Simulations of the edge plasma: the role of atomic, molecular and surface physics

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Contributors to the EFDA TF ITM

Introduction

- Fusion & Energy Production
- Simulations of the Edge Plasma
  – SOLPS
- EFDA TF ITM
  – Data needs
  – Proposed access mechanism

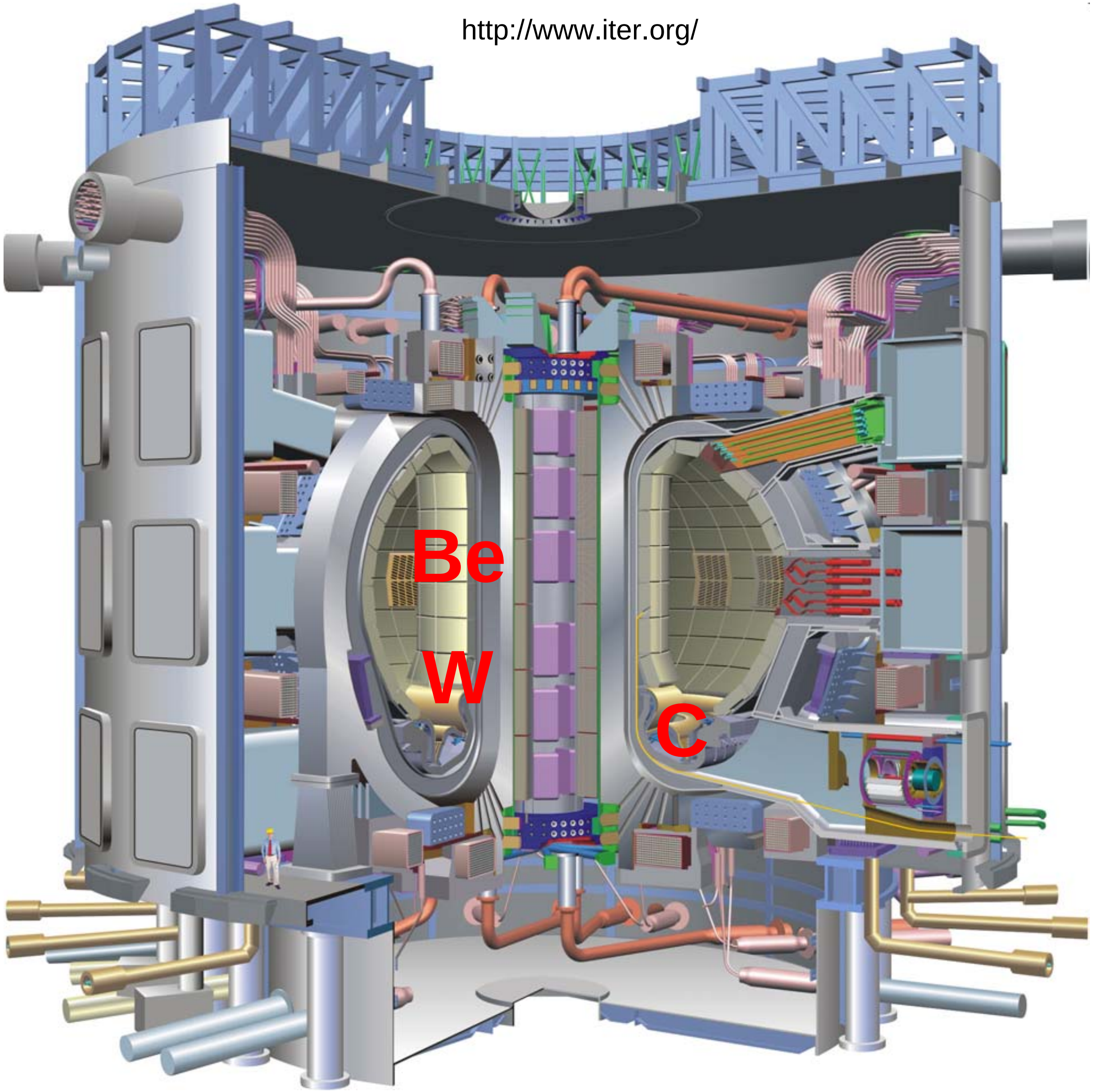
Fusion & Energy Production

- Controlled Thermonuclear Fusion presents a possible base load electric power provider
- Next step of the Magnetic Confinement approach is ITER, currently being built by 7 parties
  - –First plasma predicted for 2018

ITER

		Units
Plasma Major Radius	6.2	m
Plasma Minor Radius	2.0	m
Plasma Volume	840	m3
Plasma Current	15.0	MA
Toroidal Field on Axis	5.3	T
Fusion Power	500	MW
Burn Flat Top	>400	s
Power Amplification	>10	

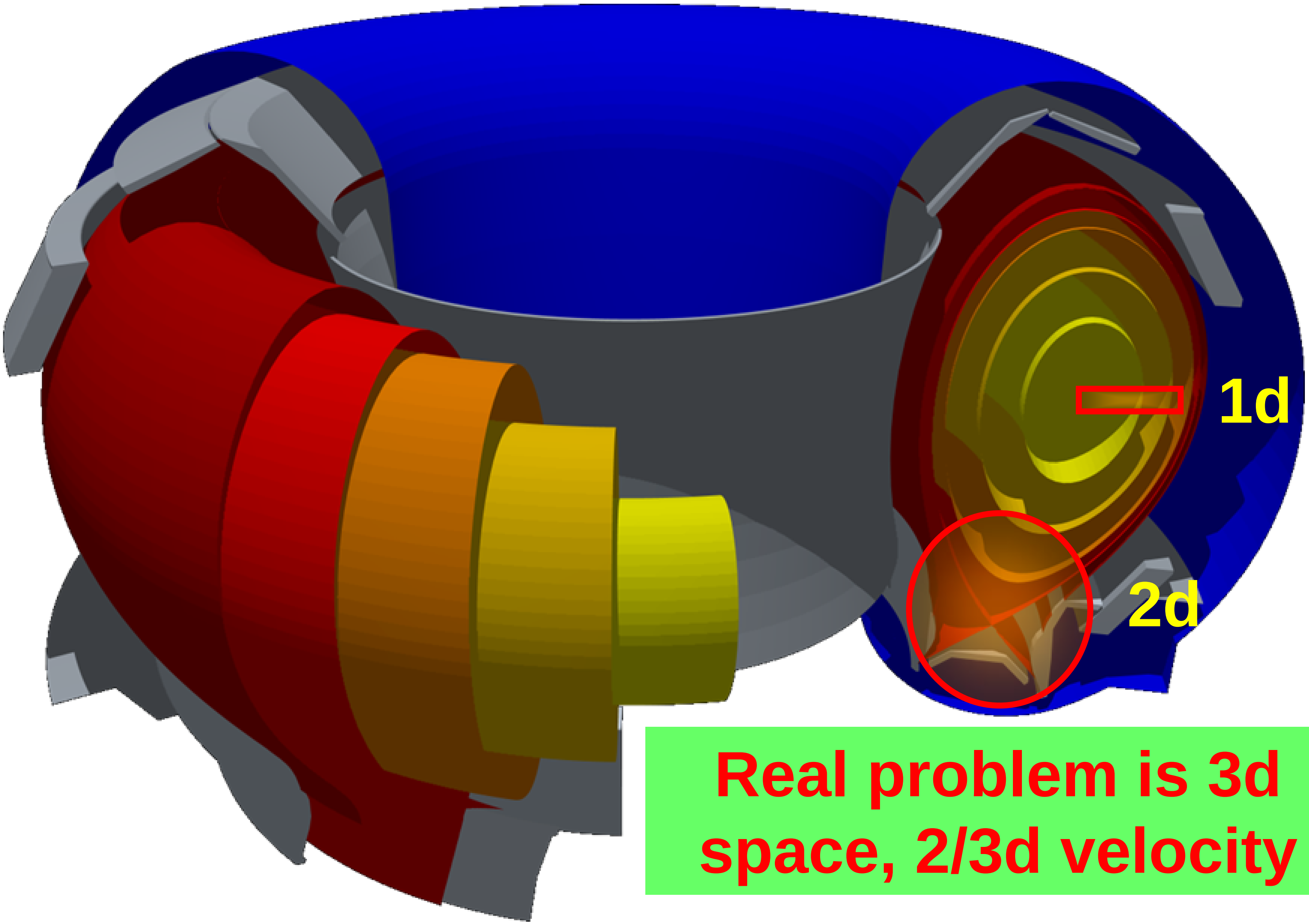
http://www.iter.org/



Implications of the material choice for ITER

- Walls/Targets
  - W
    - Many charge states
    - Data still somewhat uncertain
  - Be
    - Alloying with W
  - C
    - Hydrocarbon chemistry ($C_iD_jT_k$)
    - Tritium co-deposition
      - Hence probable removal before DT phase
- Unavoidable
  - D, T
    - Molecules (D_2, DT, T_2)
  - H (at the beginning)
  - He
- Added (radiation cooling)
    - Ne, Ar, Kr
      - Increase sputtering of W
    - N (?)
      - Molecules
      - Uncertain sticking
- Others
  - H, O, F, Fe, Ni, Cu

Simulations



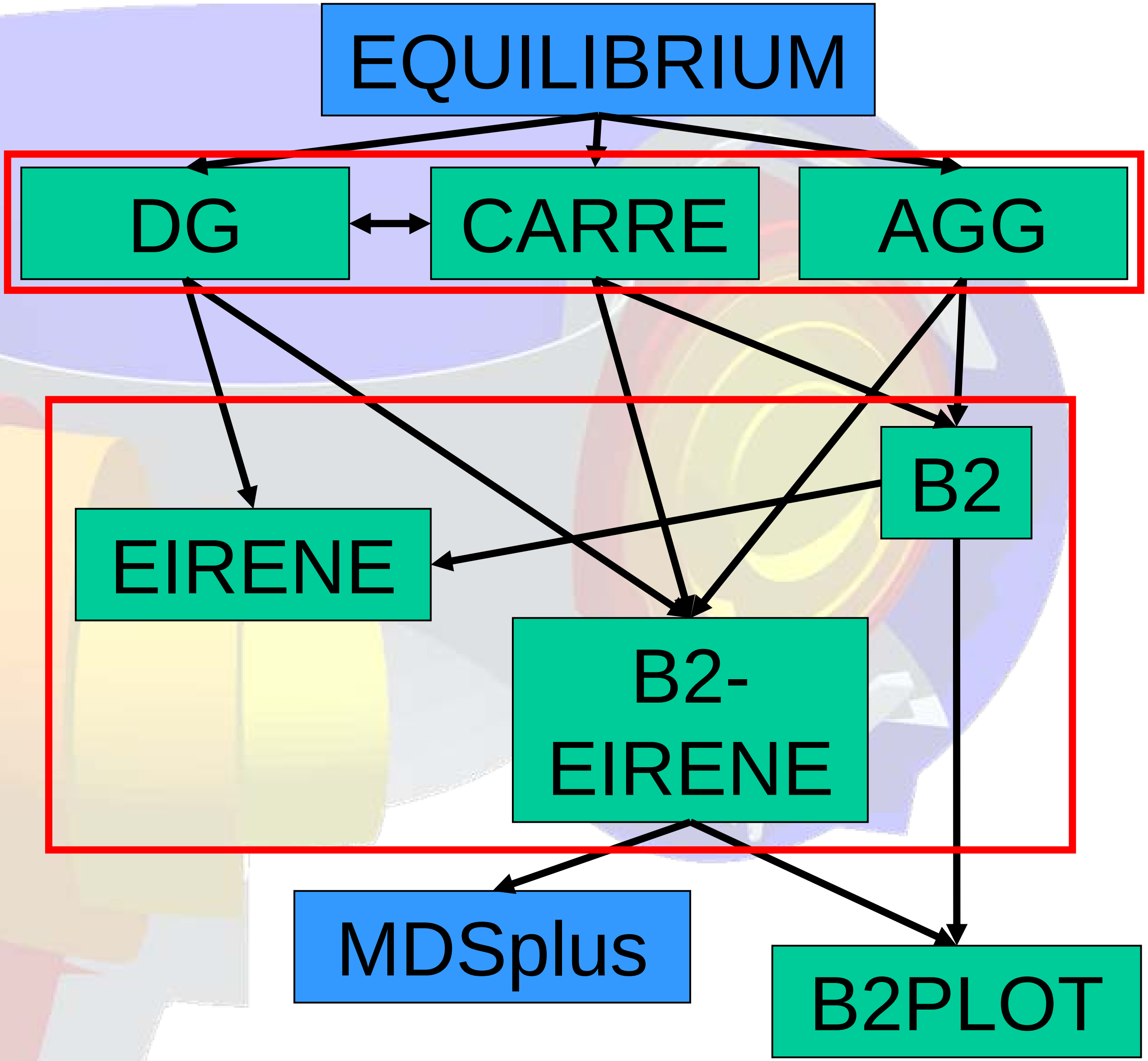
Real problem is 3d space, 2/3d velocity

2d Edge Simulations

- Plasma
  - Fluid description
    - Density of ion charge states
    - Parallel momentum of ion charge states
    - Electron and ion temperatures
    - Potential
- Neutrals
  - Either
    - Fluid (2d)
    - **Kinetic** (3d mapped to 2d)
  - Include
    - Recycling
    - Sputtering
    - (photon transport)

SOLPS

- Grid preparation
  - CARRE
  - DG
  - AGG
  - (TRIANG)
- Plasma
  - B2, B2.5
- Neutrals
  - EIRENE
- Coupled
  - B2-EIRENE
- Visualization
  - B2PLOT



SOLPS: A&M Data

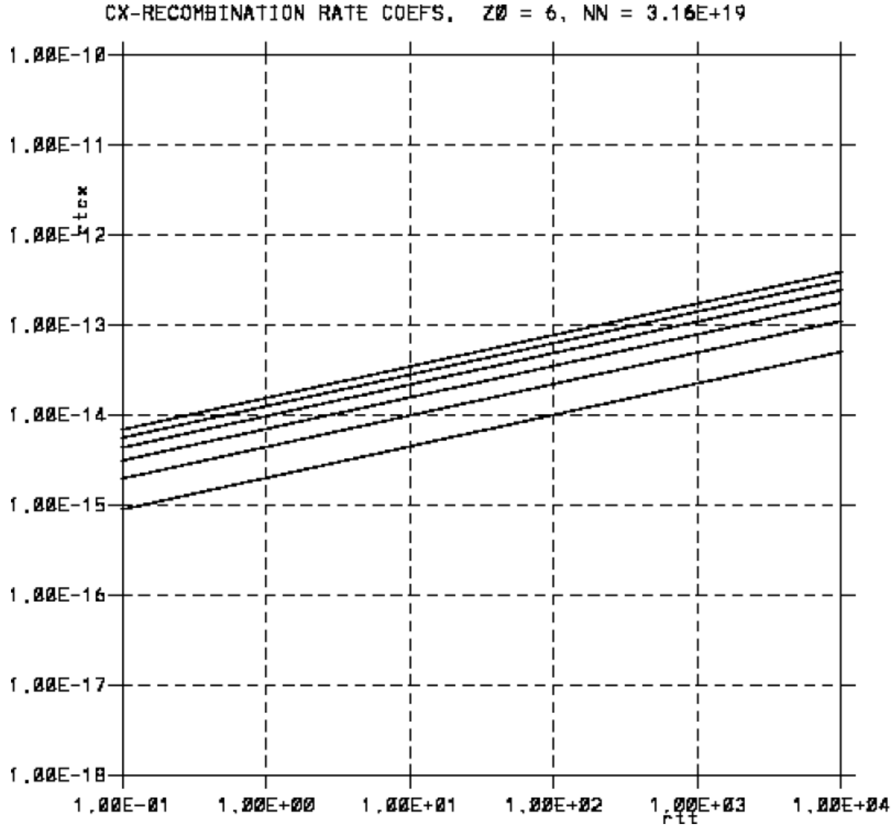
- Plasma code (B2)
  - Rate coefficients
    - Ionization, recombination, electron cooling, charge exchange
  - Rates
    - Sputtering, reflection
- Post-processing
  - Spectral line emissivity
- Neutrals code (EIRENE)
  - Rate coefficients
    - Ionization, recombination, electron cooling, **molecular break-up**
  - Cross Sections
    - Charge exchange, elastic collisions
  - Rates
    - Sputtering, reflection
  - Photon emissivity, *etc* for photon transport

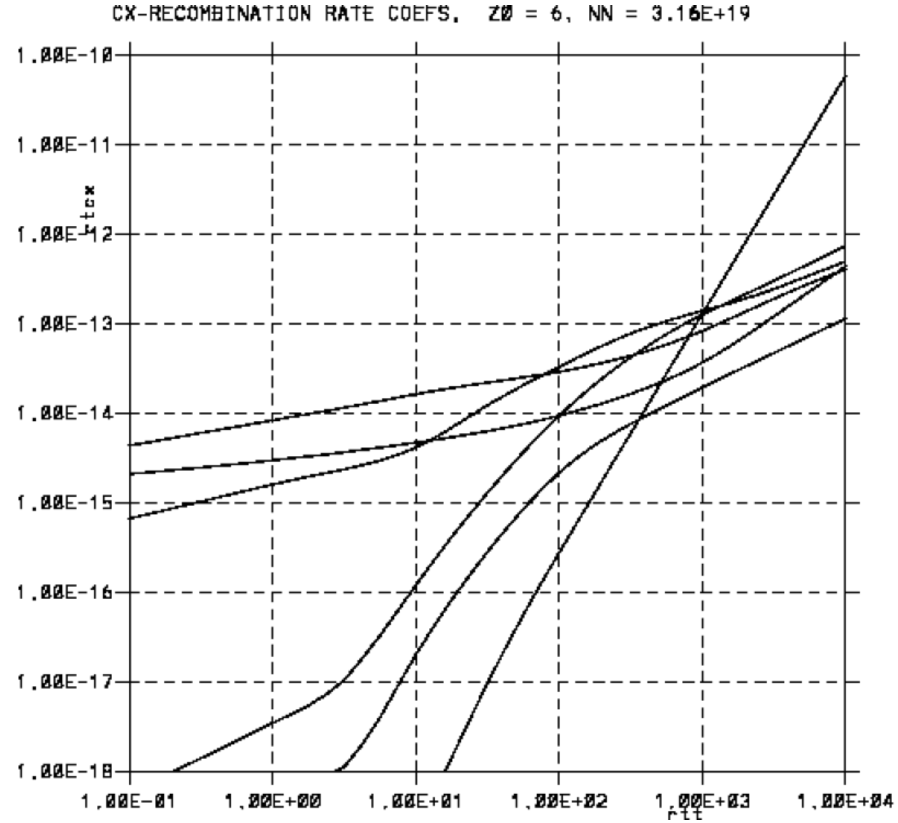
SOLPS: A&M Data, in more detail

- B2 atomic data
  - Pre-processor (b2ar) prepares tables
    - from one of
      - ADPAK
      - STRAHL
      - ADAS
    - H/D/T data overwritten by a standard model (“Weisheit”)
      - Option to prevent this
    - Energy in recombination was assumed to be radiated
      - Fixed

- Charge exchange data was provided by a simple fit
  - Good for D
  - Not so good for everything else →
  - Replaced by the use of ADAS data
    - » Turned out that there was not that much CX data in ADAS
    - » And some of it was set to 0
    - » And for D the only non-zero data was wrong

CX data for C





- Left: fit
- Right: ADAS

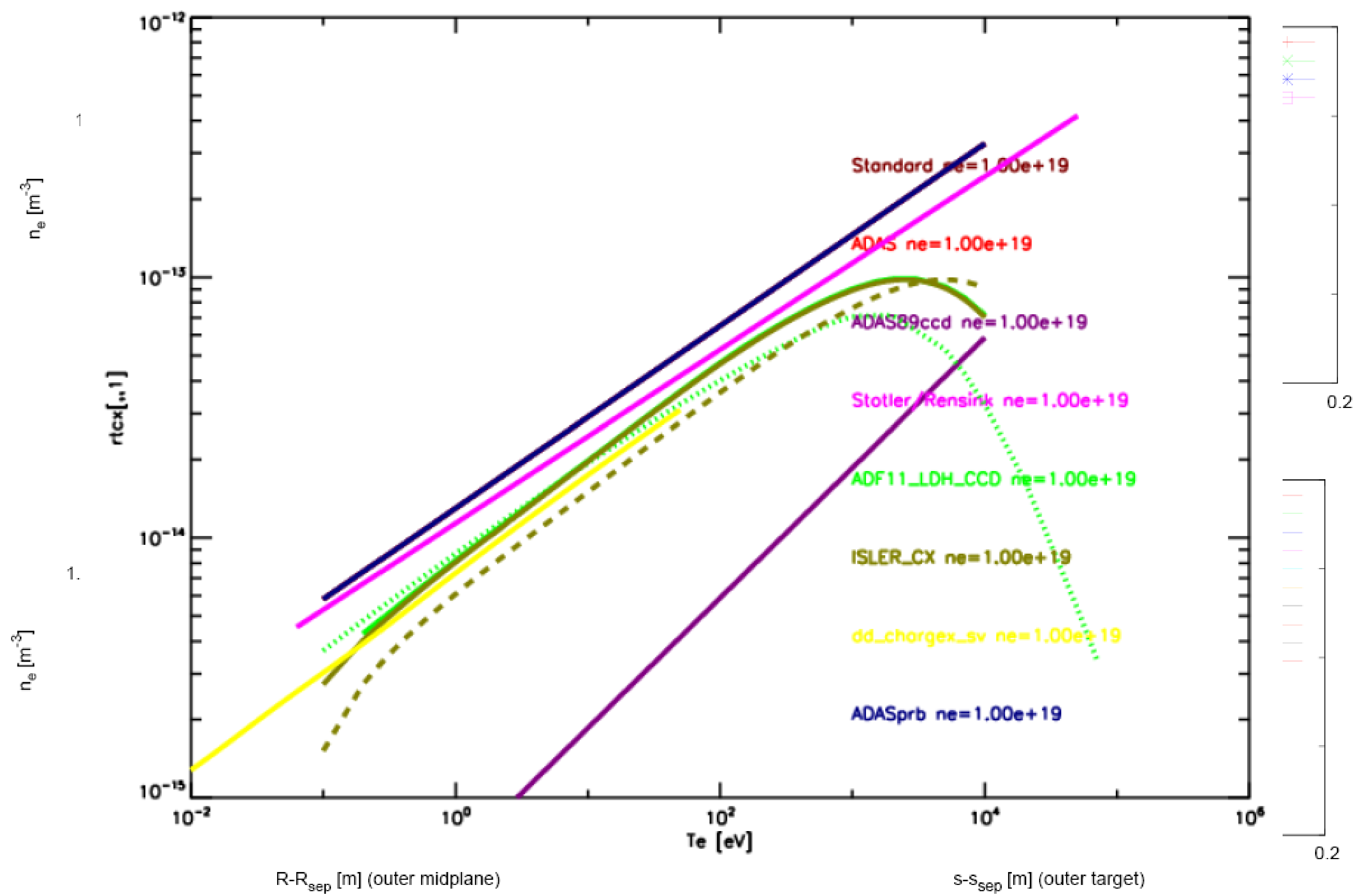
- Fit not very good!
- **Not only need good data, but also need the good data in the codes!**

SOLPS: A&M Data

- B2 surface data
  - TRIM tables accessed at run time
  - Models for chemical sputtering (Roth formula or constant yield)
  - Simple model for mixed materials
    - Simple model for Be suppression of chemical sputtering
  - Thermal model for plates also needs data
    - Thermal conductivity
  - Multiple external files needed at run time

- EIRENE
  - Most of the A&M data from polynomial fits
    - 9th order polynomials of 1 variable
    - 9x9th order polynomials of 2 variables
      - Problems with extrapolation
  - Surface data from external files
    - TRIM (one file)
    - MARLOWE
    - Individual files for TRIM

Some examples ...



EFDA-ITM-TF Charge

Originally prepared for the General Meeting of the Integrated Tokamak Modelling Taskforce (September 2008) by Par Strand (Task Force Leader)

Aims of ITM-TF

- ***Co-ordinate the development of a coherent set of validated simulation tools***
- ***Benchmark these tools on existing tokamak experiments***
- ***Provide a comprehensive simulation package for ITER and DEMO plasmas.***

Remit

- ***Development of the necessary standardized software tools for***
  - ***interfacing code modules and***
  - ***accessing experimental data.***

Medium term

- ***support the development of ITER-relevant scenarios in current experiments,***

EFDA(03)-21/4.9.2 (June 24th, 2003)

Introduction

- A wide range of AMNS data are needed by the ITM-TF.
- AMNS data are needed by several IMPs, especially IMP#3 (transport) and IMP#5 (sources).
- The AMNS task was therefore placed directly under the TF leadership.
- The task was started this year, and we have so far had three remote meetings.

- Originally prepared for the General Meeting of the Integrated Tokamak Modelling Taskforce (September 2008) by Lars-Goran Eriksson (Deputy Task Force Leader and coordinator of the AMNS Working Group)
- Modified and presented by DPC at the 2008 ADAS Workshop

IMP needs

- IMP#3 (the ITM-TF project dealing with modelling of plasma transport and discharge evolution) has been reviewed. In particular, for the ETS (European Transport Solver), which should deal with core transport, the following is needed:
- Rate coefficients (as a function of n and T) for
  - ionization,
  - recombination,
  - charge-exchange,
  - nuclear reaction rates
  - cooling rates
- ionization potential
- The elements needed are:
  - High priority (needed in 2008)
    - H, D, T, He, C
  - Lower priority (not needed until 2009 or later)
    - Be, O, N, Ne, Ar, Mo, Ni, Li, Si, B, W

- IMP#5 deals with Heating, Current Drive and Fast particles
- The main needs of atomic data are for Neutral Beam Injection, charge exchange losses, and synthetic diagnostics (e.g. of high energy NPA at JET)
  - Electron impact ionisation cross sections
  - Ion impact ionisation cross sections
  - Charge exchange cross sections
- Nuclear data for fusion reactions and other nuclear reactions between fast ions and impurities for diagnostics.

On the use of Atomic, Molecular, Surface and Nuclear (AMNS) data in the ITM-TF

- Version control of data imported to the ITM-TF data base is mandatory.
- The provenance of the data must be accurate and stored in the ITM database
- For “production” runs with ITM-TF codes using AMNS data it is important that the data have been given a stamp of approval by an expert.
- The AMNS data must be communicated to ITM-TF codes via a standardised interface (this should also ensure coherence between different ITM-TF codes needing the same type of data)

Accessing the AMNS data

Physics code

- Access to AMNS data only via interface
  - initialization (2)
  - finalization (2)
  - querying parameters (2)
  - setting parameters (2)
  - **getting data** (1)
- Separation between use of the data and the implementation of the data
- Code author doesn't need to become an expert in AMNS
- Ensures compatibility between codes

AMNS implementation

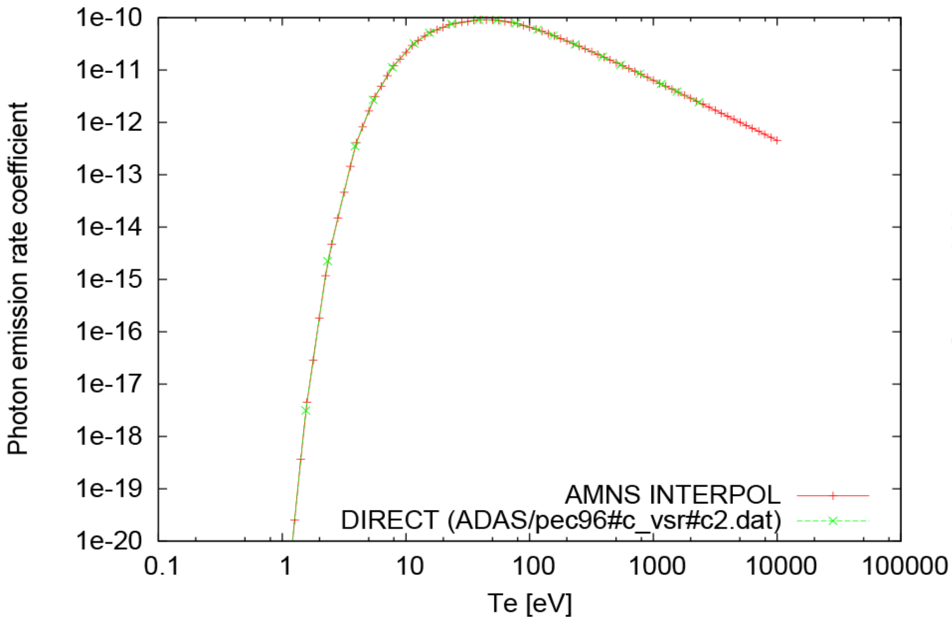
- Only accessed by a set of defined calls
- Implementation by AMNS experts
- Different versions can be supported
- Different implementations possible
  - Analytic formulae
  - Table lookup
- "Old" versions should always be recoverable (even if wrong)
- Should become easier to implement "new" data

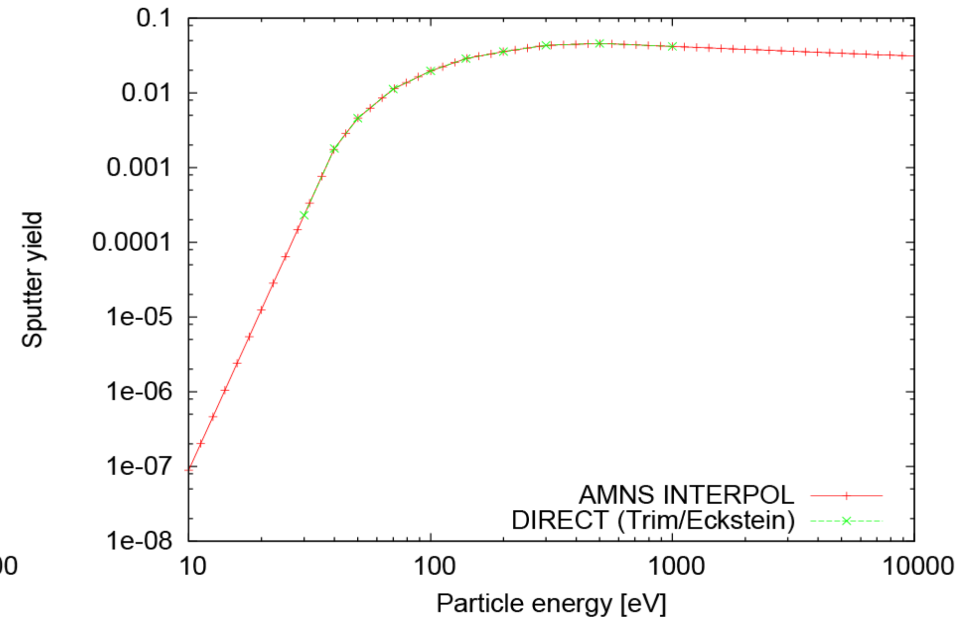
An example

- A prototype has been implemented
  - As a F90 module using derived types
  - **Interface will handle error estimates in the AMNS data!**

```
call ITM_AMNS_SETUP(amns)
query%string='version'
call ITM_AMNS_QUERY(amns,query,answer)
...
call ITM_AMNS_SETUP_TABLE(amns, lr_rx, species_lr, amns_lr)
query%string='source'
call ITM_AMNS_QUERY_TABLE(amns_lr,query,answer)
...
set%string='nowarn'
call ITM_AMNS_SET_TABLE(amns_lr,set)
...
call ITM_AMNS_RX(amns_lr,rate(:,:,0),ne,te)
...
call ITM_AMNS_FINISH_TABLE(amns_lr))
call ITM_AMNS_FINISH(amns)
```

Results of the prototype





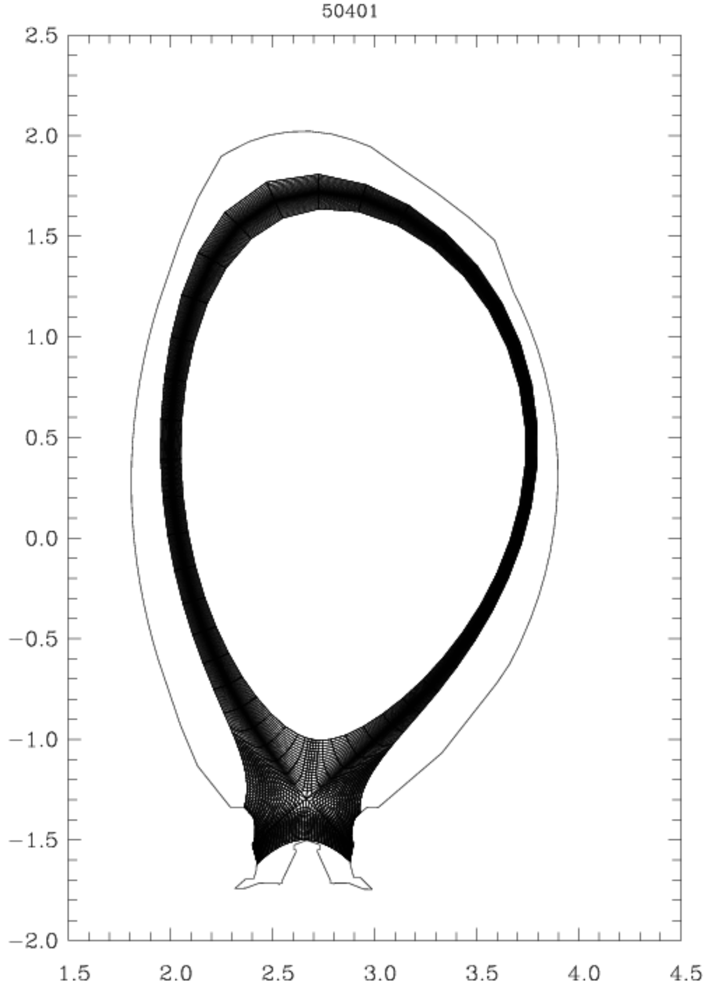
Left: comparison with ADAS (A)

Right: comparison with TRIM (S)

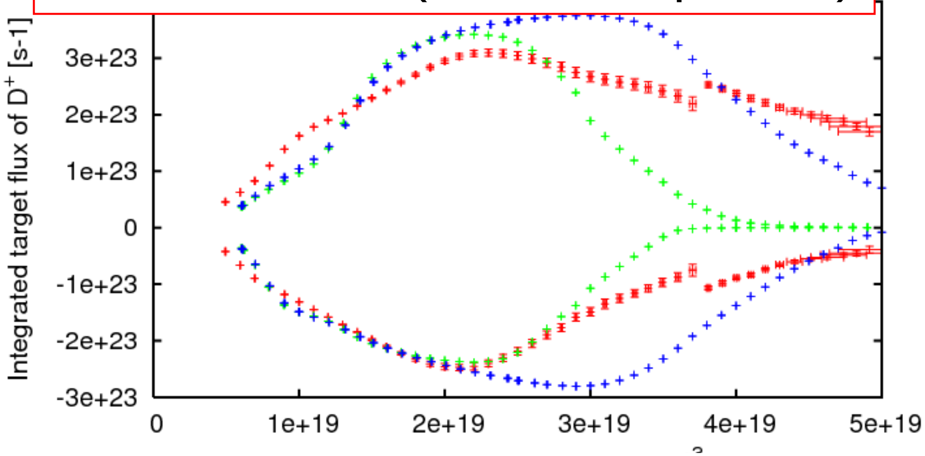
Will also be able to handle 3d (& more) dependencies

Back to some SOLPS results, JET

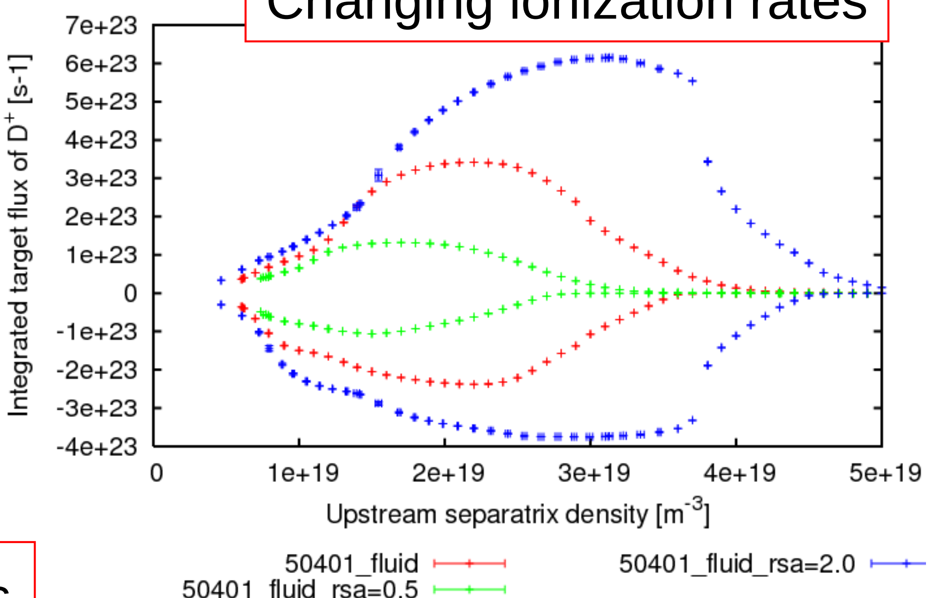
- Detachment simulations



Kinetic vs fluid (old and improved)



Changing ionization rates



- pure D with different atomic physics

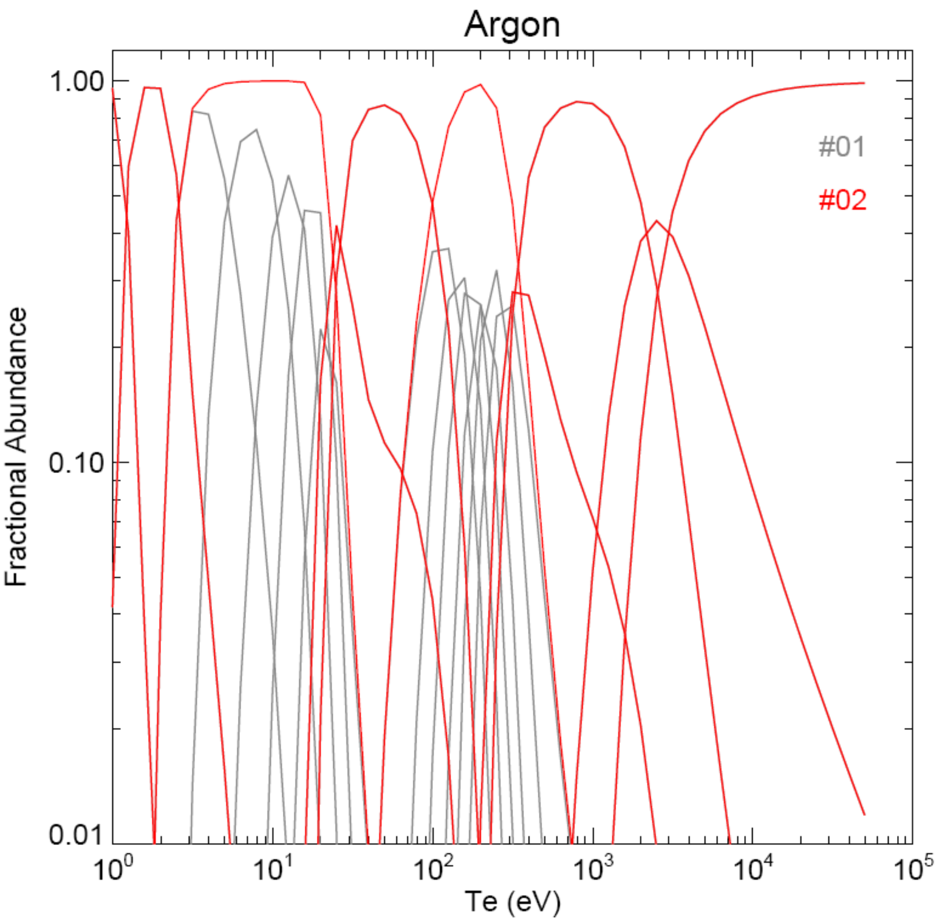
Implementation of the bundled charge state model in SOLPS5.0

- ✓ Full backward compatibility and user transparency
  - Old species data format: Z_a, Z_n, A_m, Z_a^2
  - New data format: $Z_{a,min}$, $Z_{a,max}$, Z_n, A_m
- ✓ Full recovery of old results
- ✓ New ADAS rate arrays $Z_a(n_e,T_e)$, $Z_a^2(n_e,T_e)$, $E_i(n_e,T_e)$
- ✓ Now need n_e saved in plasma state file and properly updated! (Quasi-neutrality equation becomes recursive)
- ✓ Conversion tools to change between bundling schemes
- ✓ No bundling allowed with neutrals (too different physics)

Originally presented at the ADAS Workshop, Ringberg, 10-12 October 2007 (X. Bonnin)

D+Ar test case

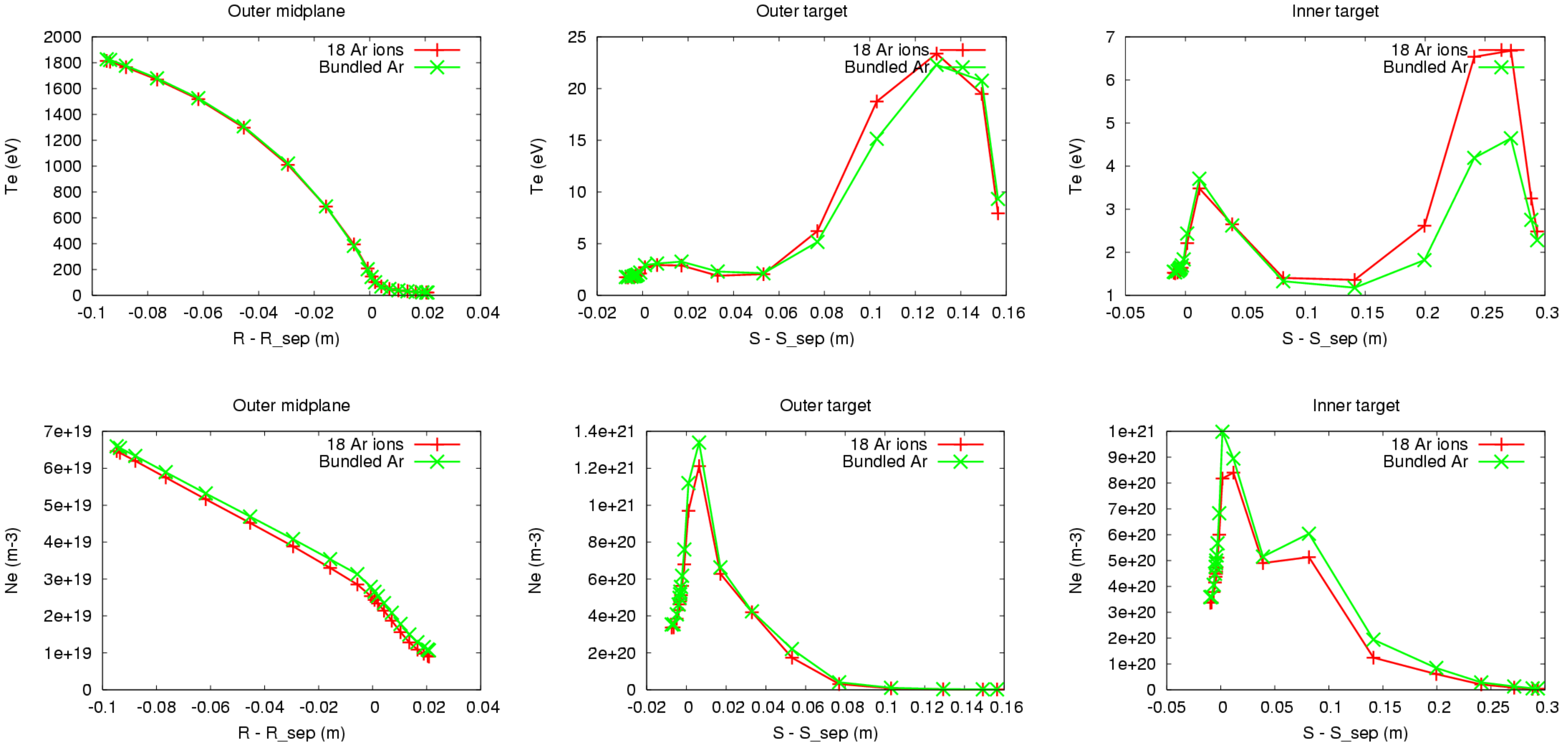
- AUG #16151
  - Reference: All charge states:
    - D_0, D^+, Ar_0, Ar^{+1}, Ar^{+2}, ..., Ar^{+18}
  - « Natural » bundling: →
    - D_0, D^+, Ar_0, Ar^{+1}, $Ar^{+2\text{-}+6}$, Ar^{+7}, Ar^{+8}, $Ar^{+9\text{-}+14}$, Ar^{+15}, ..., Ar^{+18}
  - Both cases:
    - Identical boundary conditions and transport
    - Fluid neutrals
    - Converged to machine accuracy



Still issue with CX within bundles
Need (T_e,n_e,n_0)?

Originally presented at the ADAS Workshop, Ringberg, 10-12 October 2007 (X. Bonnin)

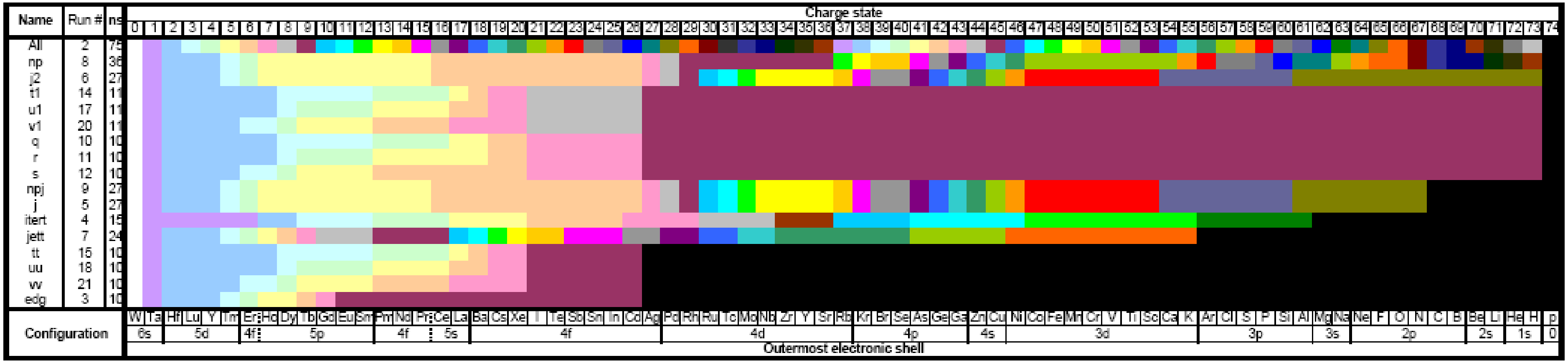
Results comparison (OMP T_e and n_e, targets)



Bundling yields quite a good approximation !

Originally presented at the ADAS Workshop, Ringberg, 10-12 October 2007 (X. Bonnin)

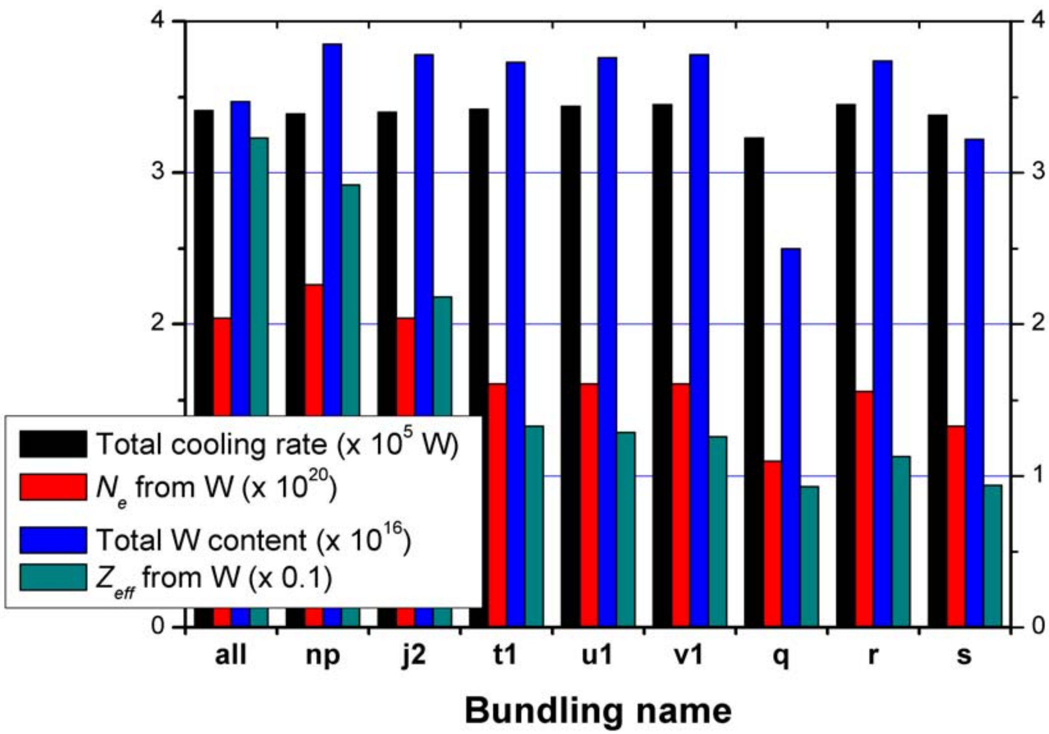
W Bundled charge state modelling



From **Xavier Bonnin** (CNRS, Paris)

Calculations for AUG are in progress with SOLPS using different bundling options for W

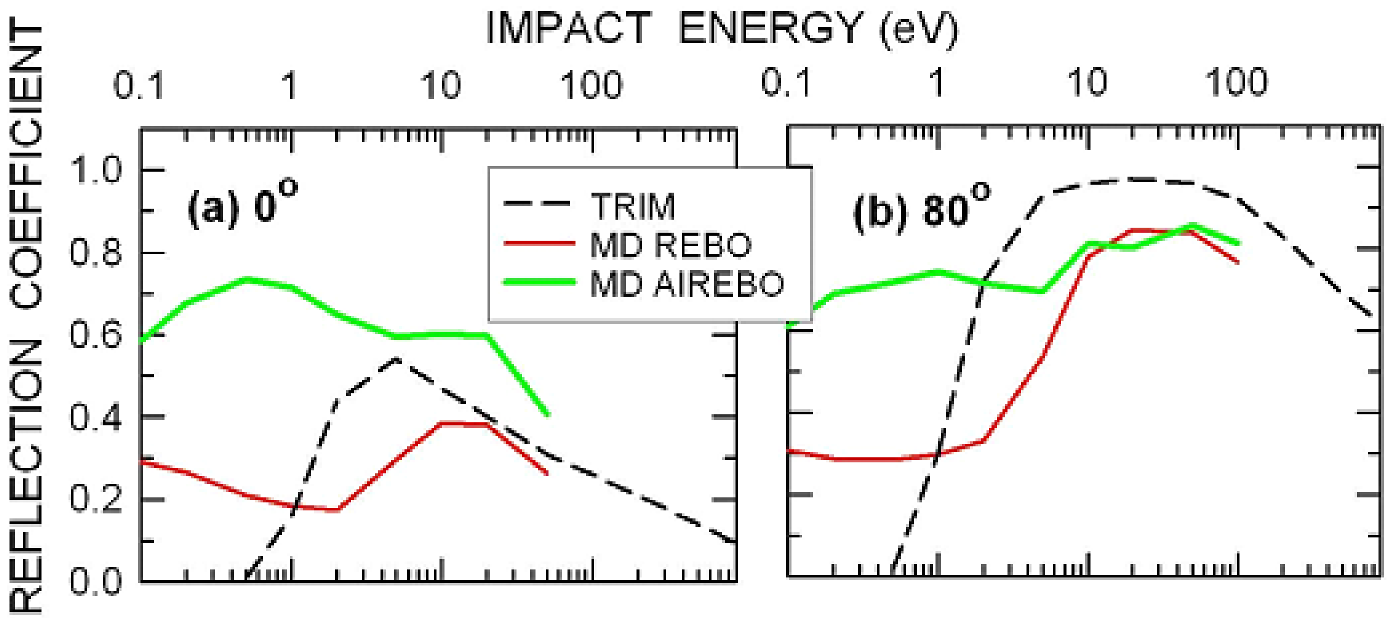
Results are very preliminary!



Challenges: survey responses

- Atomic cross-section data
  - What AMNS data do you (or will you) need? Which species, reactions, etc? [From a questionnaire sent out to data consumers in IMP3]
    - the differential cross-sections for plasma-neutral, neutral-neutral and plasma-impurity reactions (elastic, excitation, ionization, dissociation, ...) for H, D, T, He, C, W, Be, ...
    - Energy and incident angle dependent recycling coefficients for H, D, T, H_2, D_2, T_2, HD, HT, DT, He on C, W, Be. Energy (particle flux) and incident angle dependent (total = chemical + physical) sputtering coefficients for C, W, Be. I need the velocity distribution function of recycled and sputtered particles.
- Much more data on mixed materials H/Be/C/W alloying and material properties.
- The possibility to have a dependency of atomic rates not only on local properties (T_e/n_e/...) but also on non-local properties (∇T_e/ ∇n_e or gradient lengths). Is that feasible at all?

Challenges in the data: Surface data



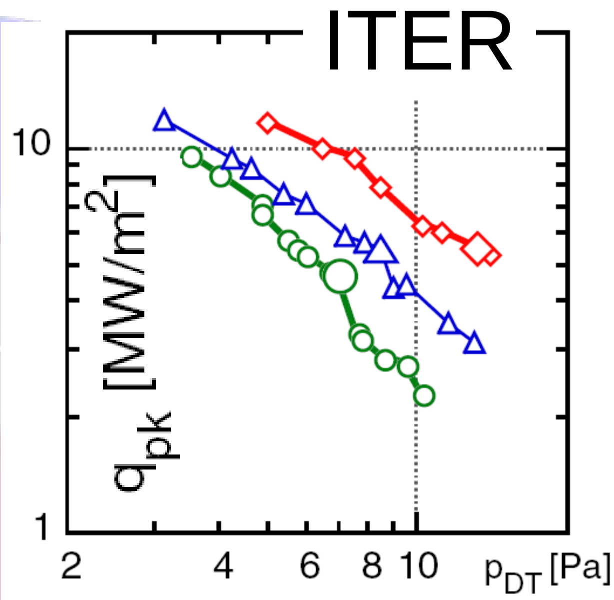
(a) and (b) Reflection coefficient as a function of impact energy for H atoms impinging on pure amorphous carbon (a-C) at two incident angles with respect to the surface normal. Results are displayed for MD simulations using REBO and AIREBO potentials and TRIM calculations

From: HYDROGEN REFLECTION IN LOW-ENERGY COLLISIONS WITH AMORPHOUS CARBON, C. O. Reinhold, P. S. Krstic, and S. J. Stuart

Summary

Hopefully this talk has given

- An indication of the needs of (a part of) the fusion community for Atomic, Molecular, (Nuclear) and Surface data
- Some sense of new developments & needs
- A sense of how the fusion modelling community in Europe is planning to use AMNS data in the future
- Help in identifying where we might not be using the "best" data
- AMNS "improvements" (such as the release of the ADAS W data) allow us to explore new physics!



Kukushkin et al, NF 45 (2005) 608-616

Introducing new atomic physics does change the results!