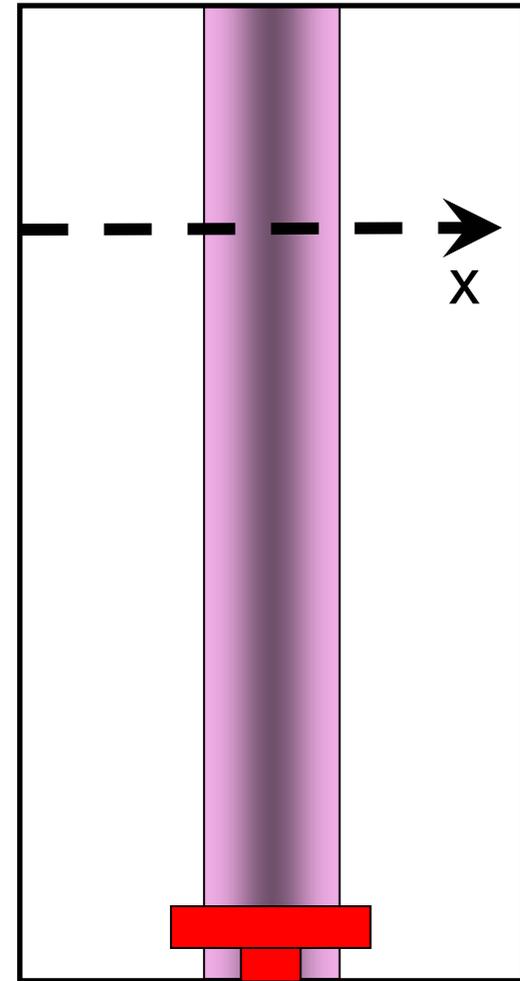


The ERO modelling is in a good agreement with experiment (PSI-2008)

Be sputtering from target



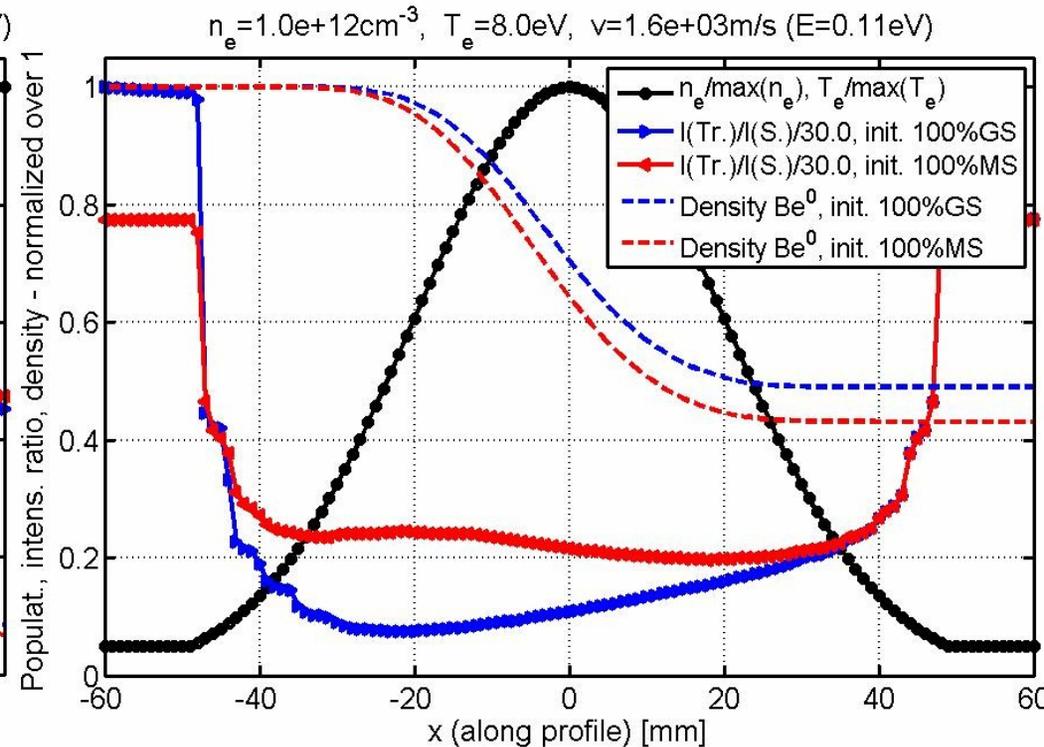
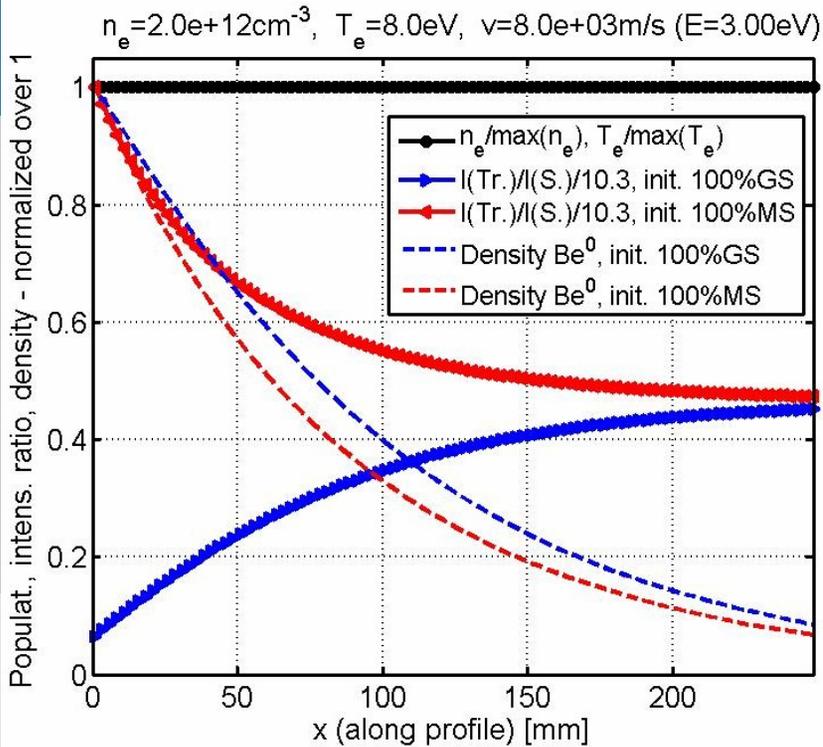
Be injection cross plasma



A narrow monoenergetic beam of Be^0 , coming through plasma.

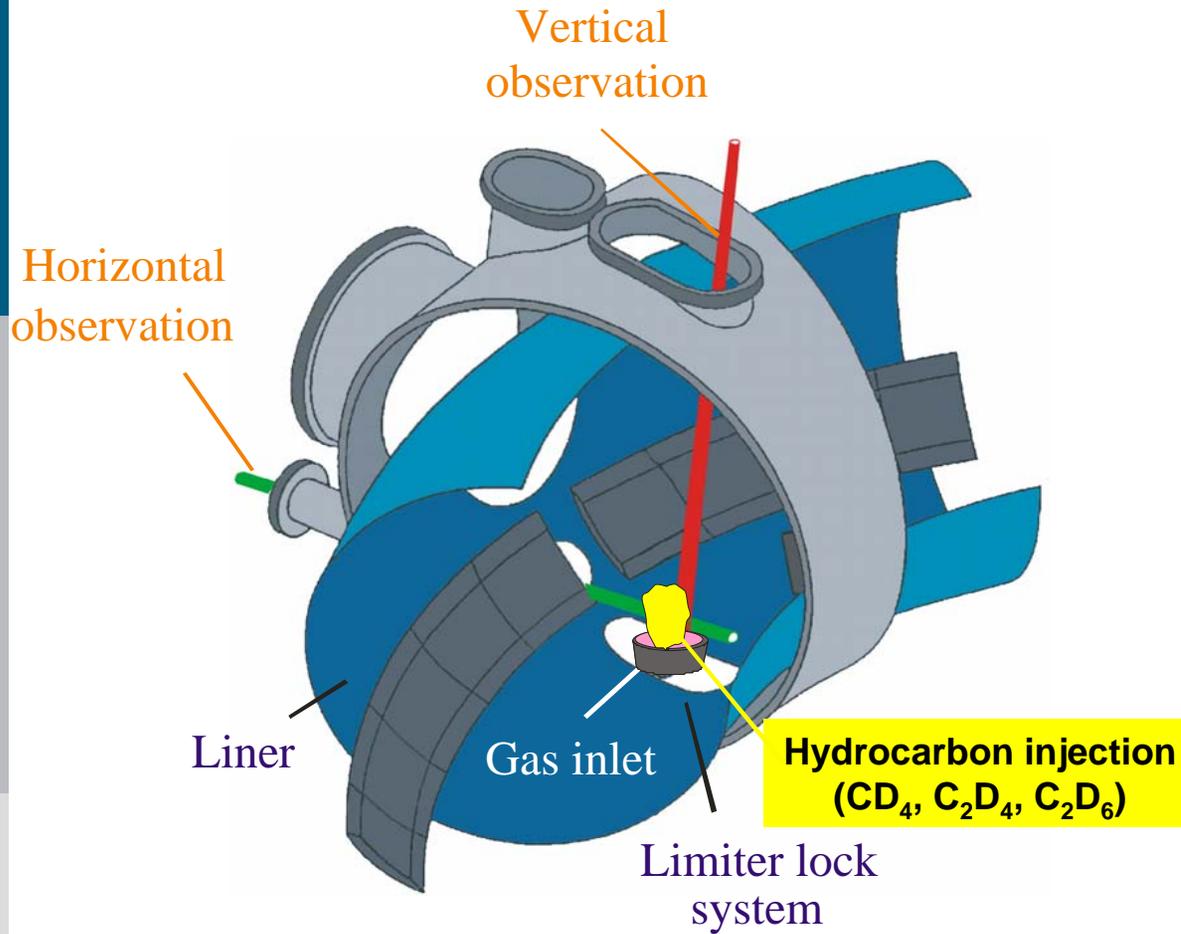
Relevant for sputtering from Be target . . .

Relevant for seeding from Be oven . . .



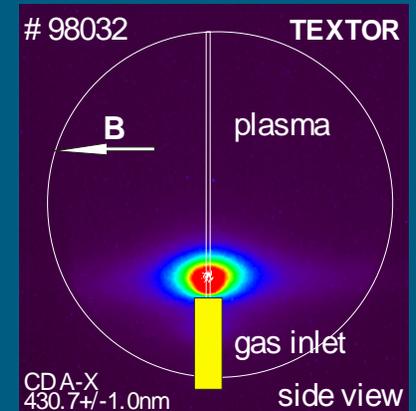
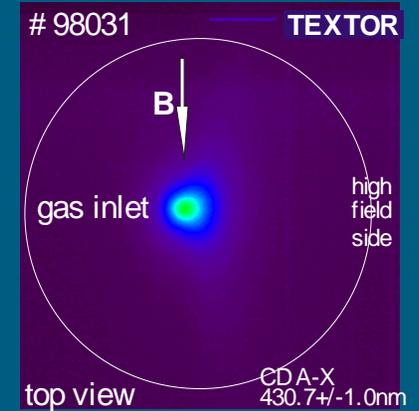
Initial MS population and plasma parameters gradient strongly affect:

- 1) Triplet/singlet line intensity ratio (4573Å and 3322Å)**
- 2) Be^0 density (MS population affects ionization)**

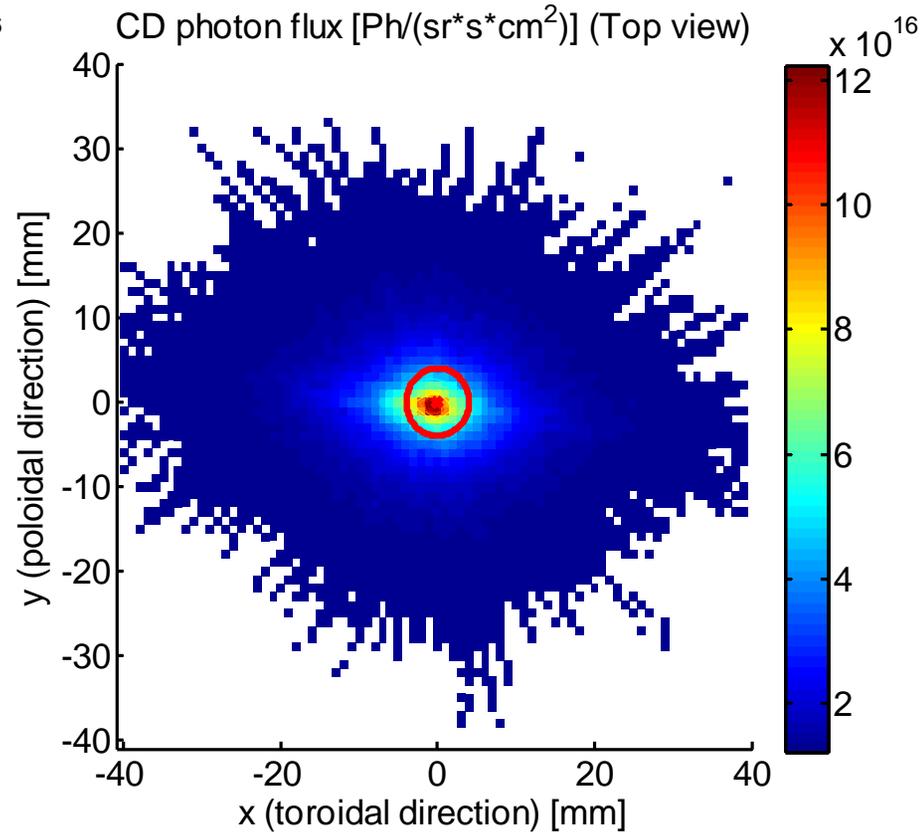
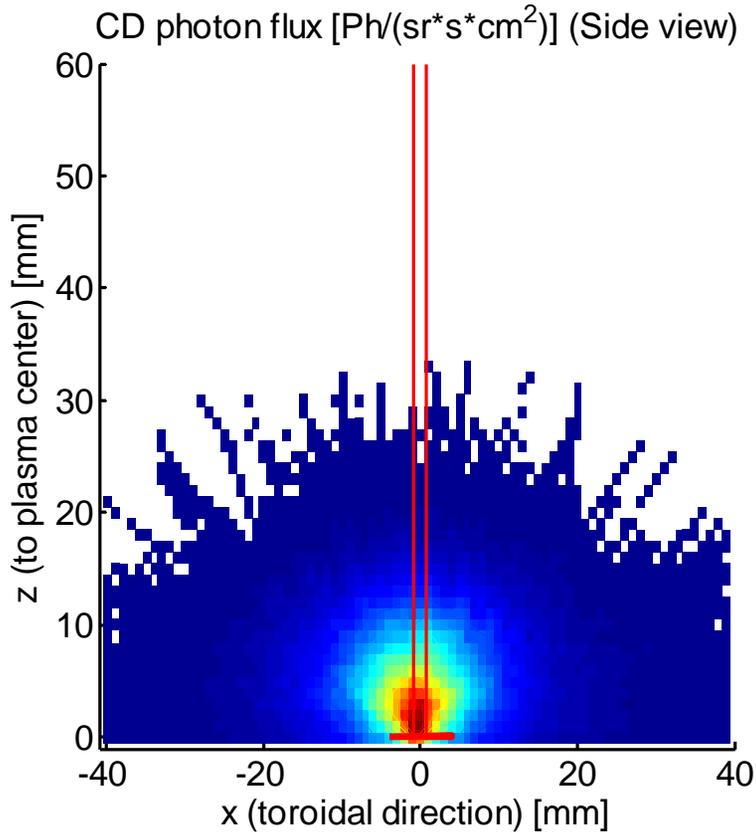


$$\left[\frac{D}{XB} \right]_{A-X}^{CD_4 \rightarrow CD} = \frac{\Gamma_{CD_4}}{\phi_{A-X}^{CD}}$$

CD light emission (CD₄ injection)

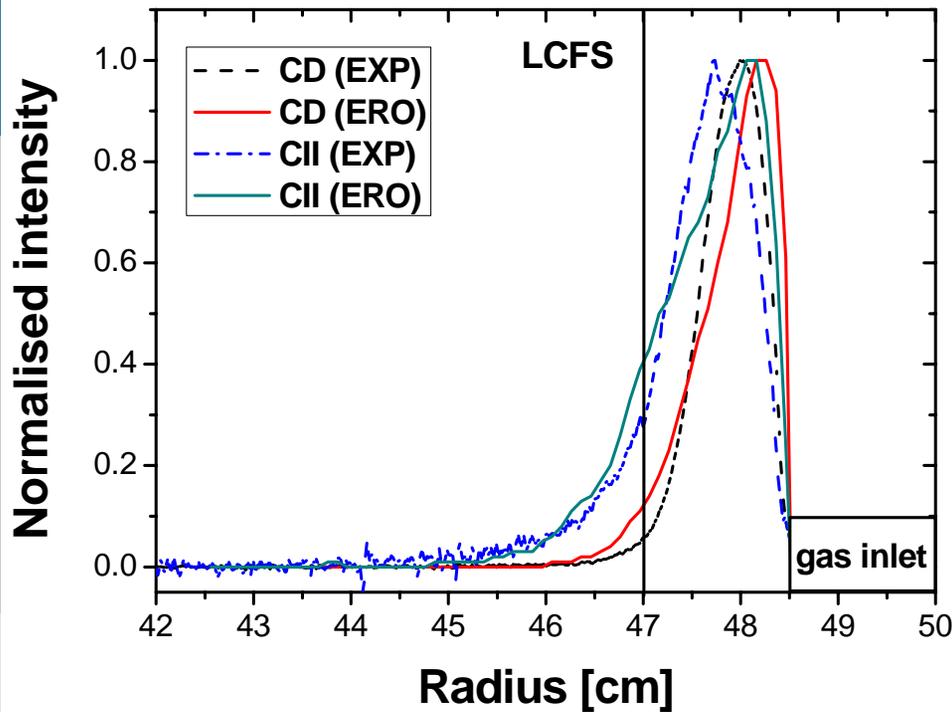


Modelled 2D light emission of CD A-X band from CD₄ injection at TEXTOR

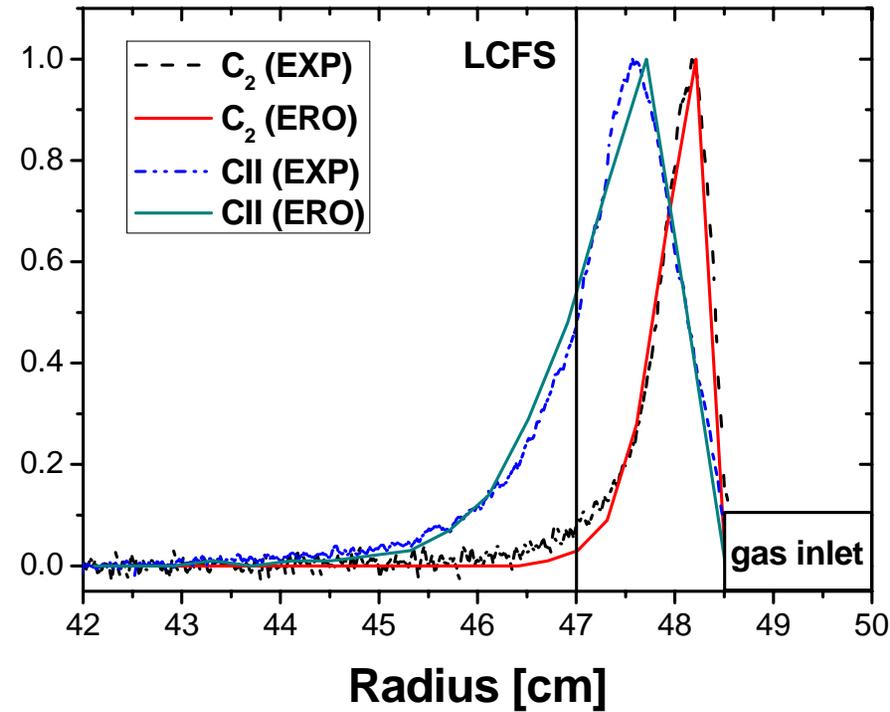


LCFS at 15 mm above inlet tip
 T_e (LCFS) = 55 eV

Modelling vs. experiment: radial profiles of CD, C₂ and CII emission



CD₄ injection



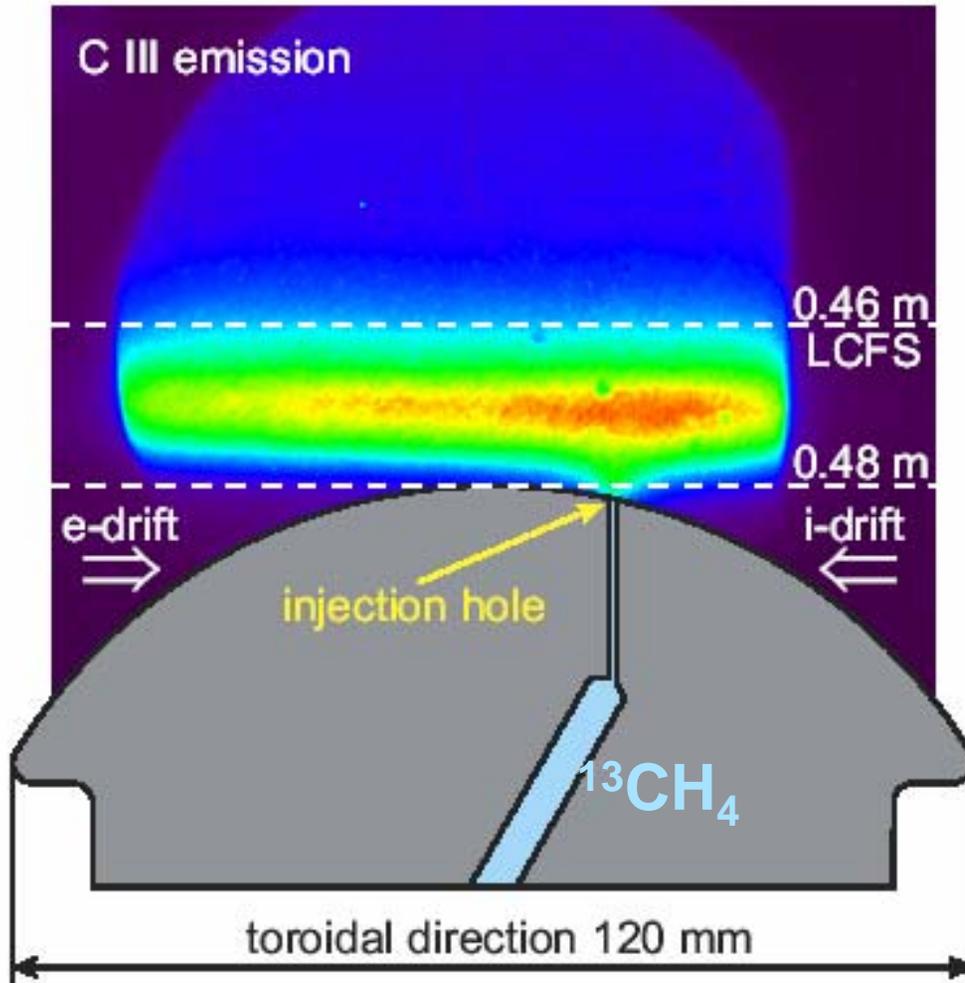
C₂D₄ injection

Good agreement between modelled and observed penetration depths

Comparison of effective D/XB values for CD A-X and C₂ d-a

Injected species	D/XB (CD A-X band)		D/XB (C ₂ d-a band)	
	Experiment	ERO	Experiment	ERO
CD ₄	36	65	930	-
C ₂ D ₄	31	80	48	45
C ₂ D ₆	27	76	65	62

$^{13}\text{CH}_4$ injection experiments: deposition and erosion of carbon layers



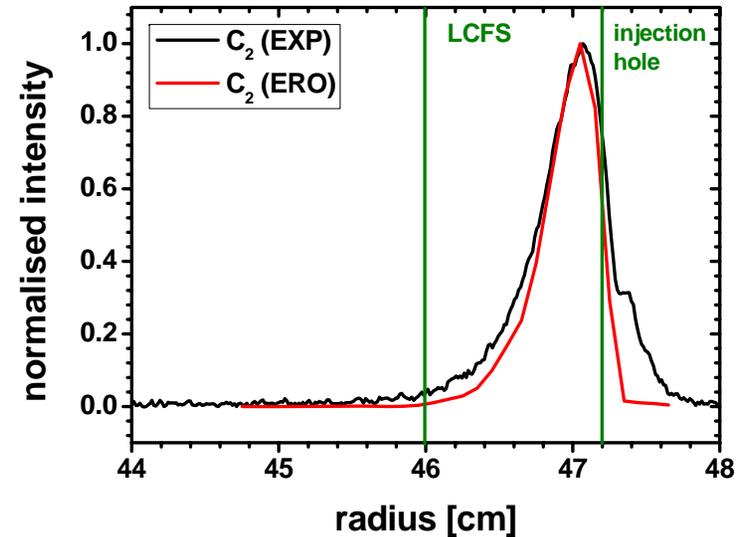
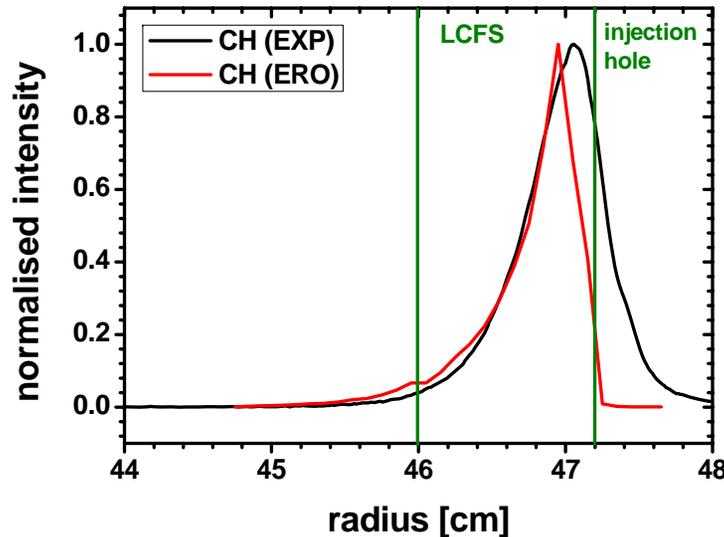
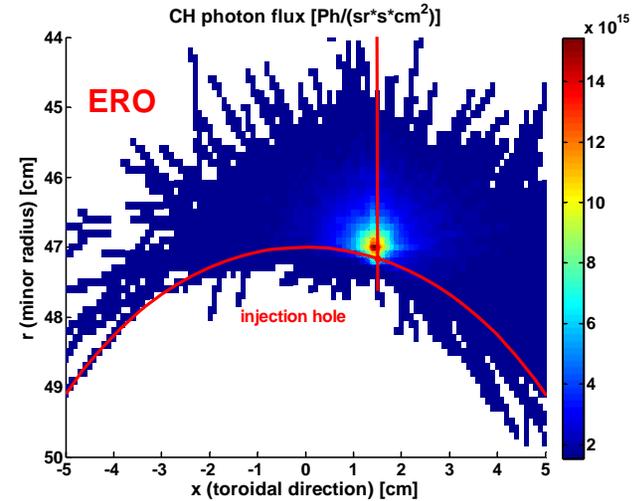
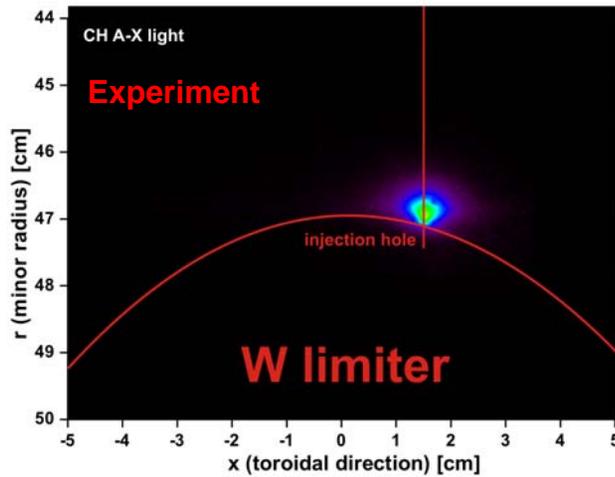
- In-situ observation of light emission above test limiter (dissociation products of CH_4).

- Post-mortem surface analysis of ^{13}C (and ^{12}C) deposition.

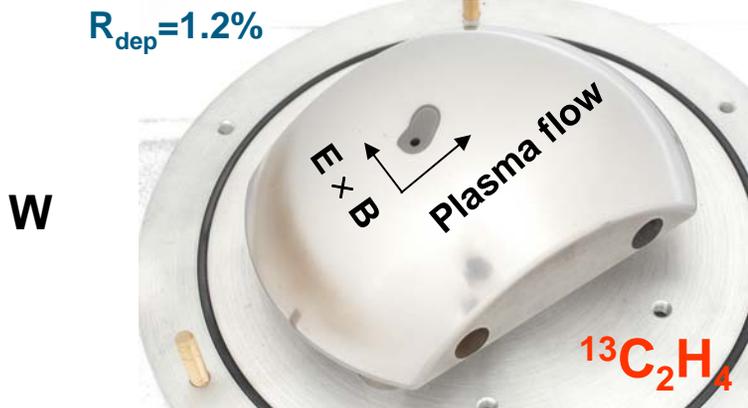
A. Kreter

Comparison of light emission: benchmark for n_e, T_e

$^{13}\text{C}_2\text{H}_4$ injection



Injection of $^{13}\text{C}_2\text{H}_4$ and $^{13}\text{CH}_4$ through C and W limiters ^{13}C deposition measured by NRA

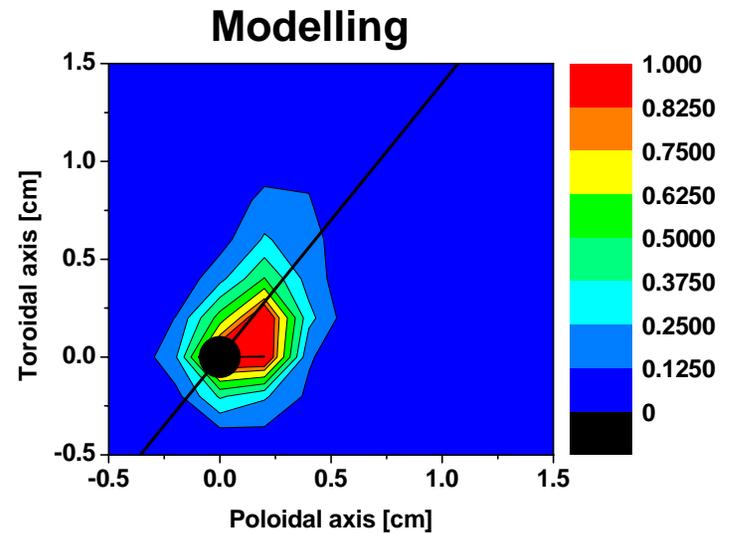
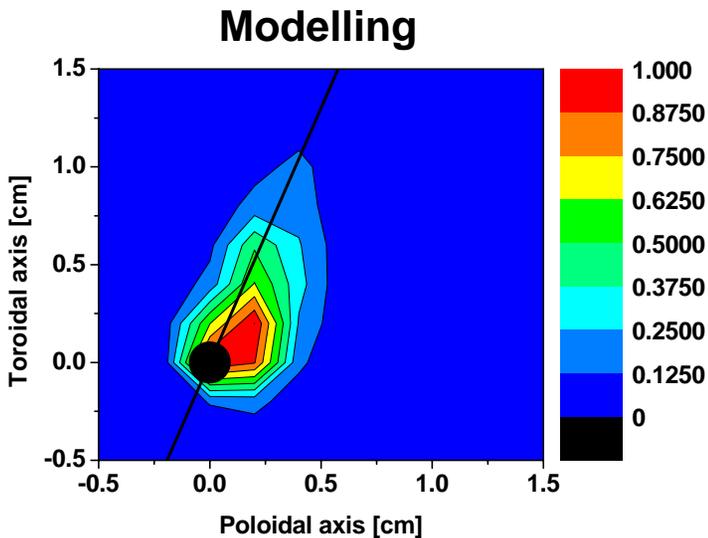
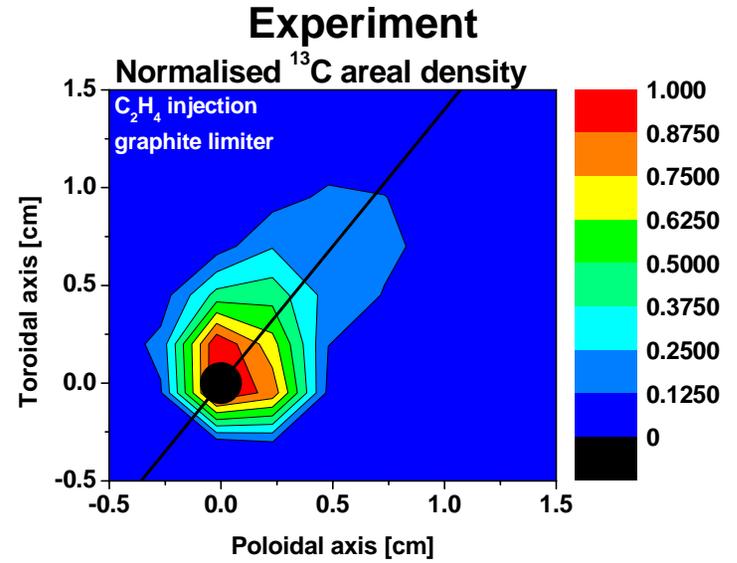
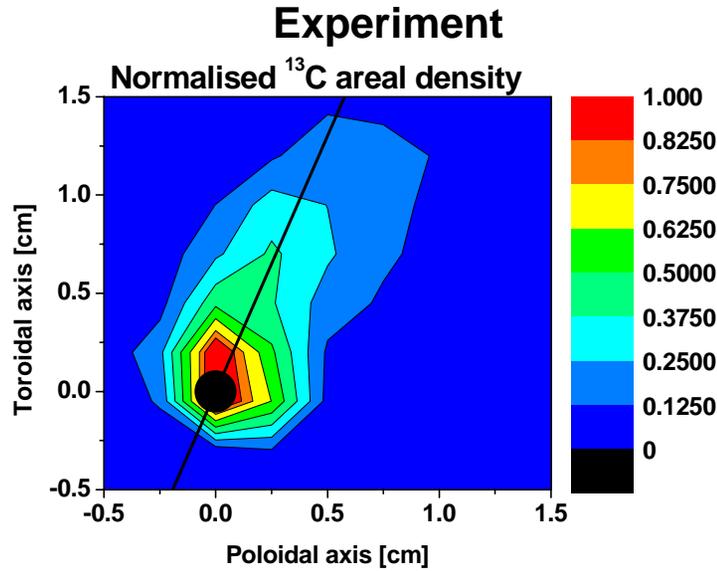


$$\text{Local } ^{13}\text{C} \text{ deposition efficiency } R_{\text{dep}} = \frac{\text{Locally deposited } ^{13}\text{C}}{\text{injected } ^{13}\text{C}}$$

R_{dep} is higher for $^{13}\text{C}_2\text{H}_4$ than for $^{13}\text{CH}_4$
 and higher on C than on W limiter

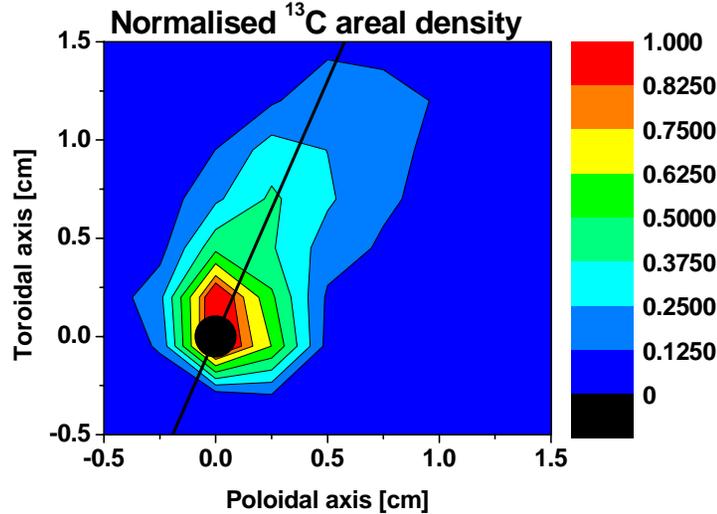
$^{13}\text{CH}_4$ injection through graphite limiter

$^{13}\text{C}_2\text{H}_4$ injection through graphite limiter

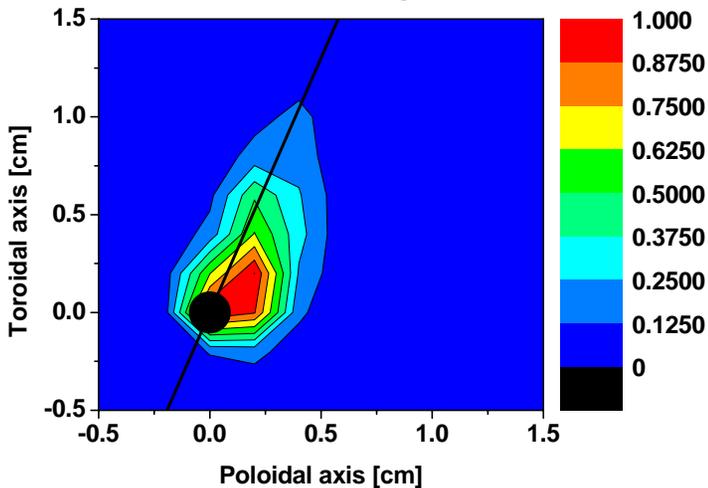


$^{13}\text{CH}_4$ injection through graphite limiter

Experiment

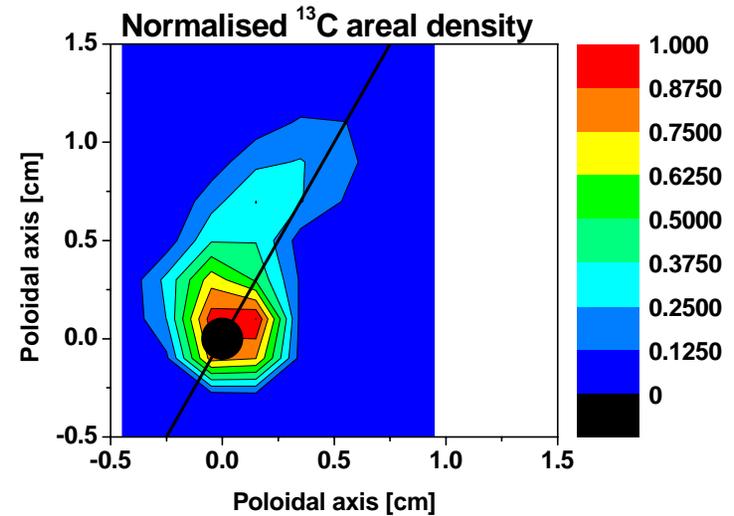


Modelling

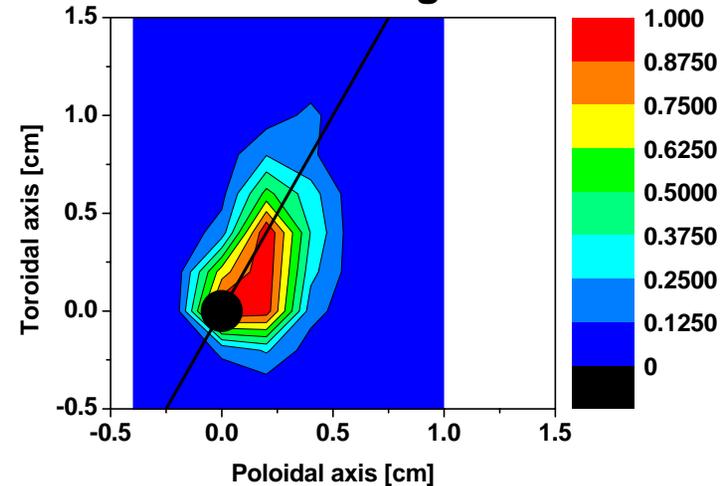


$^{13}\text{CH}_4$ injection through tungsten limiter

Experiment



Modelling



$$\text{Local } ^{13}\text{C deposition efficiency } R_{\text{dep}} = \frac{\text{Locally deposited } ^{13}\text{C}}{\text{injected } ^{13}\text{C}}$$

Gas	Limiter	R_{dep}	
		Experiment	ERO
$^{13}\text{CH}_4$	C	1.7 %	1.9 %
	W	0.8 %	1.1 %
$^{13}\text{C}_2\text{H}_4$	C	2.1 %	2.3 %
	W	1.2 %	1.3 %

$$S_{\text{eff}} = 0.15$$

$$Y_{\text{enh}} = 15\%$$

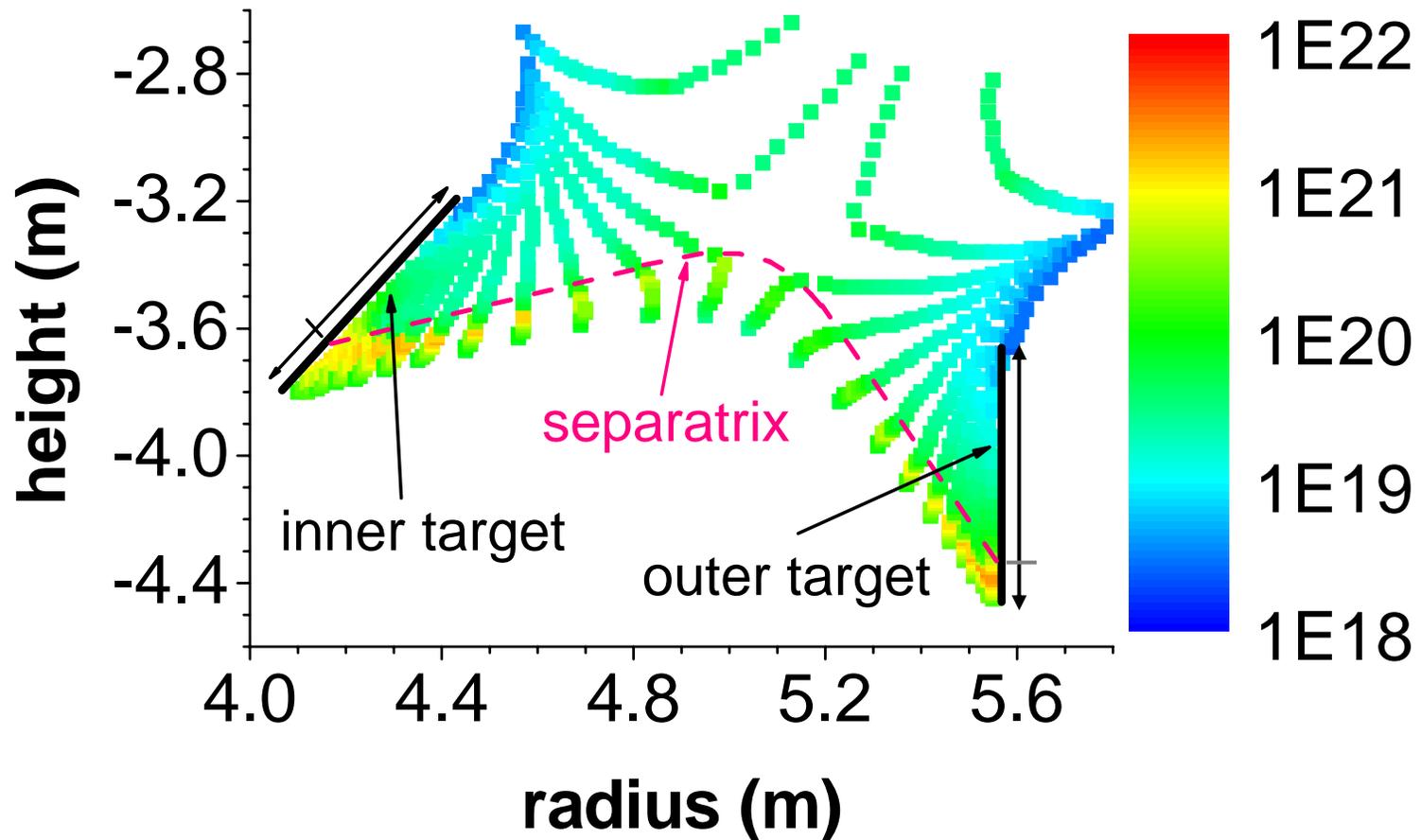
- Good agreement between experiment and modelling
- The dependency on substrate material and gases on R_{dep} is reproduced with ERO



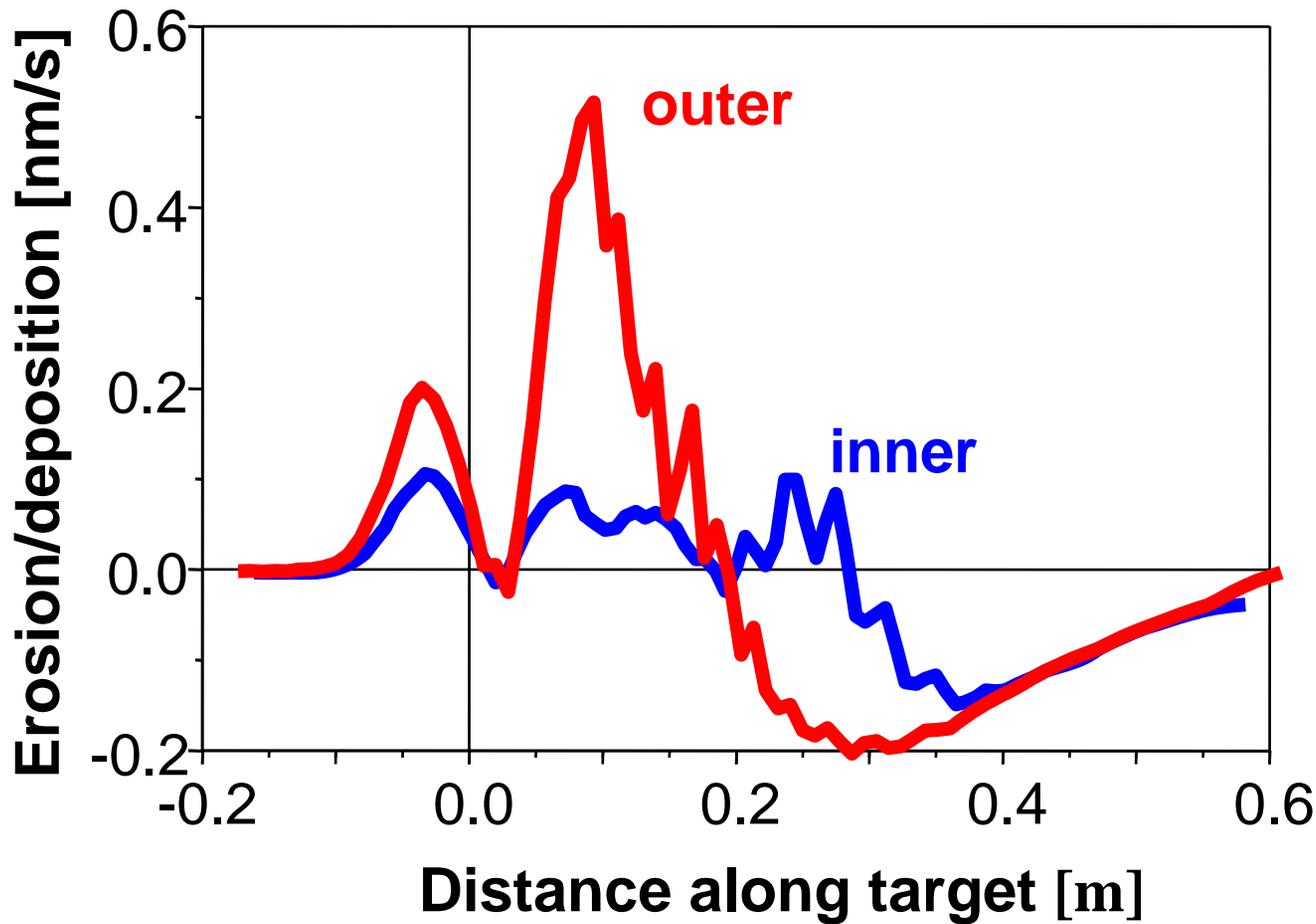
ITER availability

B2-EIRENE simulations

Electron density (m^{-3})

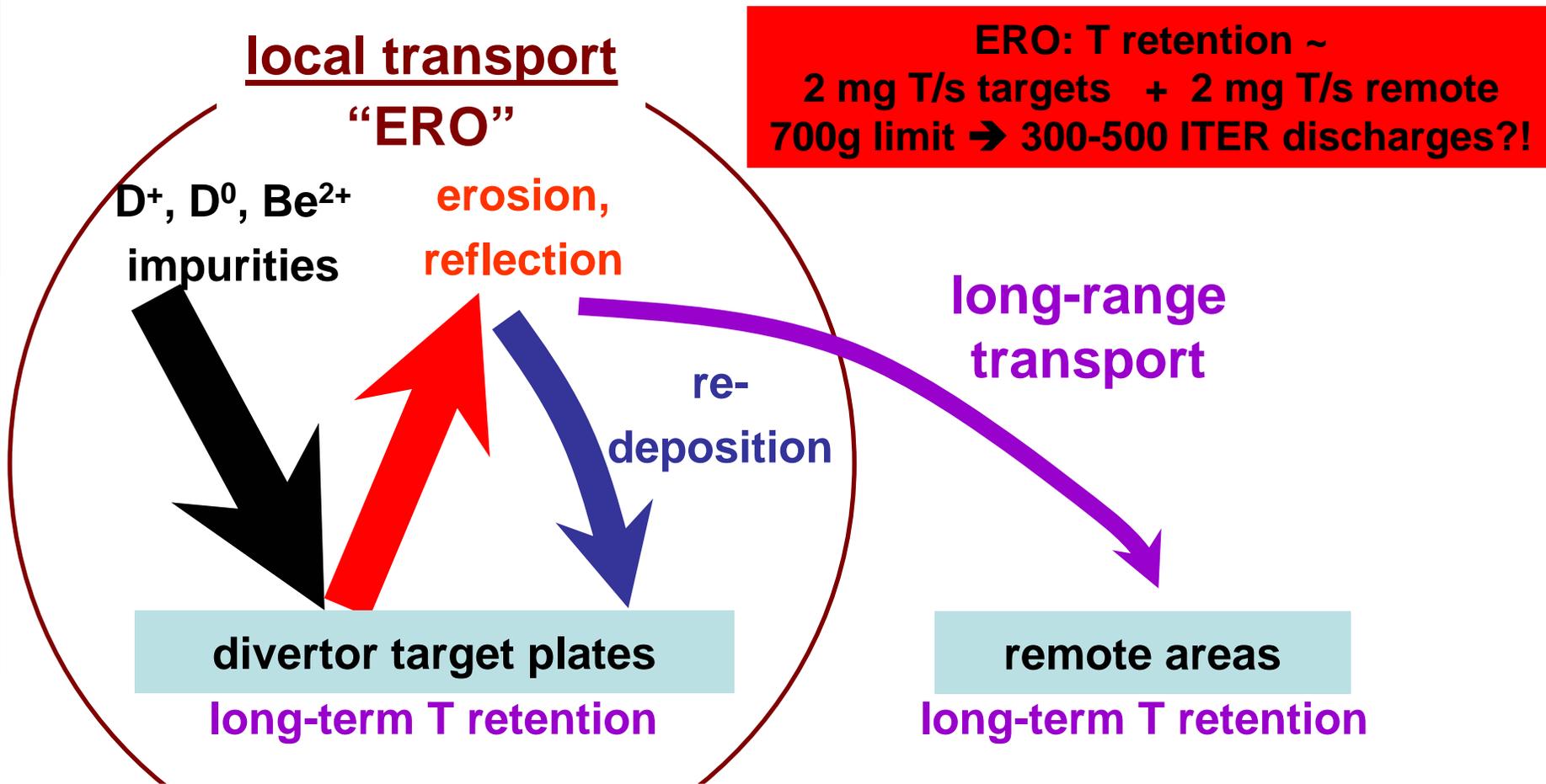


ERO modelling of target erosion (0.1% of Be)



Target plates (0.5 cm) should survive at least 6900 discharges

Sweeping of strike point can increase lifetime

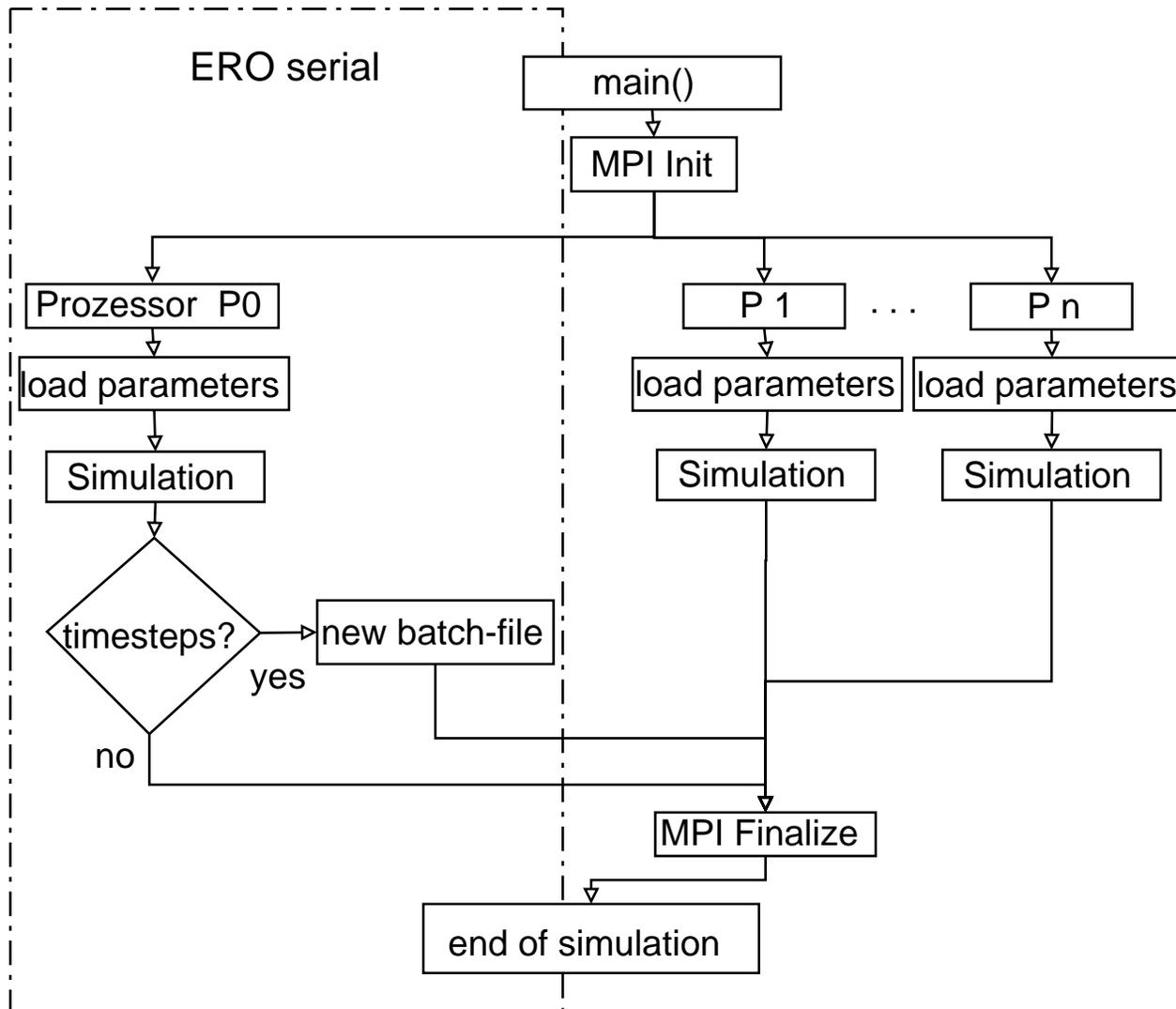


ERO:

- local transport near to divertor plates
- background plasma as input (B2 Eirene)
- layer formation (C and Be) ⇒ T retention using T/C, T/Be



Technicalities



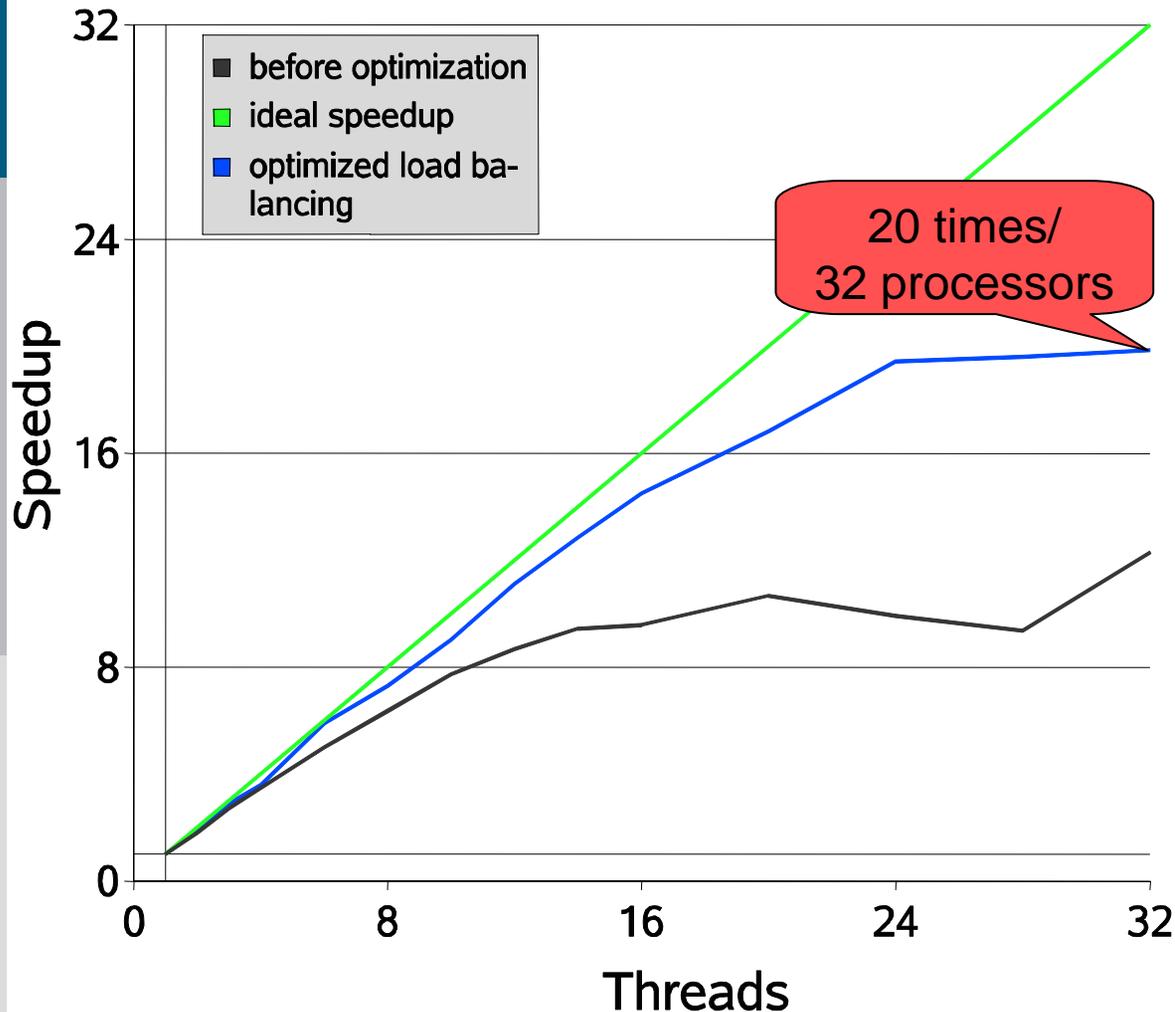
N ERO runs are substituted by 1 run on N processors
(calculation time remains the same!)

Each processor gets modified parameter file, working directory, generates all usual ERO output files.

For automatization a special **“starter”** program is developed

Data exchange between processors is minimal – MPI (message passing interface) is optimal

Speedup comparison



Processors get portions (“chunks”) of MC test particles for calculation

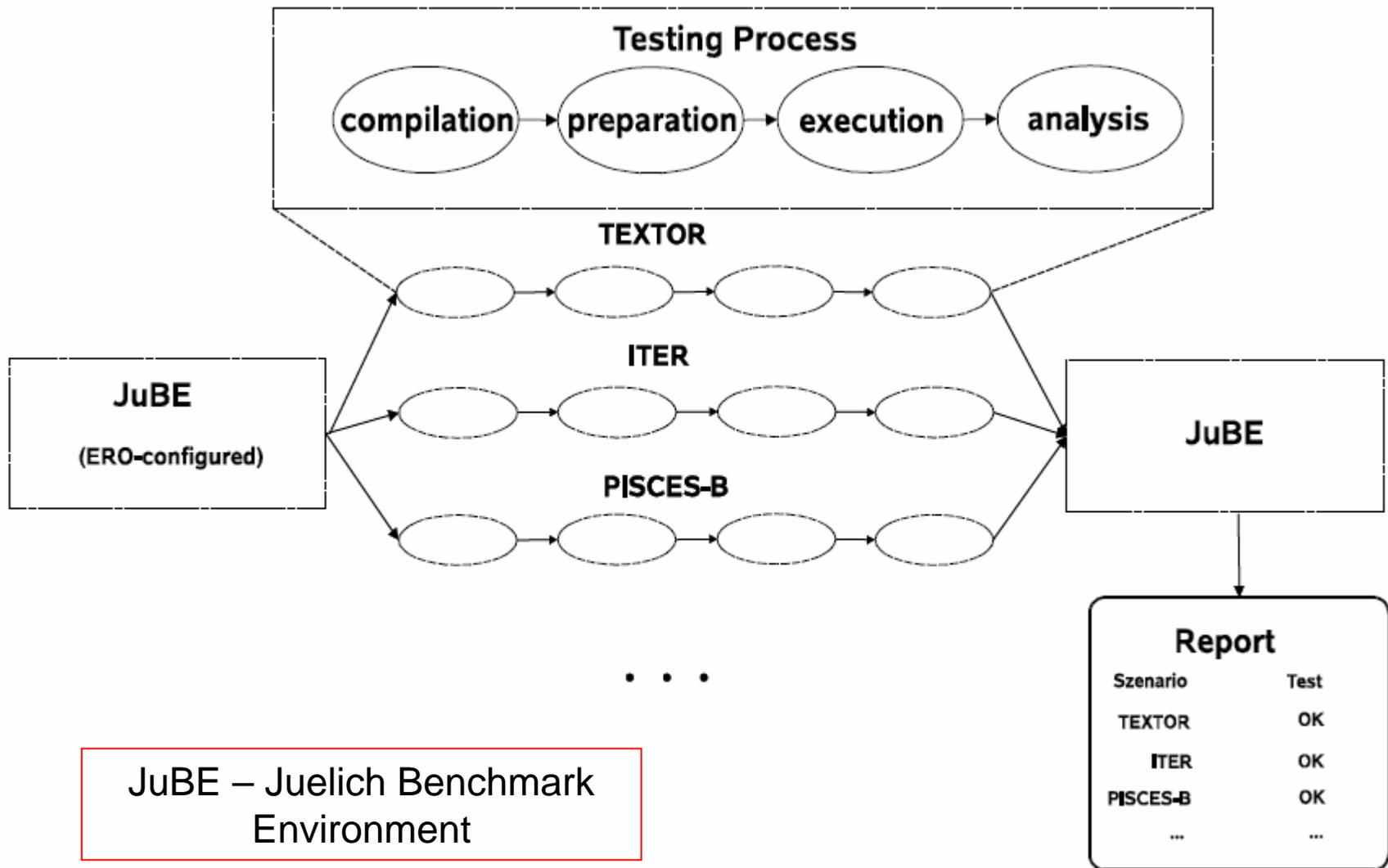
Particles are not fully independent!

They change the volume and surface meshes (occupying most part of memory used by ERO)

Shared memory (OpenMP) approach is optimal

Optimization:

- Minimization of serial part
- Processor load balancing
- Cache memory usage



(Matlab visualization GUI for ERO)

MERO 1.0
Surface Options | Volume Options

MERO (Matlab visualisation for ERO)

Task Selection:
 Task 1: Name: Cnd2MS1, File: :\ERO_RUN\PSC09\Quadro\Cnd2_MS1\Cnd2MS1Emission_fm1_step0.m
 Task2: Name: Empty, File: Empty
 Task3: Name: Empty, File: Empty

Buttons: Load task..., Reload, Add plasma parameter, Get profile, Penetration depth, Draw limiter, Add to plot list, Edit file, Save picture..., About MERO, Exit MERO

Load surface data:
 Surface analysis | TRIM data

Load volume data:
 Volume analysis | Spectroscopy

Plot Options:
 Time evolution | Movie | Plot List | Profile | Pen.dept...

Operations:
 + - * /
 Value: 1

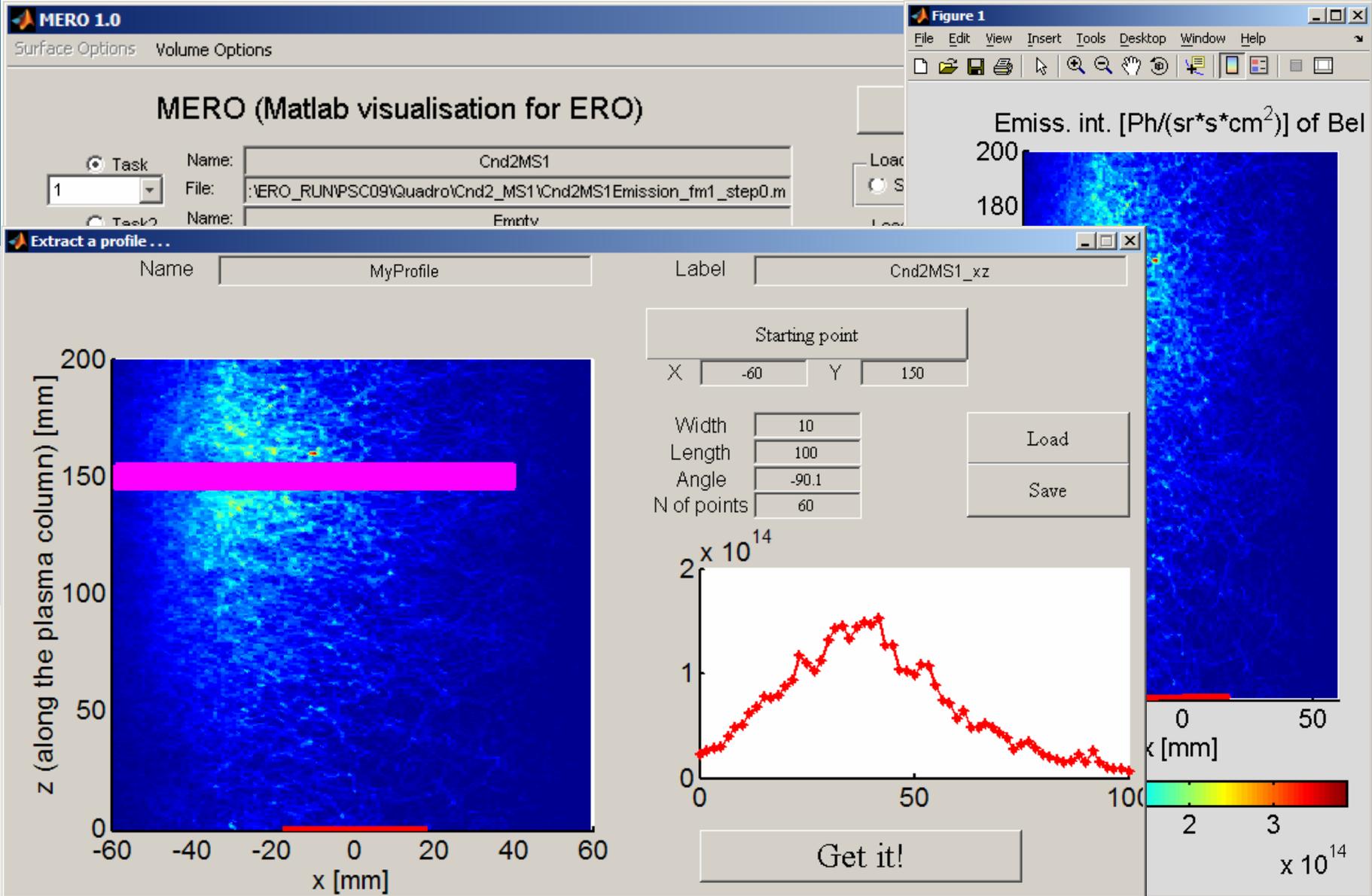
Options:
 Start new figure
 Scale the marker size
 Draw limiter contour
 Compare on one figure
 Logarithmic scale
 Normalize to 1
 Find asymptotics
 Enable sound

Element List:
 Bel 4573.0A G
 Bel 3322.0A M
 Bel UNR
 Bel 4573.0A U
 Bel 3322.0A U

Integration plane:
 xy
 xz
 yz
 3D

Steps:
 Insert... | Empty | Look for...
 Delete
 Clear
 Load
 Save
 Average
 2nd axis

Language: EN



How important is ADAS for ERO?

- 1) **Ionization/recombination** processes directly influence the particle **transport** in plasma.
- 2) For some species (e.g. H) **opacity** is not zero – radiation is an energy **transport channel**.
- 3) Spectroscopy gives **indispensable information** for model **benchmarking** (both qualitative and quantitative).



End