Member of the Helmholtz Association

Ongoing and pending data base activities @ FZ Jülich

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IAEA Technical Meeting on Technical Aspects of Atomic and Molecular Data Processing and Exchange (23rd Meeting of the A+M Data Centres), Vienna, Nov. 2 - 4 th 2015

OUTLOOK

- **Generals:** on AM-S data use in fusion plasma models

  "internal consistency", completeness (competing processes)

- **Surface Data:** Reflection, Sputtering:

  multidimensional distributions: online "TRIM" database

  maintained, and still occasionally upgraded upon demand.

- **AM Data:**

  FZJ: data evaluation, data generation, database compilation "sui generis"

  was initiated by Ratko Janev:

  C_xH_y (database is frozen, some low T updates for particle rearrangement collisions are pending),

  SiH_y (database frozen)

  H, H^-, H_2, H_2^+, H_3^+…→ ongoing, (now mainly: asymptotics, documentation)

  Be, Be_xH_y : unfinished

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  Data processing/formatting, asymptotics, internal CR modules for transport simulations,…,raw data public exposure.

  Sensitivity analysis (uncertainty propagation) on linear CR or chemistry models

Status and purpose of current integrated edge models:

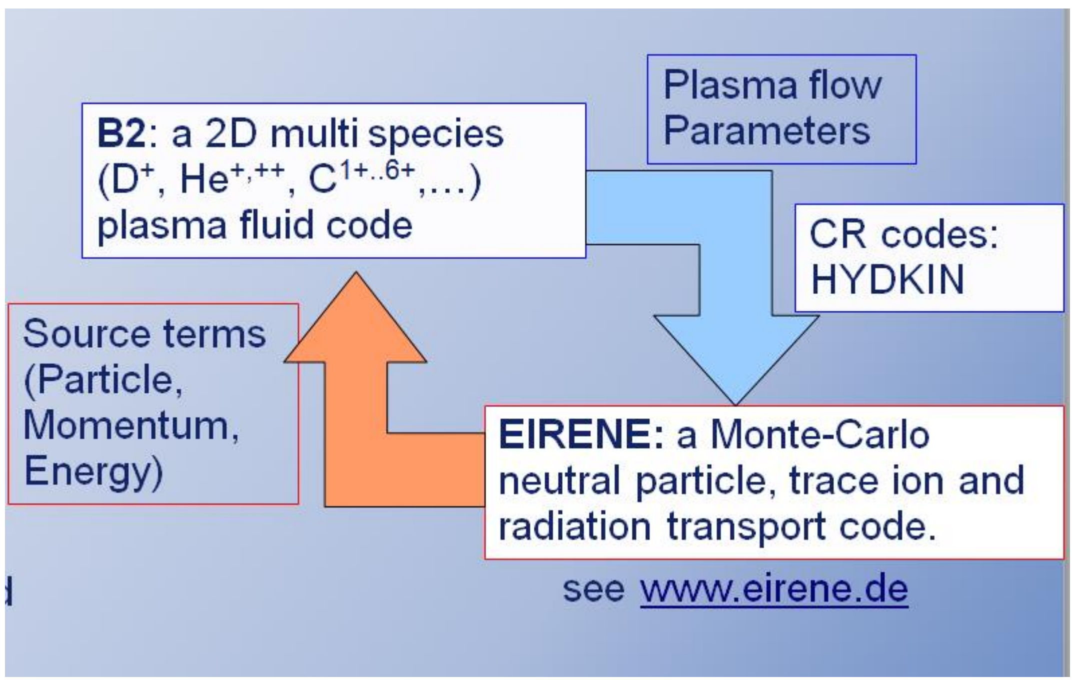
No predictive quality, due to “anomalous” cross field plasma transport (laminar? turbulent? blobby? ….?)

By detailed numerical bookkeeping current edge modelling is the tool to separate the “principal known” (PMI, A&M) from the “principle unknown” ($\perp$B plasma-transport).
If this is successful, then the latter can be isolated and determined experimentally

Method: "Operator Splitting"

Advection-diffusion: strongly implicit CFD (macroscopic flows)

Reaction part: explicit (Monte Carlo) (microscopic kinetics)



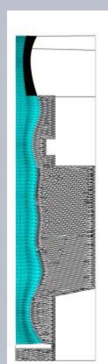
Simulation of "plasma + wall" – a multi-scale problem

JÜLICH FORSCHUNGSZENTRUM

Larger scales in time & space ←

transport codes

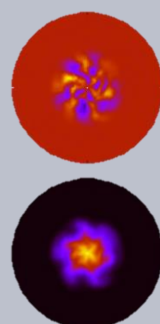
Adaption of edge transport code for linear devices



(codes: B2, EIRENE, EMC3, ERO,..)

drift-fluid models

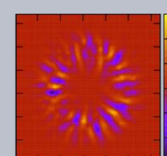
3D Simulations, currents, fields, drifts



Tokam3D (CEA), Bout++ Attempt,…

gyro-kinetic models

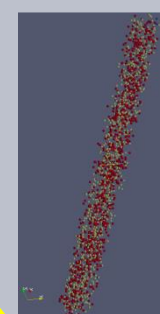
Includes non-Maxwellian effects, ExB nonlinearity and polarization drift retained



fully kinetic models (PIC/TREE)

Mesh free approach with tree code, particle based, self consistent fields

Goal: ab-initio virtual PMI lab using PEPC



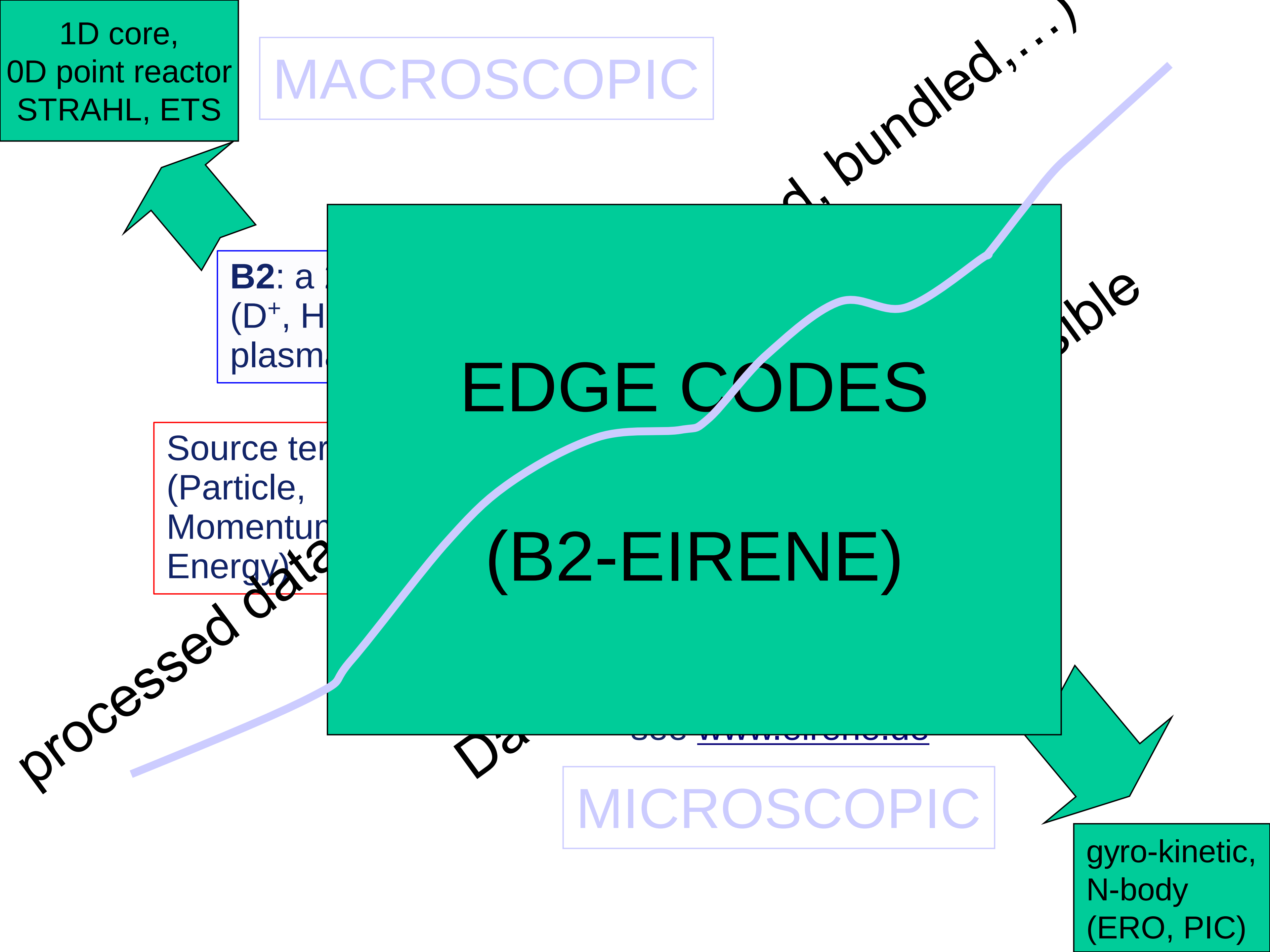
PEPC (with JSC)

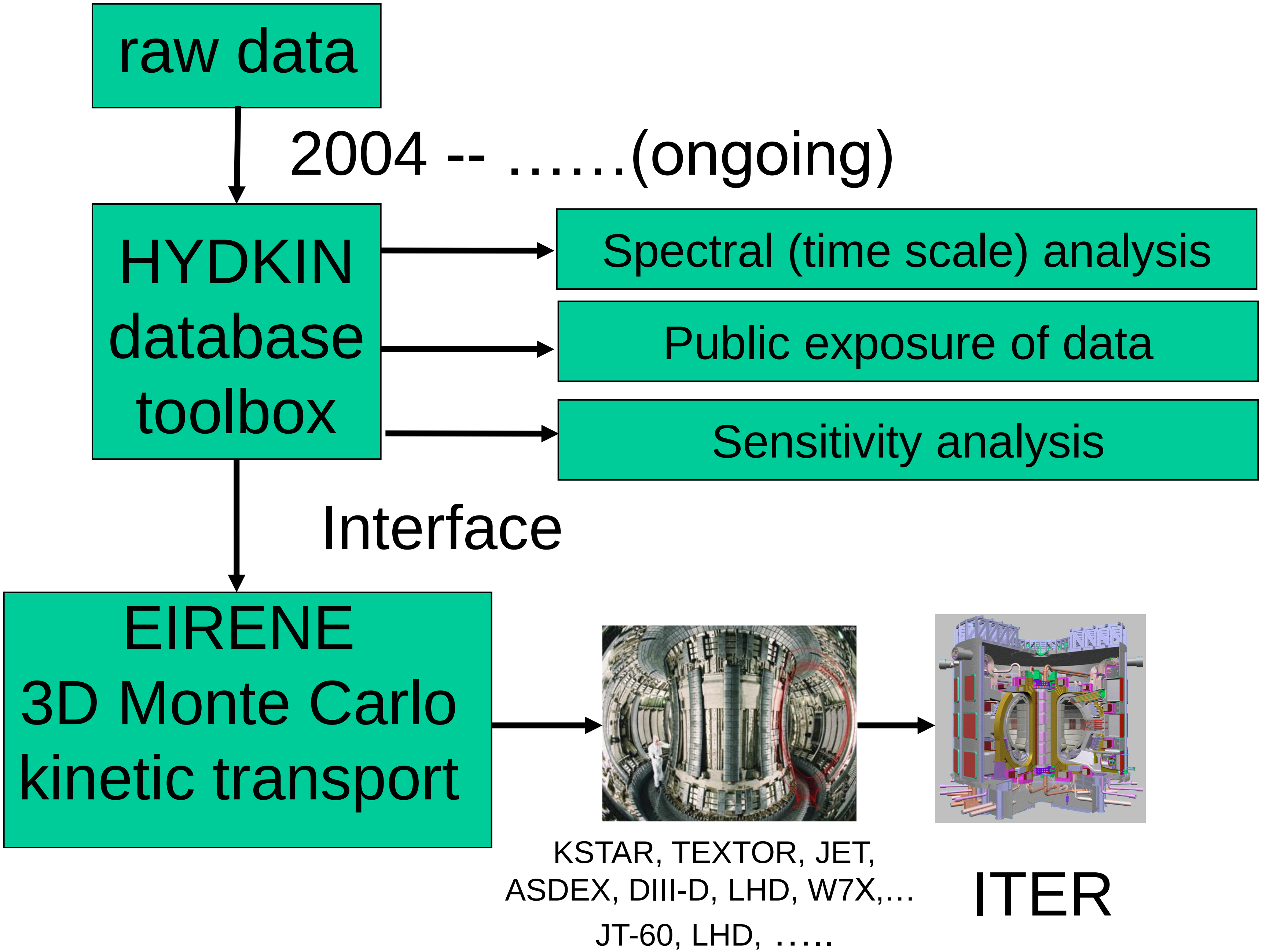
Surface and material simulations

Computational material science: multi-scale in itself:

DFT – QMD – MD – KMC …

plasma material interface


1D core,
0D point reactor
STRAHL, ETS
MACROSCOPIC
bundled,
(Particle,
Energy)
processed data
EDGE CODES
(B2-EIRENE)
MICROSCOPIC
gyro-kinetic,
N-body
(ERO, PIC)


raw data
2004 -- ……(ongoing)
HYDKIN
database
toolbox
Spectral (time scale) analysis
Public exposure of data
Sensitivity analysis
Interface
EIRENE
3D Monte Carlo
kinetic transport
KSTAR, TEXTOR, JET,
ASDEX, DIII-D, LHD, W7X,…
JT-60, LHD, …..
ITER

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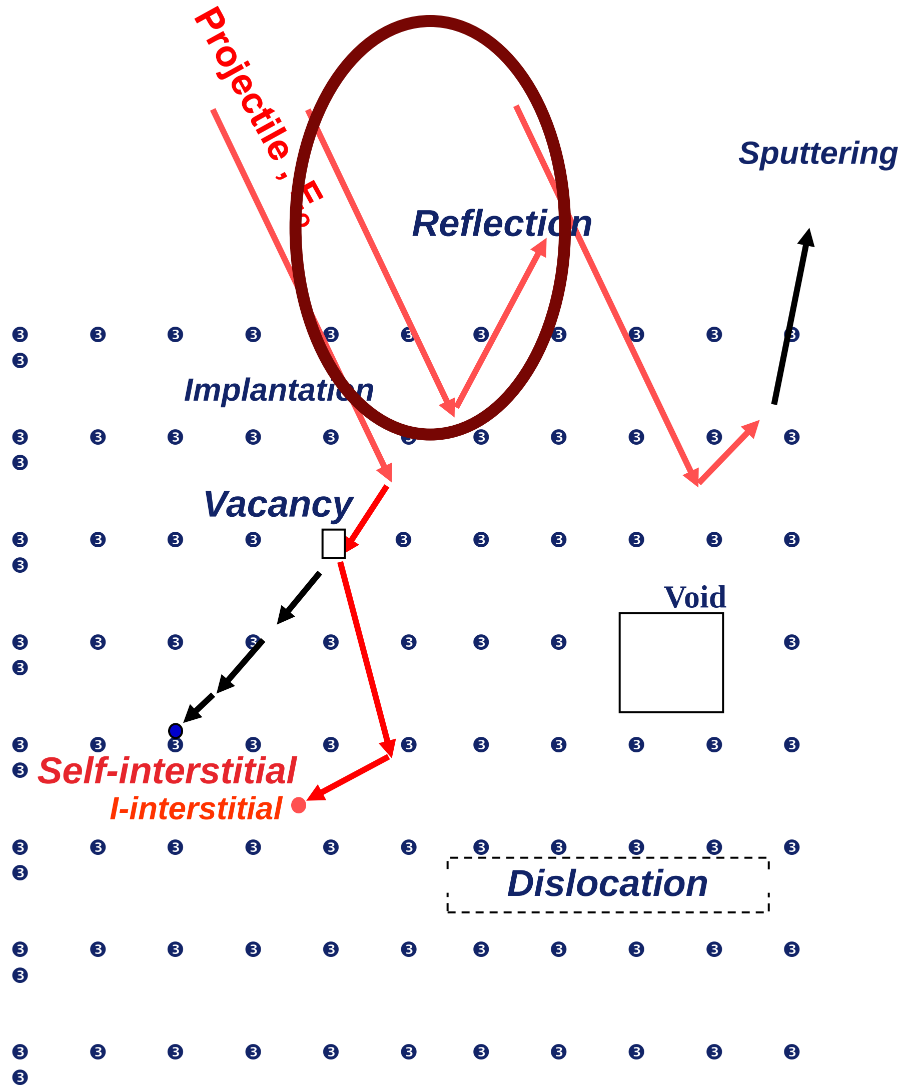
A: Basic Processes Induced in Materials by Plasma Particle Impact



Energy dissipation by elastic (with atoms) and ineleastic (with electrons) collisions

(10^{-13} sec, range 10^{-7} m, 200 eV D^{+})

Recycling: reflection and thermal re-emission of incident particles at surfaces

Elastic collisons: Creation of vacancies and interstitials

elastic collisions

(energy transfer > threshold energy for damage)

Diffusion of vacancies and interstitials

voids, dislocations, swelling, radiation, embrittlement

BCA: Binary collision approximation

Sputtering of surface atoms

(energy transfer > surface binding energy)

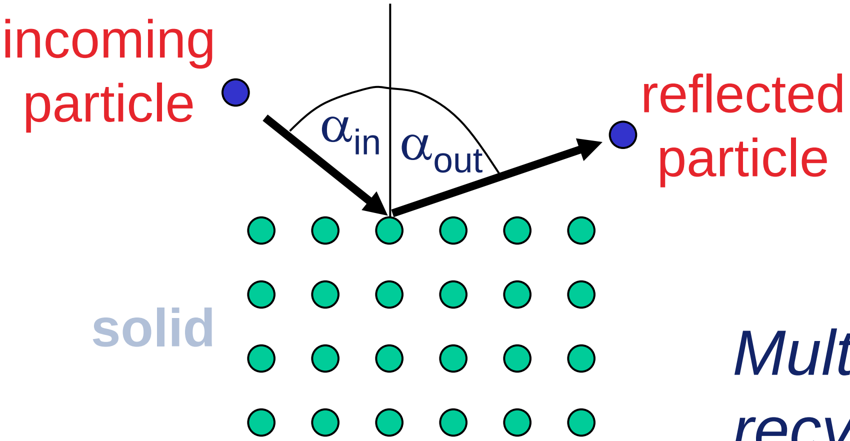
Transmutation

formation of nuclear reaction products (including H isotopes and He)

Plasma-Wall Interaction Processes

Backscattering

Reflection of impinging particles at the surface



Reflection coefficient R:

Deposition = 1 - R

$$R = \frac{\text{number of reflected particles}}{\text{number of incoming particles}}$$

Multi-differential recycling coeff.: $\frac{\partial R}{\partial E}, \frac{\partial^2 R}{\partial^2 \Omega}, \frac{\partial^3 R}{\partial E \partial^2 \Omega}$

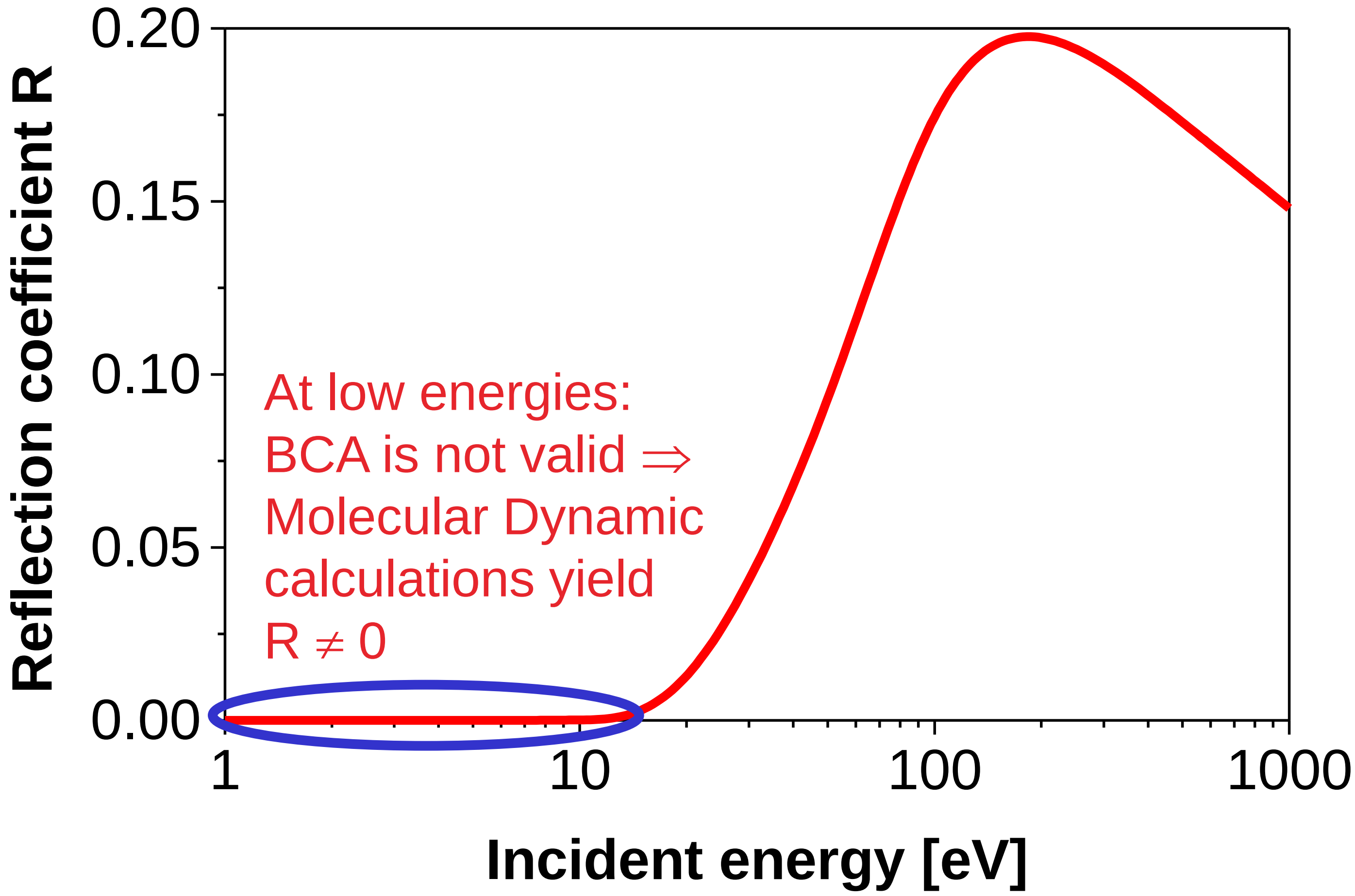
- In most cases: reflected particles are neutrals
- Reflection coefficient depends on:
  - mass of projectile and target
  - energy and angle of incident particles

Plasma-Wall Interaction Processes

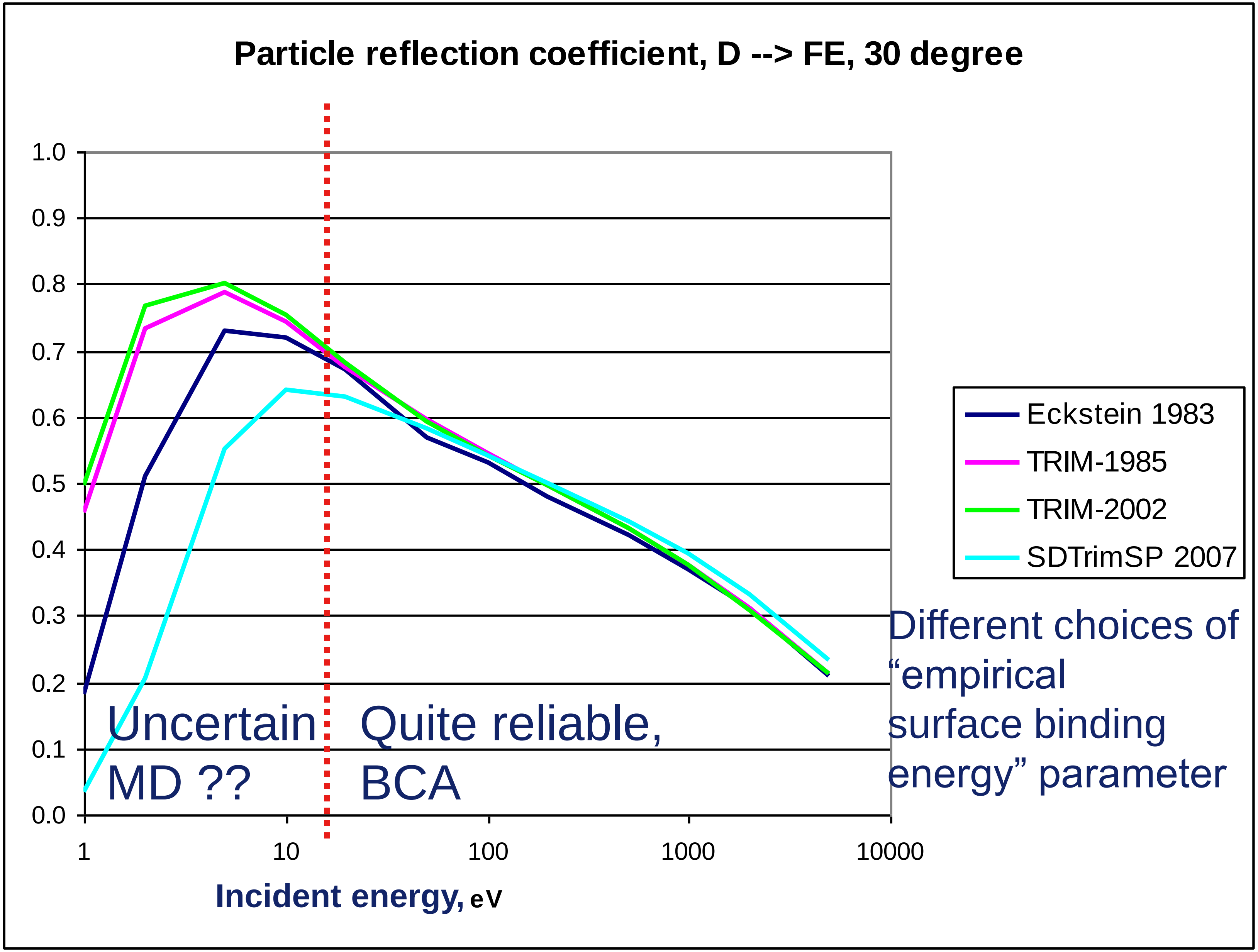
Backscattering

Dependency of reflection coefficient on incident energy

Monte Carlo simulation (BCA): C on C, α_{in} = 60°



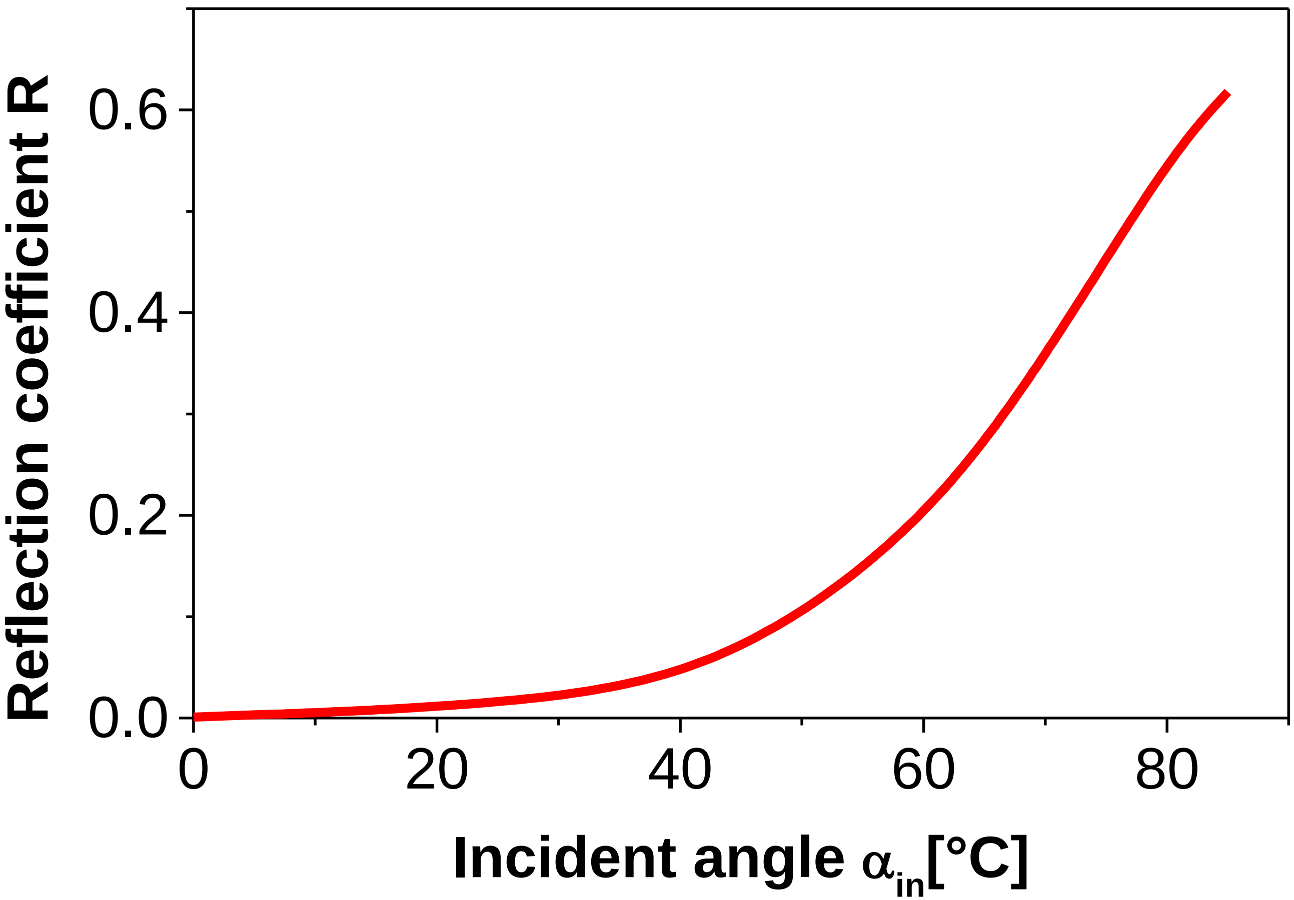
Sensitivity of reflection coefficient at low E_{in} (all within BCA, TRIM)

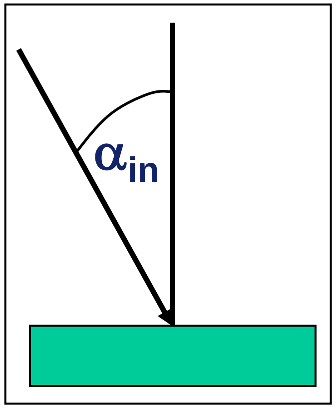


Backscattering

Dependency of reflection coefficient on incident angle

Monte Carlo simulation (BCA): C on C, E_{in} = 100 eV





Backscattering

Energy and angle distribution of reflected particles

Reasonable assumptions (IYMG*):

Energy: exponential decrease for reflected particles if incoming particle energy is Maxwell-distributed

Angle: cosine distribution for reflected particles if isotropic bombardment

Note: Reflection coefficient R can be very different from Recycling coefficient R

Recycling coefficient is typically close to one in magnetic fusion, because wall surfaces are quickly saturated.

* IYMG: If You Must Guess

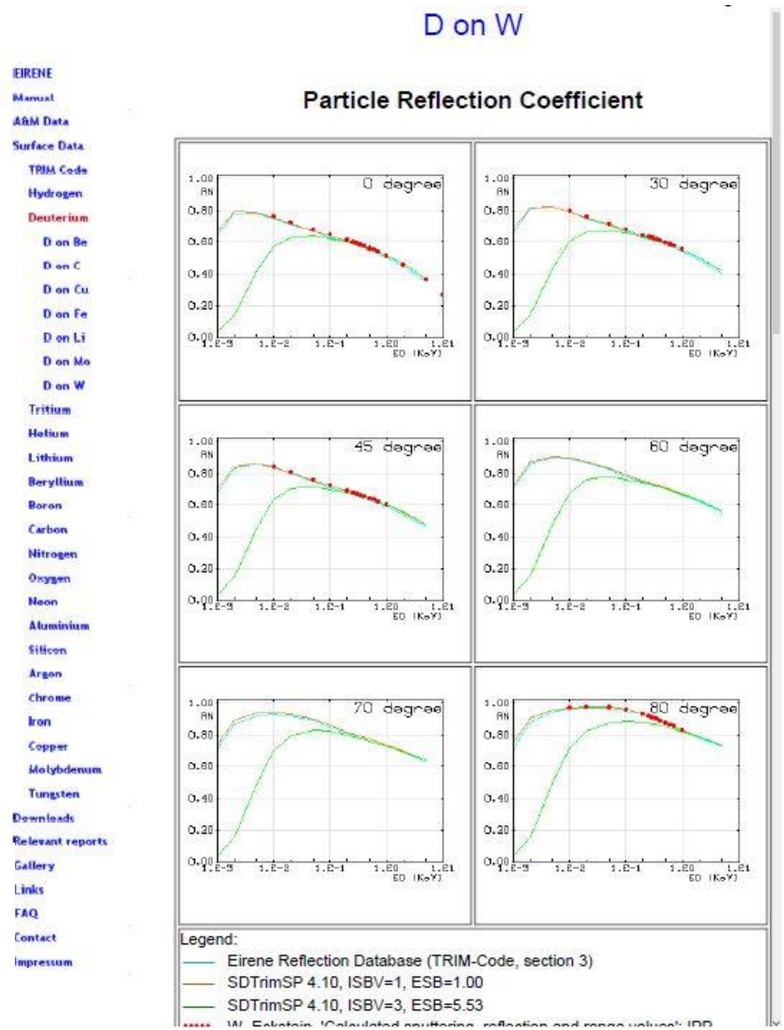
Surface processes in fusion edge codes:
Jargon in edge modelling talks/papers: “we use TRIM code data….”
(wrt. “physical sputtering and reflection”)
which means: BCA   (binary collision approximation)

Full 3V distribution of refl. part.
on: www.eirene.de/surfacedata

Reflection data

target / projectile	Li	Be	B	C	Al	Si	Cr	Fe	Cu	Mo	W
H	4	4		1 4				1 4	2	2	2 4
D	4	2		1				1 2		2	2 4
T		4		2 4				2 4		2	2 4
He				2				2		2	2
Li	4										
Be		3		3							4
B			3	3 4							
C		4	3	3	3	3	3	3	3	3	3
N		4		4							4
O		4		4							4
Ne		2		2							2 4
Al				3 4							
Si				3 4		3 4		3 4	3 4		
Ar		4		4							4
Cr				3 4			3 4			3 4	
Fe				3		3					
Cu				3		3					
Mo				3						3	
W		4		3							3

1	TRIM-Code, 1984, W. Eckstein, priv. com.
2	TRIM-Code, 1998, FZJ, PDF, sect. 3
3	TRIM-Code, 2005, FZJ, PDF, sect. 6
4	SDTRIMSP, vs. 4.10, 2010, FZJ, different ESB parameters



EIRENE
Manual
A&M Data
Surface Data
TRIM Code
Hydrogen
H on C
H on W
H on Fe
H on Mo
H on Cu
Deuterium
Tritium
Helium
Beryllium
Boron
Carbon
Neon
Aluminium
Silicon
Chrome
Iron
Copper
Molybdenum
Tungsten
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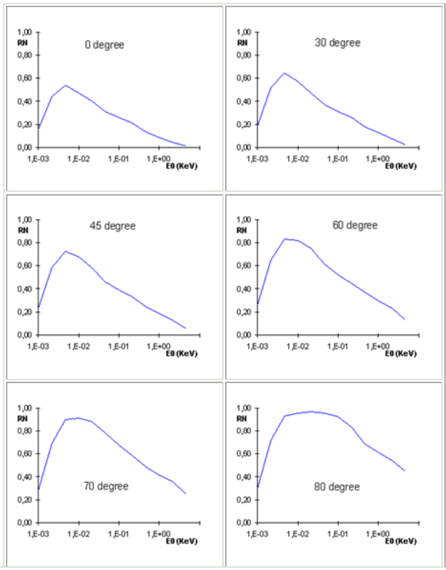
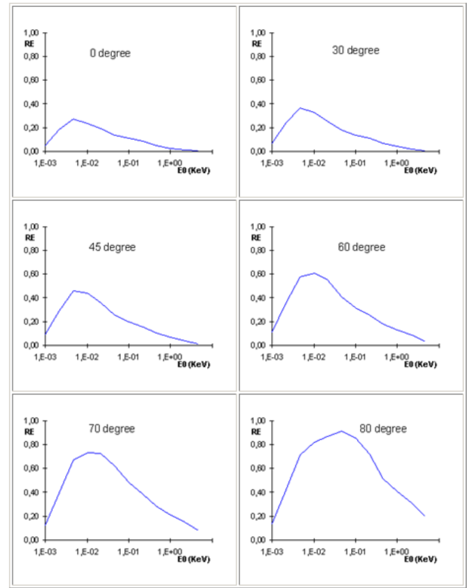
H on C

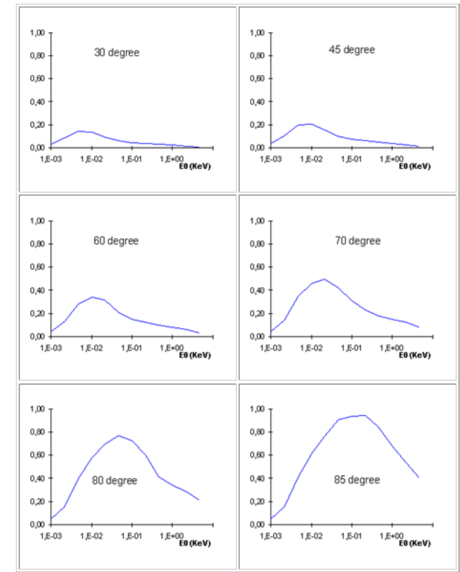
Particle Reflection Coefficient



Energy Reflection Coefficient



Momentum Reflection Coefficient



AMJUEL data file   HYDHEL data file
METHANE data file   H2VIBR data file

For the following files refer also to the surface data section:

H on C H on W H on Fe H on Mo H on Cu	D on C D on W D on Fe D on Mo D on Be	T on C T on W T on Fe T on Mo	He on C He on Mo He on W He on Fe	Be on C Be on Be	B on C B on B
C on C C on Al C on B C on Cr C on Cu C on Fe C on Mo C on Si C on W	Ne on C Ne on Be	Al on C	Si on C Si on Cu Si on Fe Si on Si	Cr on C Cr on Cr Cr on Mo	Fe on C Fe on Si
Cu on C Cu on Si	Mo on C Mo on Mo	W on C W on W			

Data files with tables of multiple differential reflection distributions, e.g. for particle simulation codes

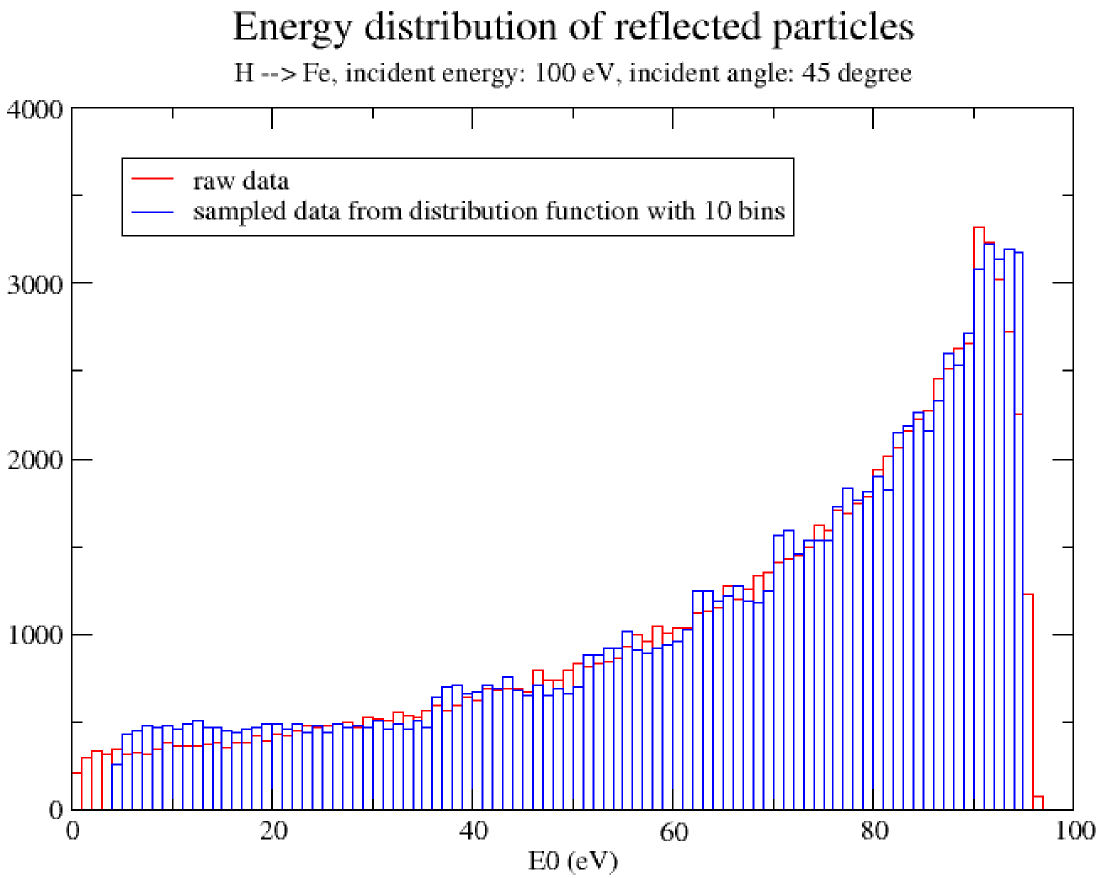
(conditional quantile format)

TRIM.xxx: reflected energy spectra

red: 200.000 TRIM particles,

blue: reconstructed from 10 quantiles

$$\frac{\partial R(E_{in}, \theta_{in}; E)}{\partial E}$$



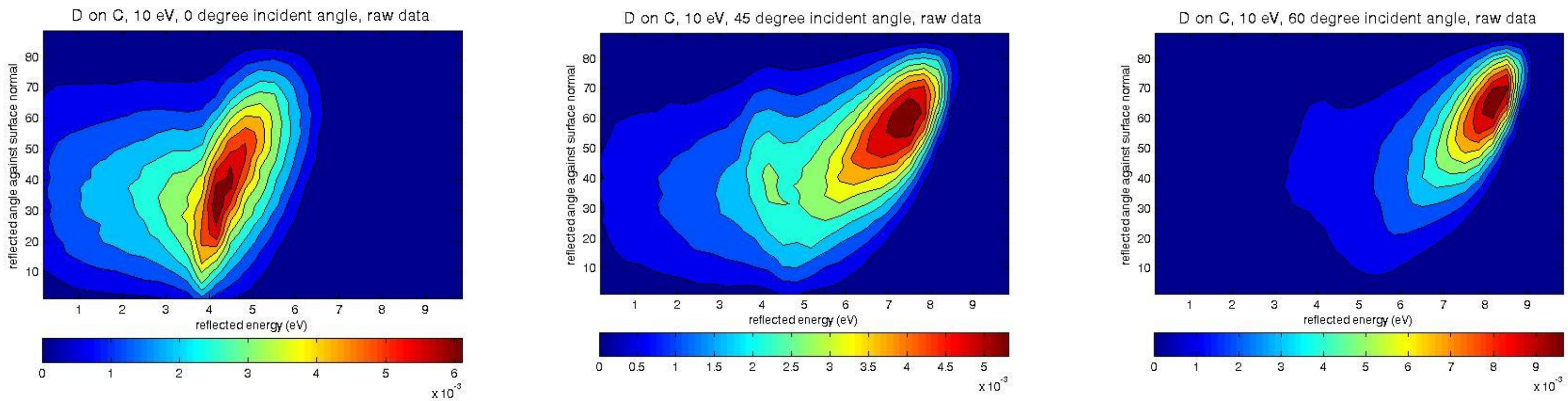
See:
www.eirene.de
Surface data
TRIM

what is the minimal dataset that allows
to re-sample the full backscattering (and sputtering) distribution ?

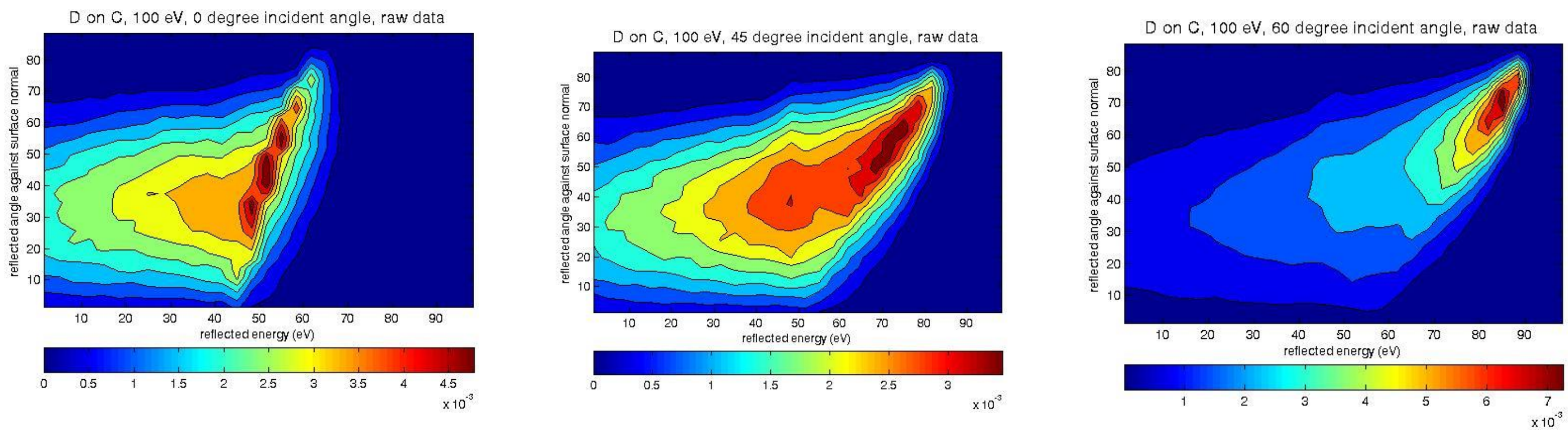
Double diff. distr.

$$\frac{\partial R(E_{in},\theta_{in};E,\theta_{out})}{\partial E\,\partial\theta_{out}}$$

D on C, 10 eV in



D on C, 100 eV in

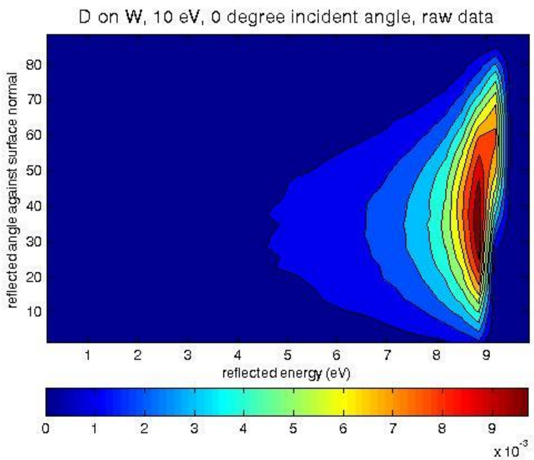


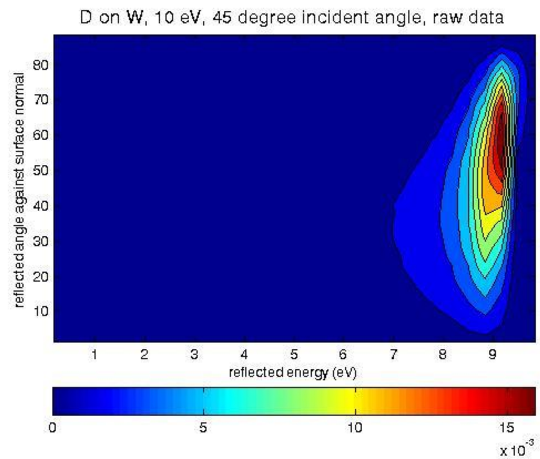
Data formatting and condensation: G. Bateman, PPPL no. 1 (1980)

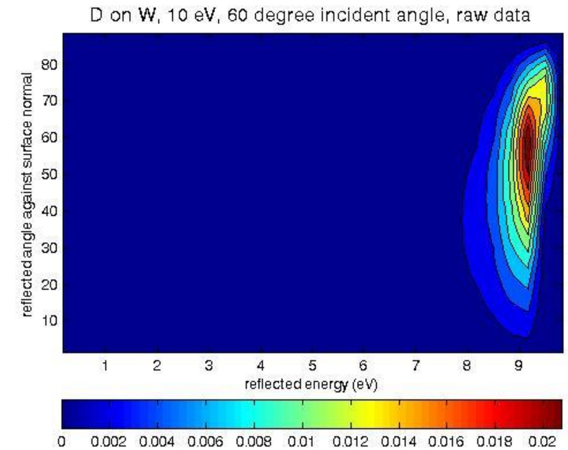
Double diff. distr.

$$\frac{\partial R(E_{in}, \theta_{in}; E, \theta_{out})}{\partial E \partial \theta_{out}}$$

D on W, 10 eV in







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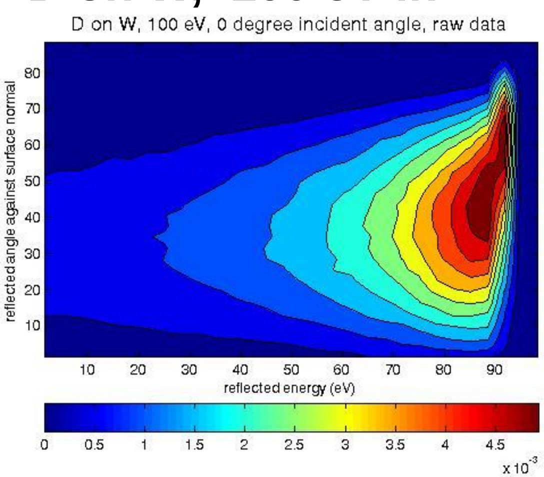

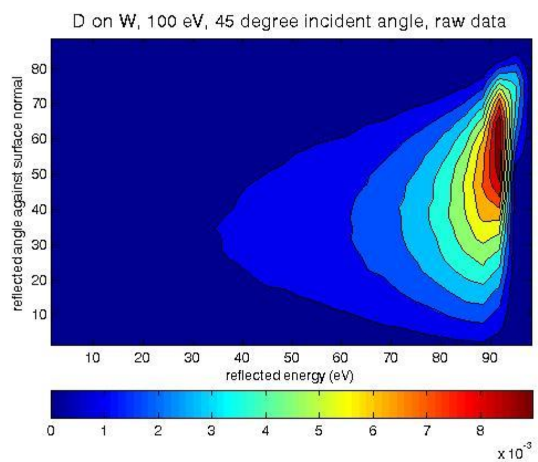

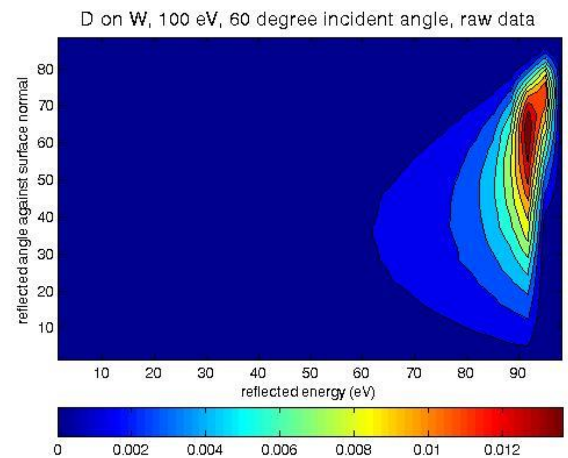

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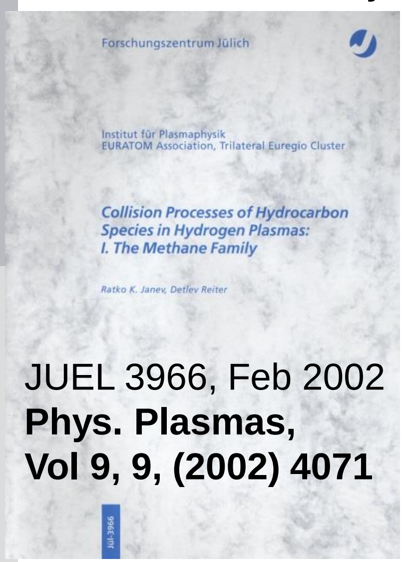
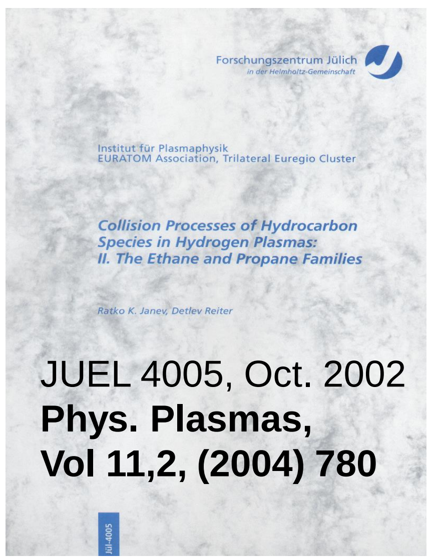
FZJ homemade "database" for fusion plasma chemistry modelling, is publicly exposed on: www.eirene.de

Reviewed EIRENE database Series 2002-…., (several IAEA CRP's)
FZ-Jülich (R. Janev, D. Reiter et al.) www.eirene.de www.hydkin.de

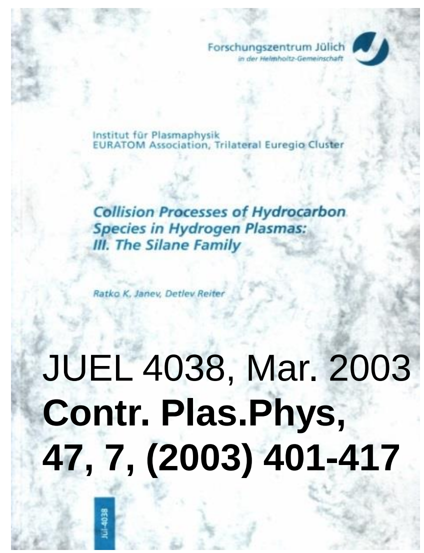
Methane (CH_y) C_2H_y C_3H_y Silane (SiH_y) p,H,H^-,H_2,H_2^+,H_3^+



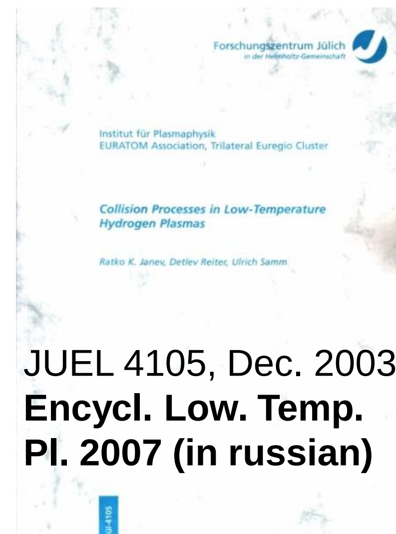
JUEL 3966, Feb 2002
Phys. Plasmas, Vol 9, 9, (2002) 4071



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. Pl. 2007 (in russian)

Ratko Janev, Detlev Reiter:

H, H_2, H_3^+… data compilation.

Mostly cross sections, few rate coefficients

Today: 471 references,

Almost all data fitted. JUEL-report: 2004.

New edition: spring 2016 (CRP H, He)

JÜLICH
FORSCHUNGSZENTRUM

raw data

2004 -- ……(ongoing)

HYDKIN
database
toolbox

- Spectral (time scale) analysis
- fragmentation pathways
- Sensitivity analysis

Interface

EIRENE
3D Monte Carlo
kinetic transport

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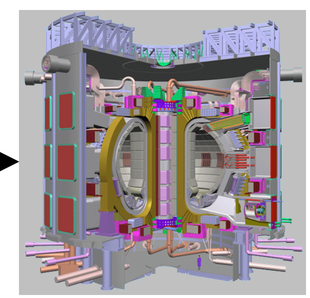

ITER

“Battle field” of hydrogen molecule: Two-electronic, strongly coupled potential-surfaces of H_3^+

$H^+ + H_2$ is the most fundamental ion-molecule system

We should know all about it P. Krstic, ORNL, US

Proton impact of molecule

$p + H_2(v) \rightarrow p + H_2(v')$

$p + H_2(v) \rightarrow H + H_2^+(v')$ Charge transfer

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

$p + H_2(v) \rightarrow H + H^+ + H^+ + e$ Dissoc Double ion

$p + H_2(v) \rightarrow p + H_2(n, v')$ Exc. elec. vib.

Processes with molecular ion

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

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

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

Numerous other processes with molecules

$H^- + H_2(v) \rightarrow H + H_2(v') + e$

$H + H_2(v) \rightarrow H + H_2(v')$

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

$H_2(v') + H_2(v'') \rightarrow H_2(v''') + H_2(v'''')$

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

Creation of H_3^+

$H_2^+(v') + H_2(v) \rightarrow H_3^+(v'') + H$

H_3^+ Series of interesting reactions:

DE, DR, branching ratios with electrons

D, DCT with H

- “Interplay” of transport and inelastic processes
- Rotational analysis is missing
- Isotopic constitution: D_2,T_2, HD, HT and DT, sensitive on vib. energy levels

"Battle field" of hydrogen molecule: Two-electronic, strongly coupled potential-surfaces of H_3^+

$H^+ + H_2$ is the most fundamental ion-molecule system
We should know all about it

P. Krstic, ORNL, US, talk @ IAEA, DCN, 2013

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

$$H_2(v') + H_2(v'') \rightarrow H_2(v''') + H_2(v'''')$$

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

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JÜLICH FORSCHUNGSZENTRUM

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Proton impact of molecule

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$p + H_2(v) \rightarrow H + H_2^+(v')$ Charge transfer

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

$p + H_2(v) \rightarrow H + H^+ + H^+ + e$ Dissoc Double ion

$p + H_2(v) \rightarrow p + H_2(n, v')$ Exc. elec. vib.

Processes with molecular ion

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

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

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

Numerous other processes with molecules

$H^- + H_2(v) \rightarrow H + H_2(v') + e$

$H + H_2(v) \rightarrow H + H_2(v')$

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

$H_2(v') + H_2(v'') \rightarrow H_2(v''') + H_2(v'''')$

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

Creation of H_3^+

$$H_2^+(v') + H_2(v) \rightarrow H_3^+(v'') + H$$

H_3^+ Series of interesting reactions:

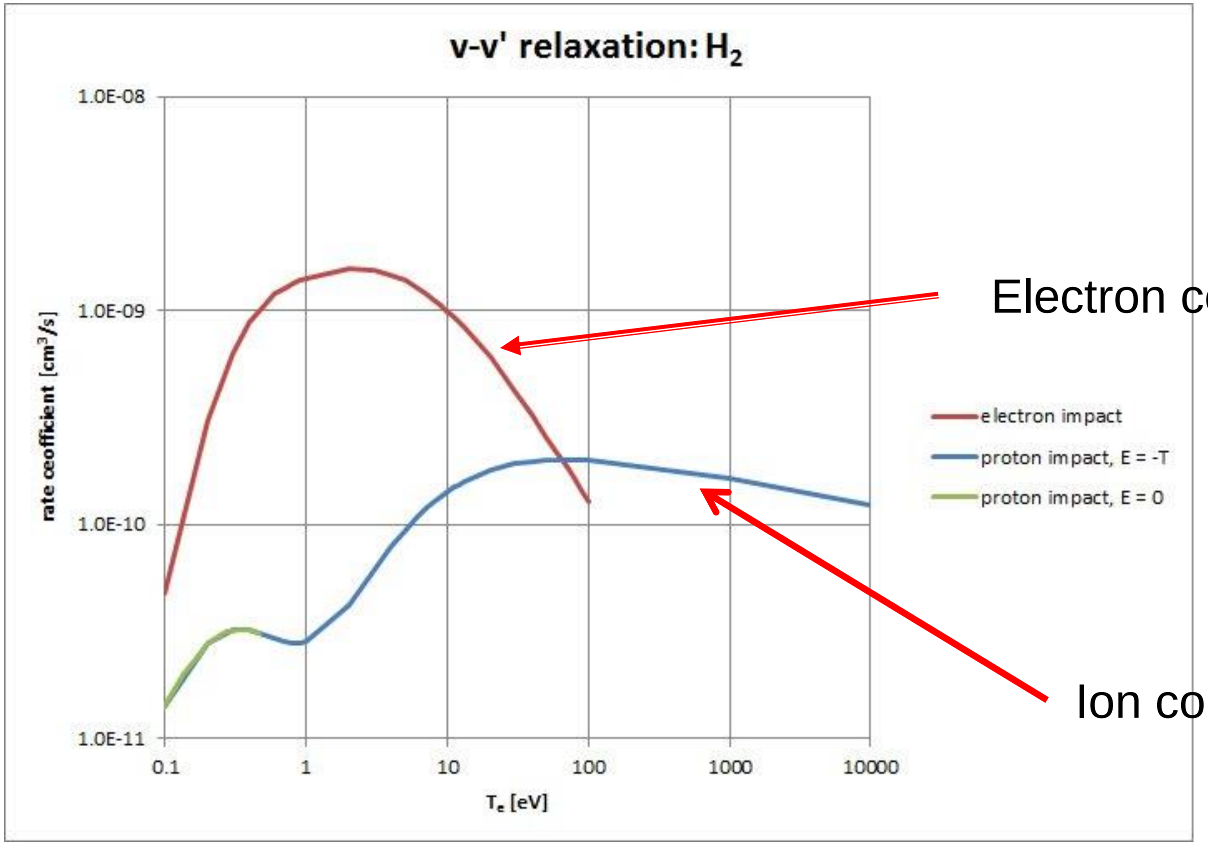
DE, DR, branching ratios with electrons

D, DCT with H

- "Interplay" of transport and inelastic processes
- Rotational analysis is missing
- Isotopic constitution: D_2, T_2, HD, HT and DT, sensitive on vib. energy levels

Spectral analysis in CR models: → model reduction

Build v-v' transition rate matrix, for e and p collisions on H_2 → HYDKIN
→ slowest timescale (smallest eigenvalue): relaxation of T_{vib} to T_e or T_i



Electron collisions on H2(v)

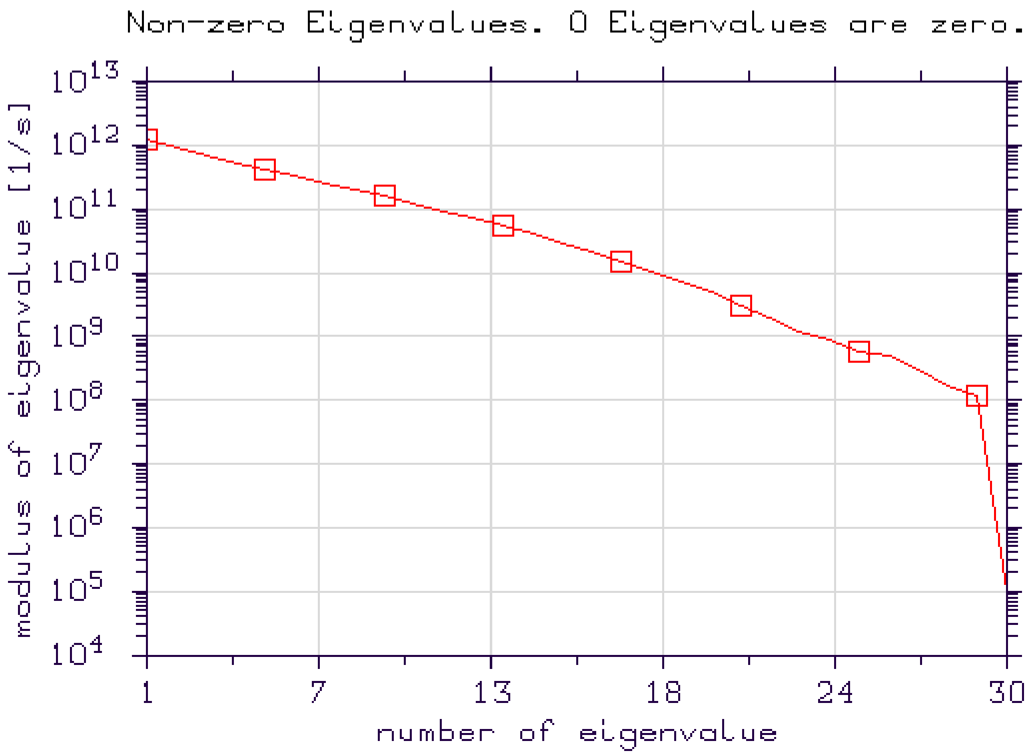
Ion collisions on H2(v)

Cross section database is scanty (very, very scanty, to say the least)
result from (spectral) analysis:
p+H2(v) cross sections large, effect on fusion plasma negligible compared to e+H2(v) (still good to have, **"reserve of knowledge",** but: main focus elsewhere

HYDKIN: spectral analysis for reaction kinetics

Warm up: H-atom, CR model: H(1),H*(2),….,H*(30),H^+

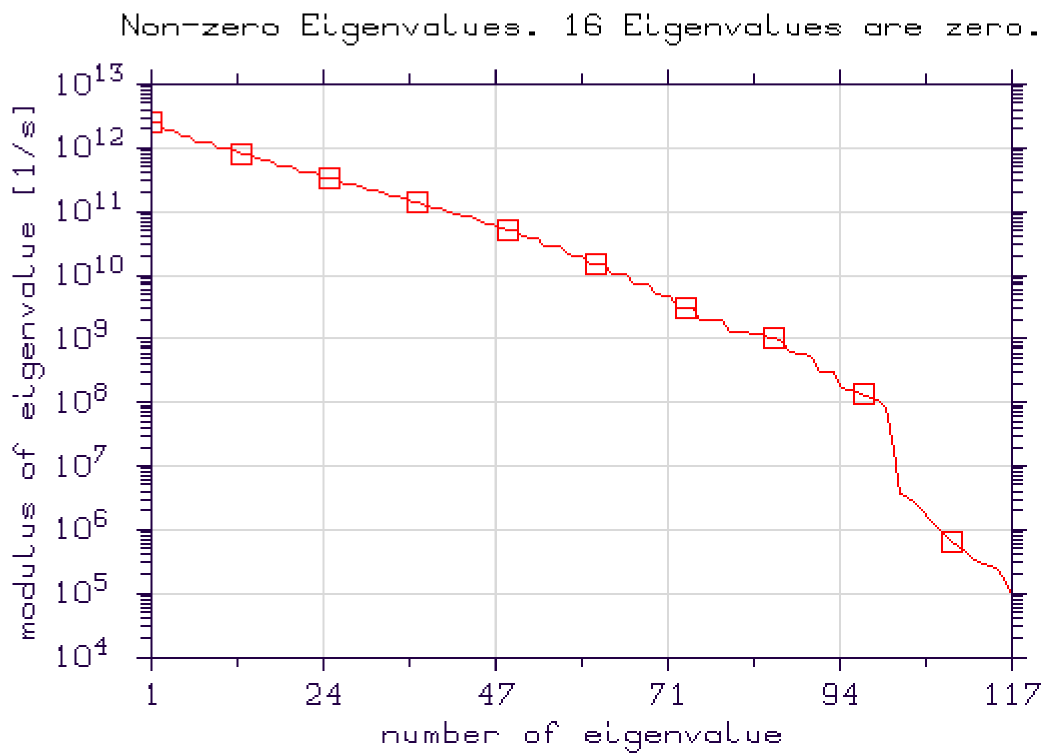
(I,k-excitation, i-ionization A_ik, and k,i de-excitation



@ Te = 10 eV,
ne = 1e13

HYDKIN: spectral analysis for reaction kinetics

Coupled H-H^+-H_2-H_2^+ CR model, @ 10 eV, 1e13 cm-3
134 species/states, 16 final states, 117 non-zero eigenvalues



H, H^-, H_2, H_3^+,….database for fusion edge plasma modelling:

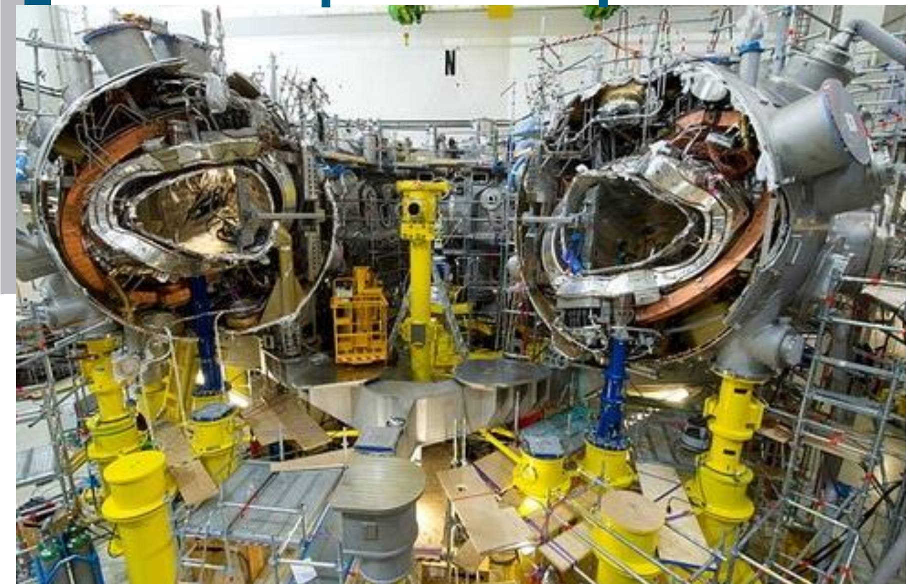
Status: cross sections, CR models, “ok, up 2011..” (at least: compiled, fitted….)

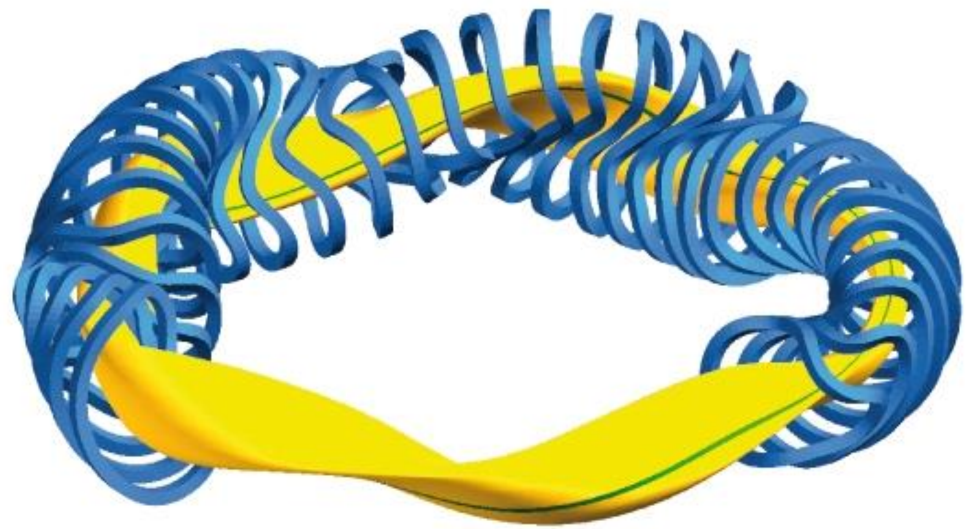
Main issues in transport modelling:

- Multi-parametric dependencies of eff. rates: T_e, T_i, n_e n_{i1}, n_{i2}, E0,…..
- Asymptotic behavior of either: fits or tables
  (what do complex codes really do with the data ??)
- Our current tendency: integrate CR model solvers inside transport solvers,
  evaluated CR rates on the fly, cell by cell,
  fully parallelized (domain decomposition) → very little CPU penalty
  Available for H, soon for He (W7X) , H_2/H (?) ,
  and we would hope for: $BeH/BeH^+/Be$…
- current applications are:
  1. e.g.: ITER diagnostic beam (100 keV) plus Halo
     (thermal gas cloud around 100 keV beam that forms from charge exchange)
  2.) main chamber erosion by neutral CX sputtering, power plant studies

SIMILAR ISSUES: $He – He^+ – He^{++}$

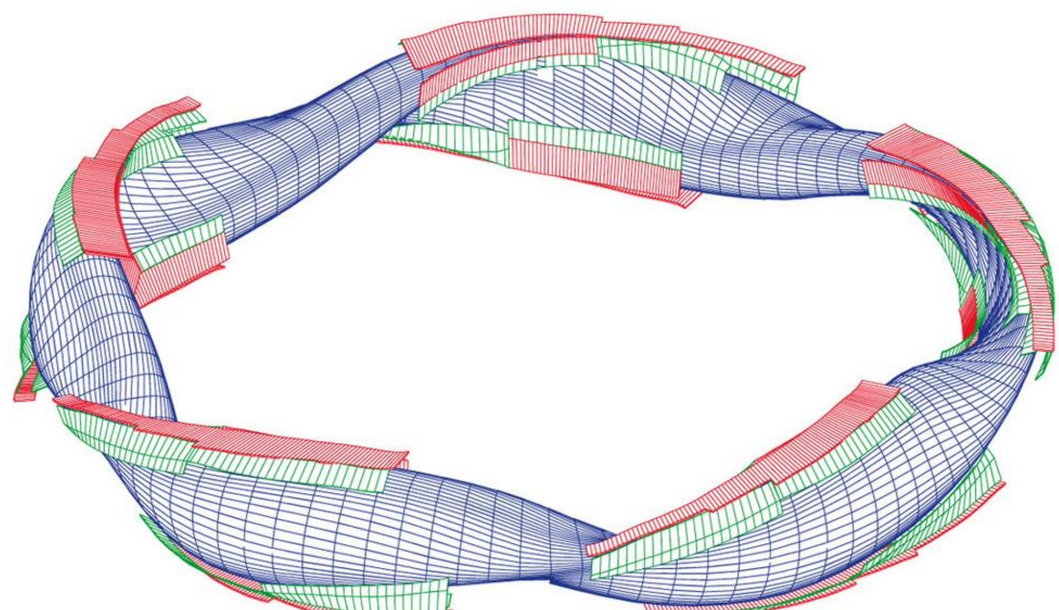
W7X, Greifswald, Germany:
start of plasma operation: October 2015: He-plasmas





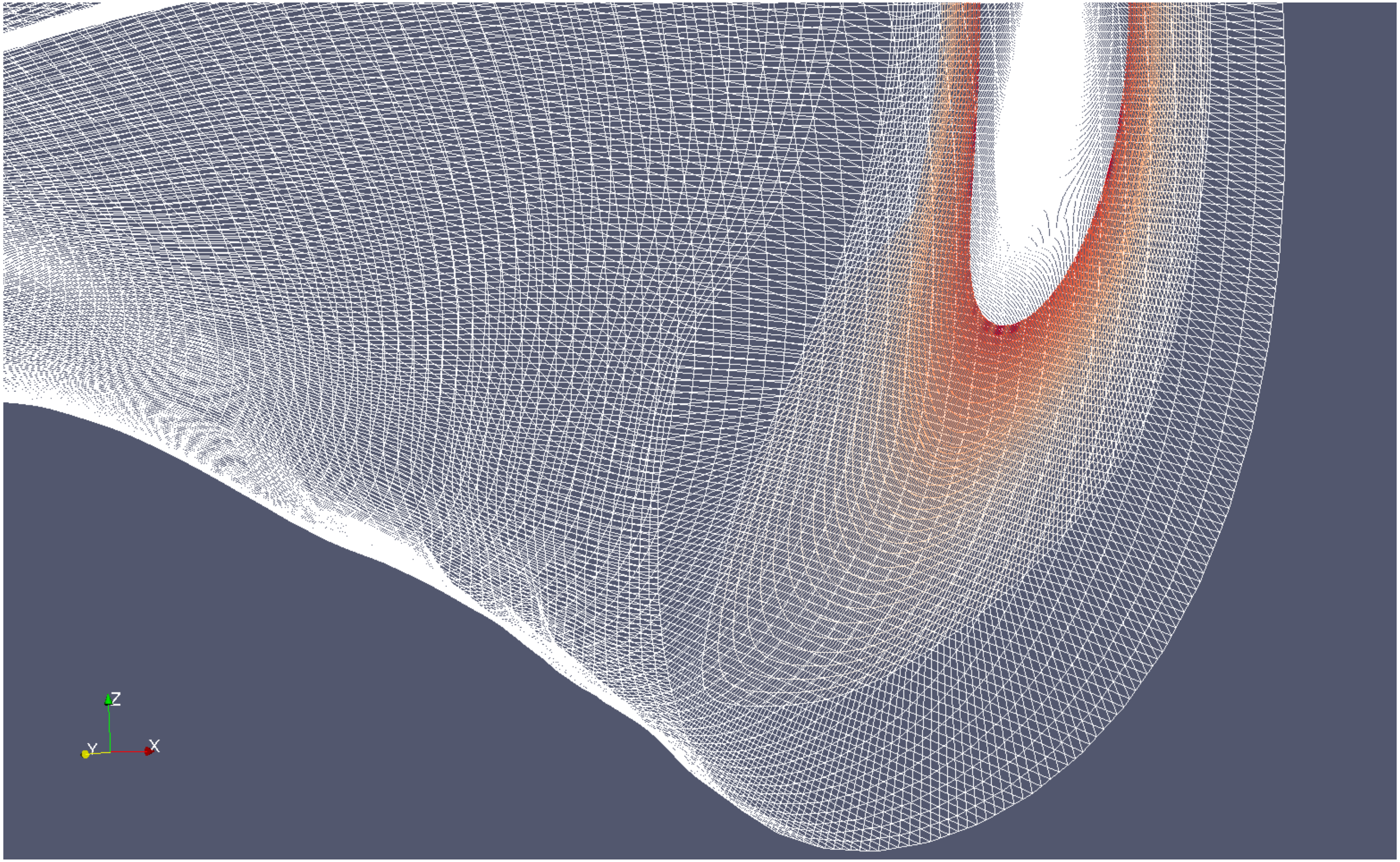
Current FZJ activity:

EMC3-EIRENE:
Fully 3D,
Helium plasmas
He -- He^+ -- He^{++}
by Oct. 2015 ??



Edge Modelling Expressionism……

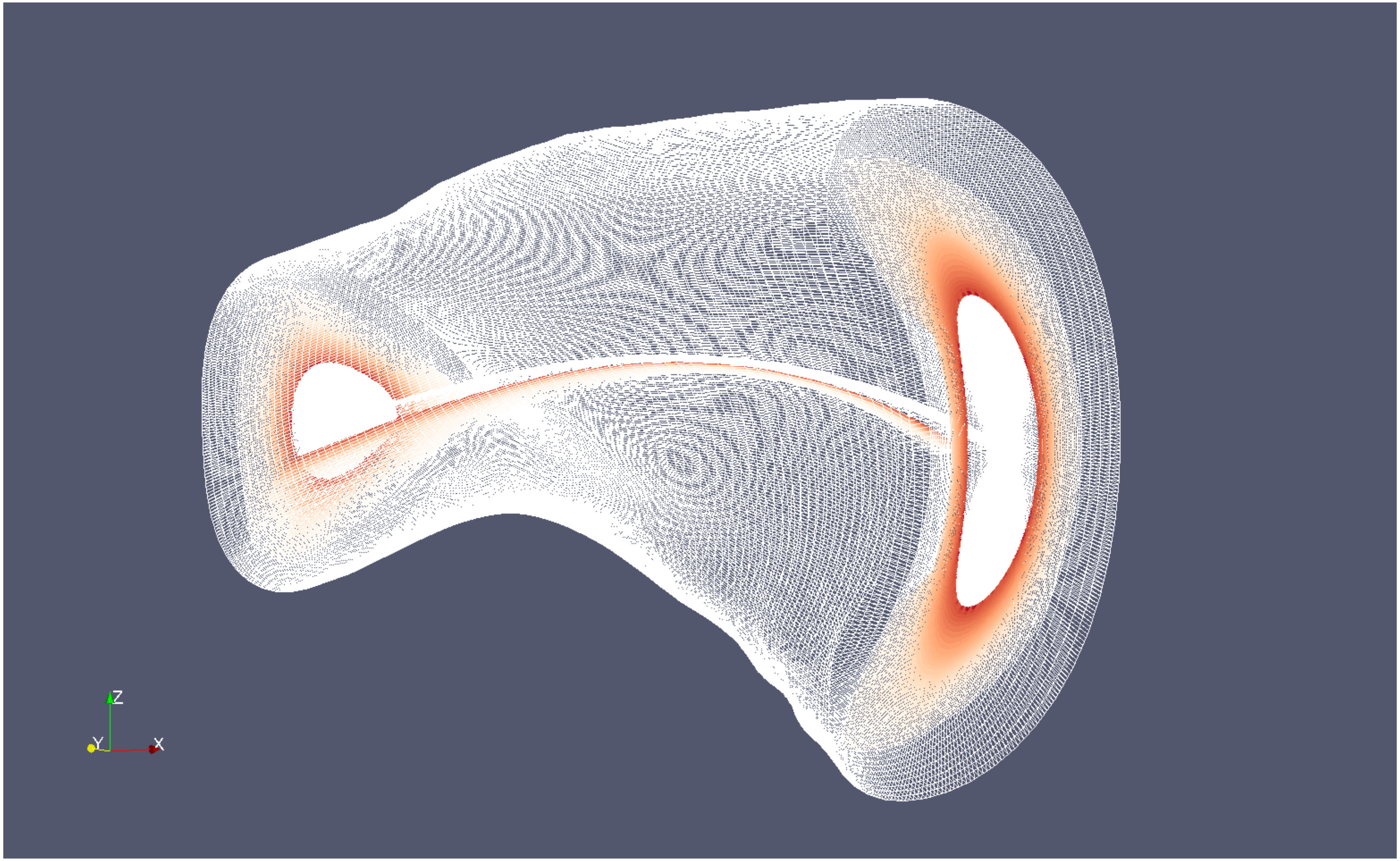
W7X: 3 D grid (trilinear hexahedrons): EMC3-EIRENE, 1-3 Mill cells



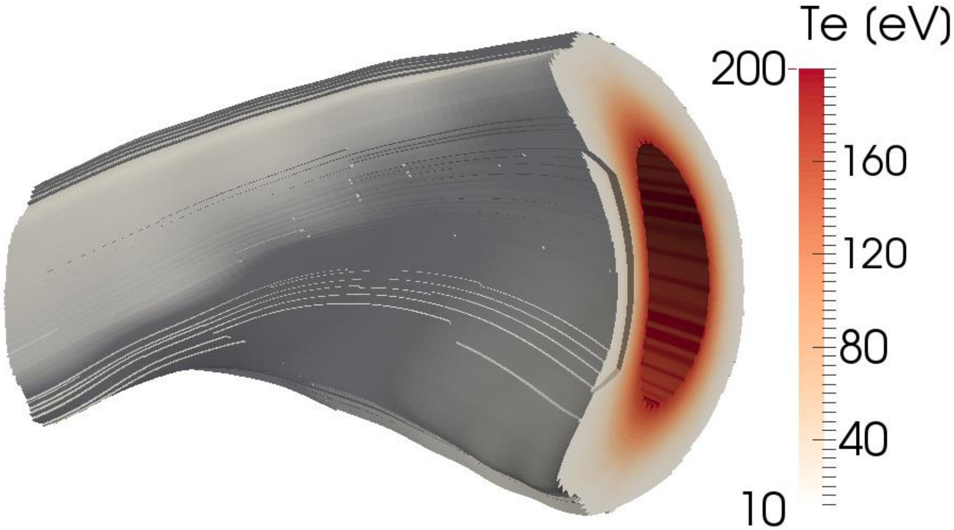
Full He CR model, 65 states, MS resolved, cell by cell, about extra 1-3 sec. CPU cost on 1028 compute cores (typical value)

Edge modelling expressionism……

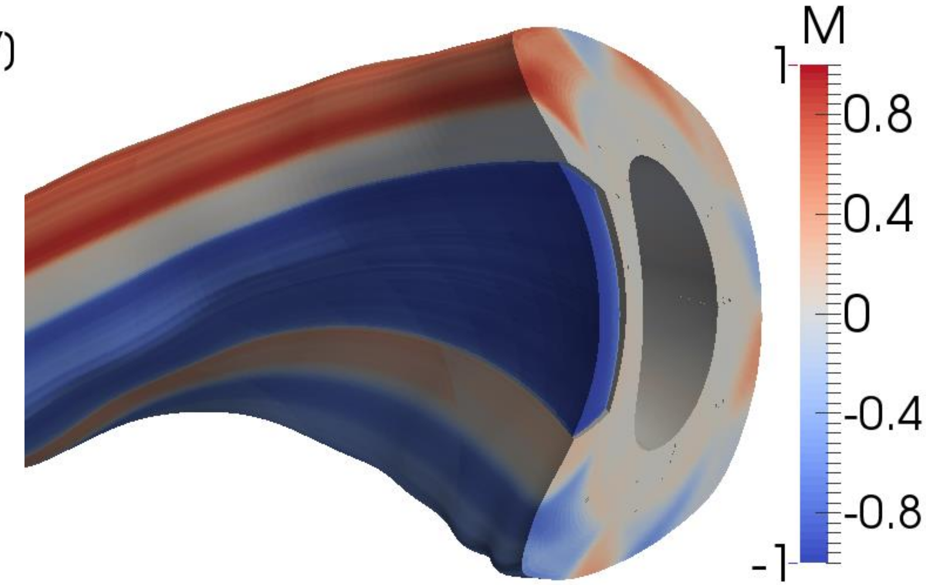
W7X, Te profile, 3D.



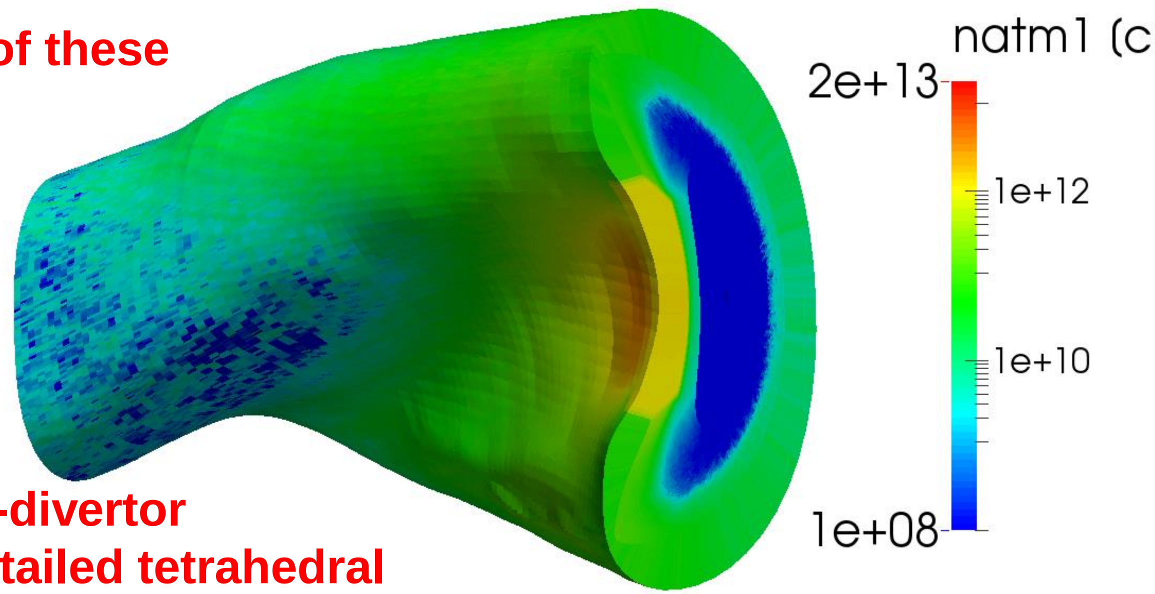
Electron temperature (eV)



Ion flow Mach number, He^{++}



Neutral He atom density, cm^{-3}



Possible future relevance of these developments also for SOLPS-ITER (?)

- **Pure He plasmas ??**
- **Gas flows in full 3D sub-divertor structures, based on detailed tetrahedral discretization?**

Starting Hypothesis at W7X Team: Edge Model for He, He+, ignore He++
(until June 2014)
Spring 2015: **FLYCHK, (AMDU): case study: must build He – He++ model, with He+ only as tracer.**
→ Use EMC3-EIRENE in hybrid fluid-kinetic mode. (M.Rack, D.Reiter, EPS 2015)

Consequences for He - He+ + He++ database:

From a consistent set of cross sections: many datasets are derived:
MS resolved, MS condensed, S/XB, rad. loss, Elect. energy loss rates, opacity, etc…
A single transition cross section upgrade → replace the full set of CR data files.

Solution: Similar to H-COL (built in CR model into transport code)
Also build He-COL (a He-CR Model, with matrix solver inside transport code,
Condensation, data processing: on the fly.

Database: provide all individual He collision processes needed to build a CR matrix.
Issues: asymptotics in rates or cross sections! detailed balancing !

Transport code does not need fits or tables (and their asymptotics)
to multidimensional CR data vs.: Te, Ti, E0, ne, ni1,ni2…..)

OUTLOOK

- **Generals:** on AM-S data use in fusion plasma models

  "internal consistency", completeness (competing processes)

- **Surface Data:** Reflection, Sputtering:

  multidimensional distributions: online "TRIM" database
  maintained, and still occasionally upgraded upon demand.

- **AM Data:**

  FZJ: data evaluation, data generation, database compilation "sui generis"
  was initiated by Ratko Janev:

  C_xH_y (database is frozen, some low T updates for particle rearrangement collisions are pending),

  SiH_y (database frozen)

  H, H^-, H_2, H_2^+, H_3^+…→ ongoing, (now mainly: asymptotics, documentation)

  Be, Be_xH_y : unfinished

- **FZJ data activity is now focused on:**

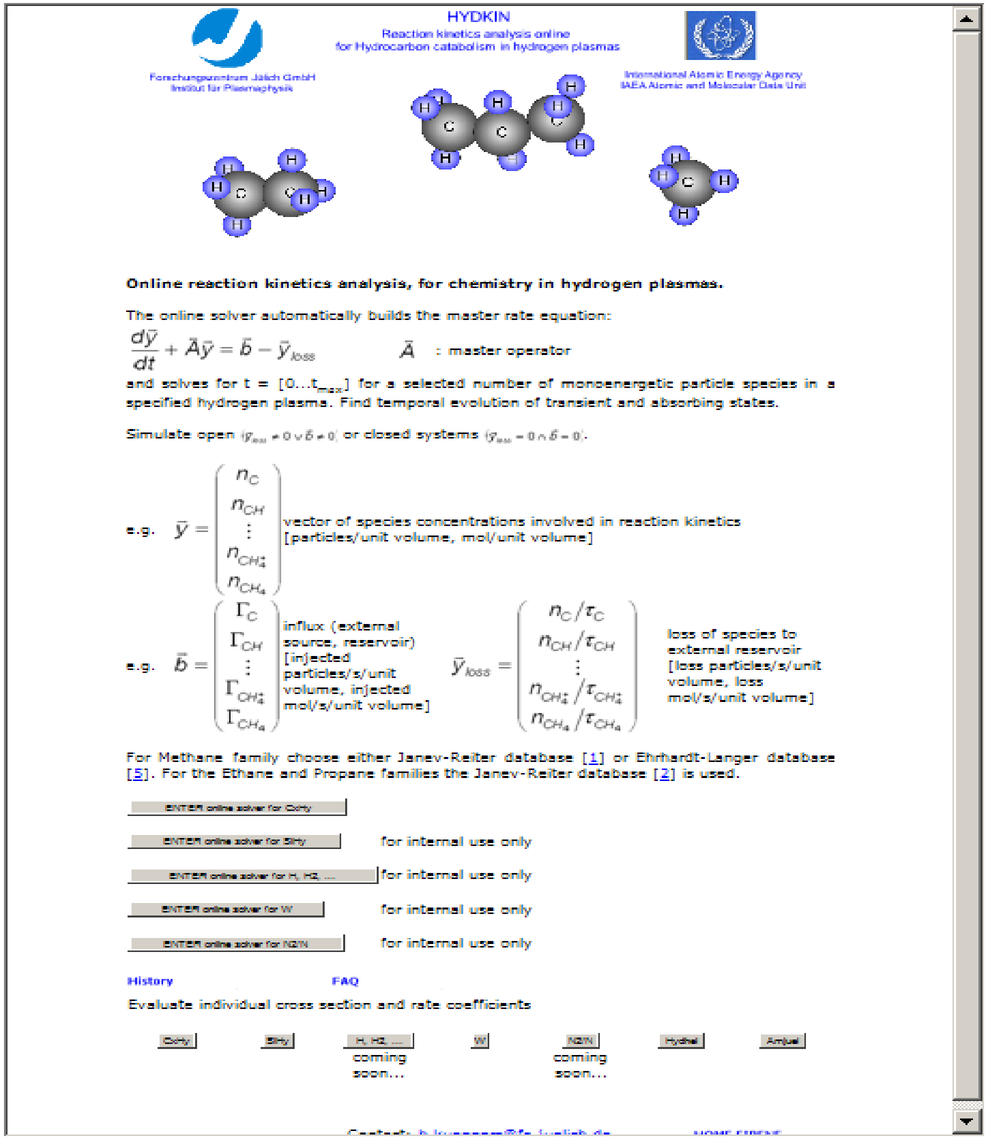
  Data processing/formatting, asymptotics, internal CR modules for transport simulations,…,raw data public exposure.

  Sensitivity analysis (uncertainty propagation) on linear CR or chemistry models

Basic input for EIRENE: A&M data, (& surface data)

JÜLICH
FORSCHUNGSZENTRUM

Goal: publicly expose raw data used in any modelling



HYDKIN
Reaction kinetics analysis online
for Hydrocarbon catabolism in hydrogen plasmas

Forschungszentrum Jülich GmbH
Institut für Plasmaphysik

International Atomic Energy Agency
IAEA Atomic and Molecular Data Unit

Online reaction kinetics analysis, for chemistry in hydrogen plasmas.

The online solver automatically builds the master rate equation:

$$\frac{d\bar{y}}{dt} + \bar{A}\bar{y} = \bar{b} - \bar{y}_{loss} \qquad \bar{A} \ : \text{master operator}$$

and solves for t = $[0 \ldots t_{max}]$ for a selected number of monoenergetic particle species in a specified hydrogen plasma. Find temporal evolution of transient and absorbing states.

Simulate open $(\bar{y}_{loss} \neq 0 \vee \bar{b} \neq 0)$ or closed systems $(\bar{y}_{loss} = 0 \wedge \bar{b} = 0)$.

e.g. $\bar{y} = \begin{pmatrix} n_C \\ n_{CH} \\ \vdots \\ n_{CH_4^+} \\ n_{CH_4} \end{pmatrix}$ vector of species concentrations involved in reaction kinetics [particles/unit volume, mol/unit volume]

e.g. $\bar{b} = \begin{pmatrix} \Gamma_C \\ \Gamma_{CH} \\ \vdots \\ \Gamma_{CH_4^+} \\ \Gamma_{CH_4} \end{pmatrix}$ influx (external source, reservoir) [injected particles/s/unit volume, injected mol/s/unit volume]

$\bar{y}_{loss} = \begin{pmatrix} n_C/\tau_C \\ n_{CH}/\tau_{CH} \\ \vdots \\ n_{CH_4^+}/\tau_{CH_4^+} \\ n_{CH_4}/\tau_{CH_4} \end{pmatrix}$ loss of species to external reservoir [loss particles/s/unit volume, loss mol/s/unit volume]

For Methane family choose either Janev-Reiter database [1] or Ehrhardt-Langer database [5]. For the Ethane and Propane families the Janev-Reiter database [2] is used.

ENTER online solver for CxHy

ENTER online solver for SiHy — for internal use only

ENTER online solver for H, H2, ... — for internal use only

ENTER online solver for W — for internal use only

ENTER online solver for N2/N — for internal use only

History FAQ

Evaluate individual cross section and rate coefficients

CxHy | SiHy | H, H2, ... (coming soon...) | W | N2/N (coming soon...) | Hydhel | Amjuel

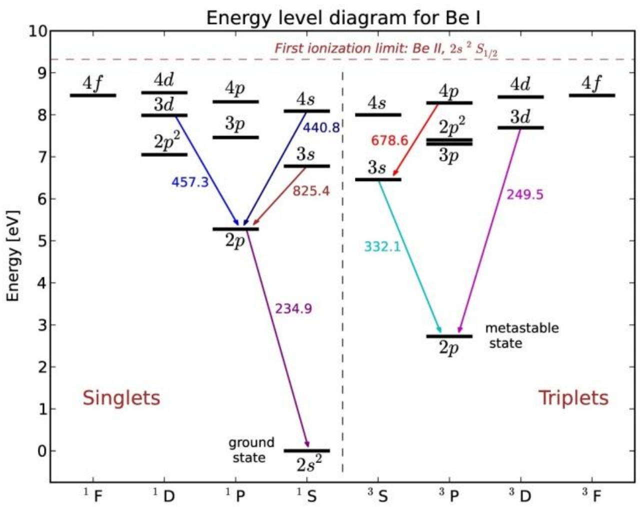
www.hydkin.de

Online data base
and data analysis tool-box:

- CR model condensation
- Sensitivity analysis
- Fragmentation pathway analysis
- Reduced models

• Hydrocarbons
• Silanes
• H, H_2, H_3^+,….
• W, W^+, ….W^{74+}
• N, N_2, activity stopped, rely on other communities…

Be-BeH-BeH^+, ……
attempted, but expert help needed for cases of doubt



Towards a Be – Be^+ CR modul for transport simulations

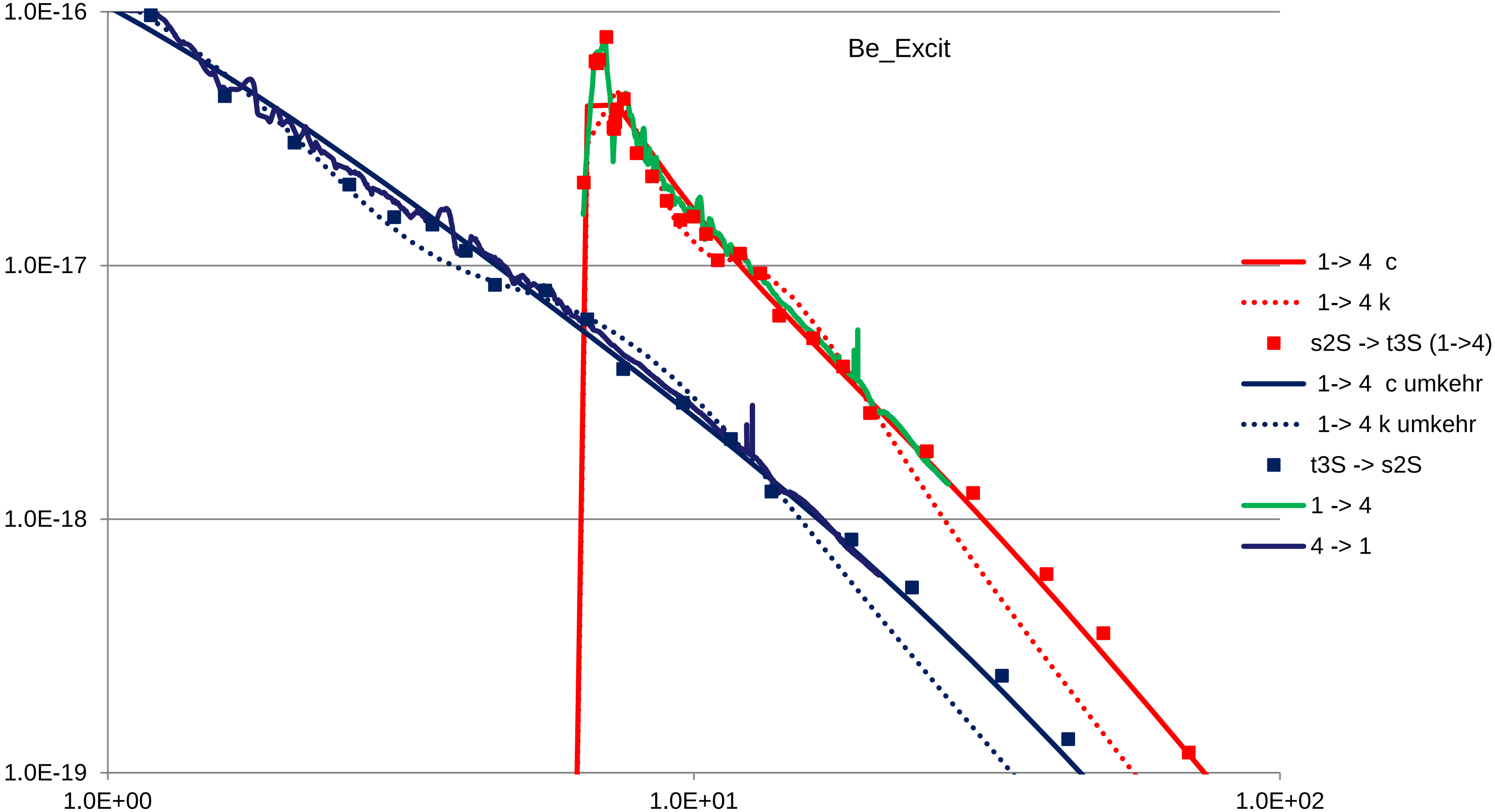
Various sets of CCC cross section data provided by I. Bray, 2013

Complementary set of R Matrix cross section data from C. Balance (2014)

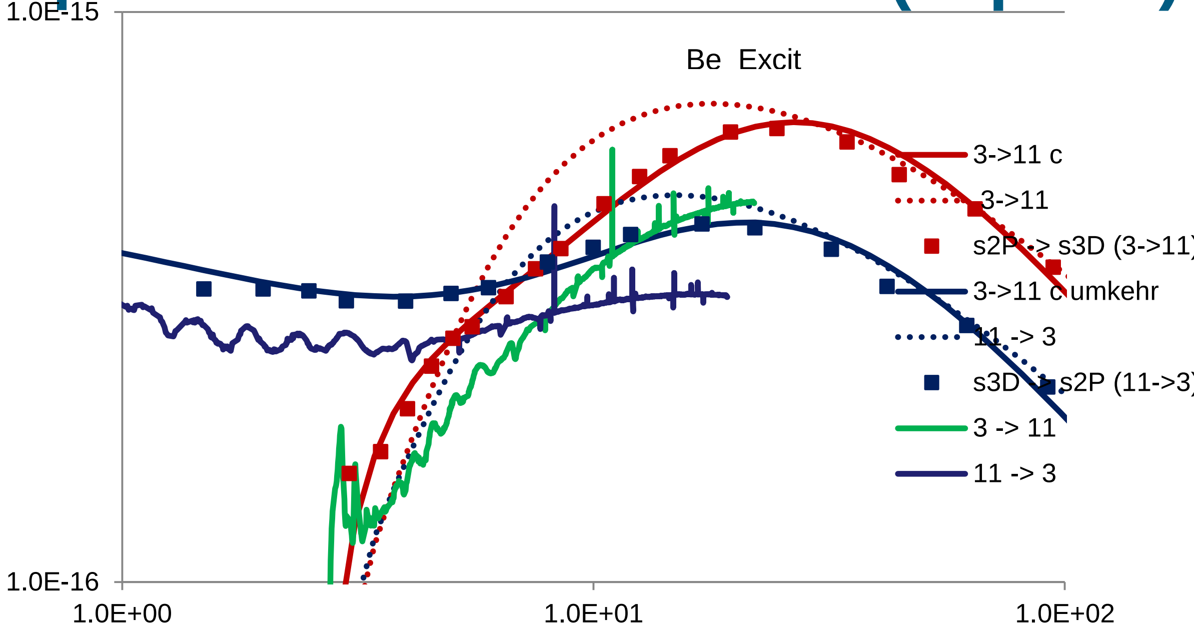
			2s21S	2s12p13P	2s12p11P	2s13s13S	2s13s11S		2s13p13P		2s13p11P	2s13d13D	2s13d11D	2s14s13S	2s14s11S	2s14p13P	2s14p11P	2s14d13D	2s14f13F	2s14f11F	2s14d11D
			s2S	t2P	s2P	t3S	s3S	S2D	t3P	T2P	s3P	t3D	s3D	t4S	s4S	t4P	s4P	t4D	t4F	s4F	s4D
			1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
2s21S	s2S	1		C 23	K 6	C 23	K 22	K22	C 23	K2	K 22	K 2	K 22	C 23	K 21 C 22	C 23	K 22 C 5	K 2	C 23	K 11 C 22	K 22 C 22
2s12p13P	t2P	2			C 23	K 21	C 23	K2	K 1	K21	C 23	K 5	C 23	C 5	K 2	C 22	C 23	C 5	C 22	C 23	C 23
2s12p11P	s2P	3				C 23	K 21	K1	C 23	K2	K 6	K 2	C22	C 23	C 5	K 2 C 23	K 21 C 22	C 23	K 2 C 23	C 22	K 6 C 5
2s13s13S	t3S	4					K23	K2	C 5	K11	C 23	K 21	K 23	K 21 C 22	K 23	C 5	K 2 C 23	C 22	C 22	K 2 C 23	K 2 C 23
2s13s11S	s3S	5						K22	C 23		K 8	C 23	K 21	C 23	K 5 C 22	K 2 C 23	C 5	K 2	C 23	C 22	K 22 C 22
	S2D	6								K22											
2s13p13P	t3P	7								K5	C 23	C 5	C23	K 22 C 5	C 23	K 1 C 22	C 23	C 5	C22	C 23	C 23
	T2P	8																			
2s13p11P	s3P	9										C 23	C 5	K 23	K 8 C 5	K 2	C 22	K 23 C 23	K 2 C 23	C 22	C 5
2s13d13D	t3D	10											C 23	C 22	K 1 C 23	K 11 C 5	C 23	K 5 C 22	K 22 C 5	C 23	C 23
2s13d11D	s3D	11													C 22	C 23	K 22 C 5	C 23	K 2 C 23	K 22 C 5	C 22
2s14s13S	t4S	12											C 23		nur K 22	nur K				nur K 2	
2s14s11S	s4S	13															nur K		nur K 22	nur K	
2s14p13P	t4P	14																	nur K		
2s14p11P	s4P	15																		nur K	nur K
2s14d13D	t4D	16																			
2s14f13F	t4F	17																			
2s14f11F	s4F	18																			
2s14d11D	s4D	19																			

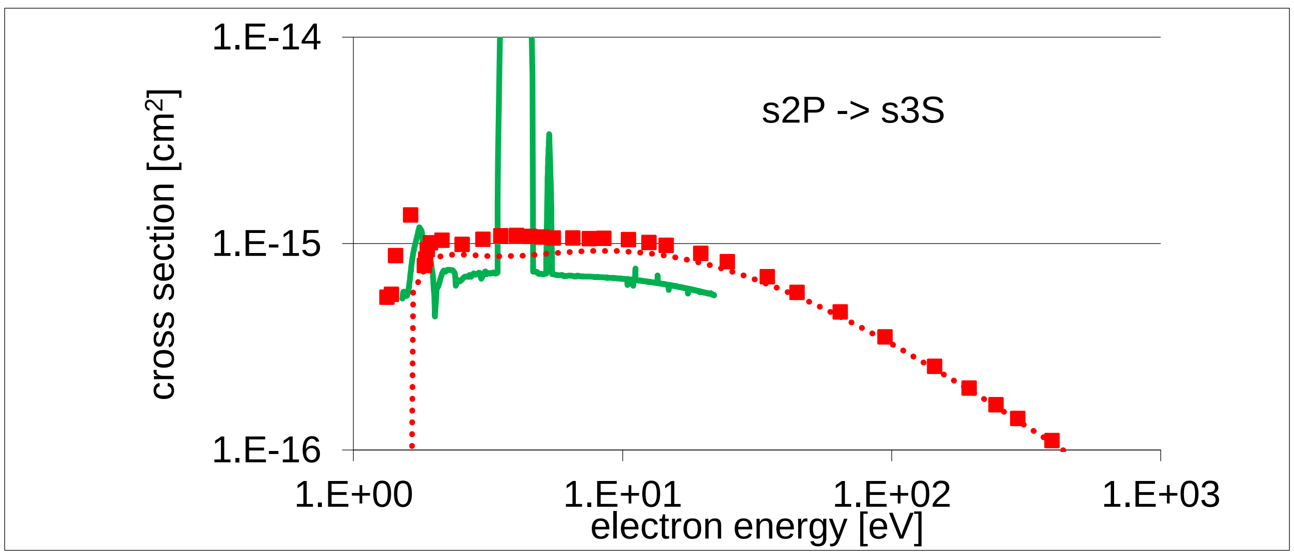
e + Be(1) → e + Be(4)

2 datasets (CCC and R-Matrix), 2 set of fits (2 tasks, c & k, independent): positive example. Easy decision



Less clear examples: CCC or R-Matrix, and poor fits…. → evaluation (experts)





So: **bring on Be – Be+ evaluated cross section database**:

with:

- either asymptotically correct fits

  or

  recommendations re threshold and high E asymptotics
- consistent forward and reverse processes
- double excited states?
- recombination (radiative, threebody, dielectronic…)

Current Nucl. Fusion N_2 database: obsolete !

see e.g.: Planetary Atmospheric Entries

Dissociative Recombination in Reactive Flows Relative to Planetary Atmospheric Entries

Nitrogen

Species, states and elementary processes

N_2, N_2^+, N, N^+ and e^-

N_2	$X^1\Sigma_g^+(v=0 \rightarrow v_{max}=67)$, $A^3\Sigma_u^+$, $B^3\Pi_g$, $W^3\Delta_u$, $B'^3\Sigma_u^-$, $a'^1\Sigma_u^-$, $a^1\Pi_g$, $w^1\Delta_u$, $G^3\Delta_g$, $C^3\Pi_u$, $E^3\Sigma_g^+$	
N_2^+	$X^2\Sigma_g^+$, $A^2\Pi_u$, $B^2\Sigma_u^+$, $a^4\Sigma_u^+$, $D^2\Pi_g$, $c^2\Sigma_u^+$	*150 states*
N	$^4S^o_{3/2}$, $^2D^o = (^2D^o_{5/2} + ^2D^o_{3/2})$, $^2P^o = (^2P^o_{1/2} + ^2P^o_{3/2})$, $^4P_{1/2}$,... (63 states)	
N^+	$^3P_0$, $^3P_1$, $^3P_2$, $^1D_2$, $^1S_0$, $^5S^o_2$, $^3D^o_3$, $^3D^o_2$, $^3D^o_1$	

CR Model Database – CoRaM – N_2

Forward rate coefficient

$$k_i(T_{A,e}) = \sqrt{\frac{8\,k_B\,T_{A,e}}{\pi\,\mu}} \int_{x_0}^{+\infty} x\,e^{-x}\,\sigma_i(x)\,dx$$

with $\sigma_i(x)$ the cross section and

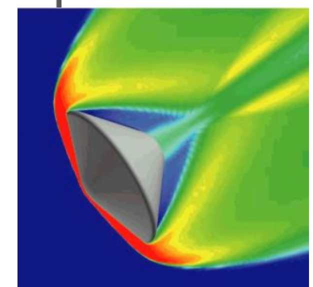
$x = \frac{\varepsilon}{k_B\,T_{A,e}}$ the reduced collision energy

Backward rate coefficient from ***Detailed Balance***

⇒ *100 000 elementary processes*

A. BULTEL *Paris – July, 10th 2013*

Vibrational processes	$N_2(X,v) + e^- \rightarrow N_2(X,w) + e^-$
	$N_2(X,v) + e^- \rightarrow 2\,N(^4S^o_{3/2}) + e^-$
	$N_2(X,v) + (N_2 \text{ or } N) \rightarrow N_2(X,w) + (N_2 \text{ or } N)$
	$N_2(X,v) + N(^4S^o_{3/2}) \rightarrow 3\,N(^4S^o_{3/2})$
	$N_2(X,v_{max}) + N_2 \rightarrow 2\,N(^4S^o_{3/2}) + N_2$
	$N_2(X,v_1) + N_2(X,v_2) \rightarrow N_2(X,w_1) + N_2(X,w_2)$
Electronic excitation	$N_2(i) + e^- \rightarrow N_2(j) + e^-$
	$N_2(i) + (N_2 \text{ or } N) \rightarrow N_2(j) + (N_2 \text{ or } N)$
	$N_2^+(i) + e^- \rightarrow N_2^+(j) + e^-$
	$N(i) + e^- \rightarrow N(j) + e^-$
	$N(i) + (N_2 \text{ or } N) \rightarrow N(j) + (N_2 \text{ or } N)$
	$N^+(i) + e^- \rightarrow N^+(j) + e^-$
	$N^+(i) + (N_2 \text{ or } N) \rightarrow N^+(j) + (N_2 \text{ or } N)$
Excitation transfer	$N_2(A) + N_2(A) \rightarrow N_2(X) + N_2(B)$
	$N_2(A) + N_2(A) \rightarrow N_2(X) + N_2(C)$
	$N_2(A) + N_2(B) \rightarrow N_2(X) + N_2(C)$
	$N_2(A) + N(^4S^o_{3/2}) \rightarrow N_2(X) + N(^2P^o)$
	$N_2(B) + N(^4S^o_{3/2}) \rightarrow N_2(X) + N(^2P^o)$
	$N_2(C) + N(^4S^o_{3/2}) \rightarrow N_2(X) + N(^2P^o)$
Dissociation	$N_2(i \neq X) + e^- \rightarrow N(j) + N(k) + e^-$
	$N_2^+(i) + e^- \rightarrow N(j) + N^+(k) + e^-$
Ionisation	$N_2(i) + e^- \rightarrow N_2^+(j) + 2\,e^-$
	$N_2(i) + (N_2 \text{ or } N) \rightarrow N_2^+(j) + e^- + (N_2 \text{ or } N)$
	$N(i) + e^- \rightarrow N^+(j) + 2\,e^-$
	$N(i) + (N_2 \text{ or } N) \rightarrow N^+(j) + e^- + (N_2 \text{ or } N)$
Charge exchange	$N_2(X) + N^+(^3P_0) \rightarrow N_2^+(X) + N(^4S^o_{3/2} \text{ or } ^2P^o)$
	$N_2(X) + N^+(^3P_0) \rightarrow N_2^+(A) + N(4S^o_{3/2})$
Dissociative recombination	$N_2^+(X) + e^- \rightarrow N(^4S^o_{3/2}) + N(^2D^o \text{ or } ^2P^o)$
	$N_2^+(X) + e^- \rightarrow N(^2D^o) + N(^2D^o)$
Radiation ***Escape factor***	$N_2(B^3\Pi_g) \rightarrow N_2(A^3\Sigma_u^+) + h\nu$ (1st positive)
	$N_2(C^3\Pi_u) \rightarrow N_2(B^3\Pi_g) + h\nu$ (2nd positive)
	$N_2^+(B^2\Sigma_u^+) \rightarrow N_2^+(X^2\Sigma_g^+) + h\nu$ (1st negative)
	$N(i) \rightarrow N(j < i) + h\nu$
	$N^+(i) \rightarrow N^+(j < i) + h\nu$



A. Bultel et al., UNIVERSITÉ DE ROUEN, UNIVERSITÉ DE AIX-MARSEILLE (FRANCE)

Thank you