ADAS and Software issues

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ADAS: The Atomic Data and Analysis Structure

Allan Whiteford, Martin O'Mullane, Hugh Summers and dozens of others*

25th March 2009

* Many people have contributed to the ADAS Project over the past 25 years — of particular note at this meeting is, of course, Manfred von Hellermann.

Contents

The ADAS Project

- The ADAS Project is a self-funding (i.e. funded by participants) project consisting of most major fusion laboratories along with other astrophysical and university groups. In its present incarnation it is over fifteen years old but the roots in JET go back almost twenty-five years.

- As an implementation, it is an interconnected set of computer codes and data collections for modelling the radiating properties of ions and atoms in plasmas.

- Historical roots are in fusion (JET) and so are the bulk of the users/members. Has also been extensively applied to astrophysics.

- Is governed by a steering committee coming from its members. Day to day running and implementation is done by the University of Strathclyde.

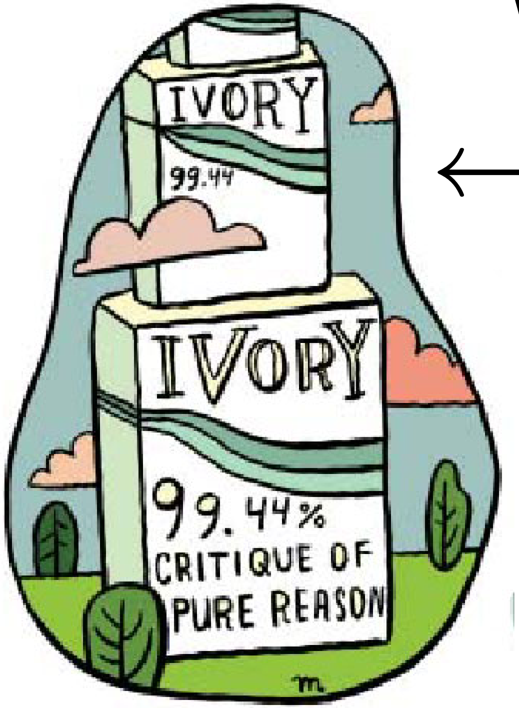
Size and Scope of use

- Rough idea of the computational 'size' of ADAS:
  - 3.0GB of data in 20,103 distinct files,
  - 425,253 lines of Fortran and 406,225 lines of IDL,
  - also contains C, Perl, csh, Matlab and C++ code,
  - tentative plans to expand to support Python.
- Used extensively in spectroscopic fusion diagnostic analysis.
- Integrated into key fusion transport codes
  - e.g. Strahl, JETTO, SANCO, **CHEAP**, EDGE2D etc.
- The Project currently has 25 members across the world.

ADAS Members

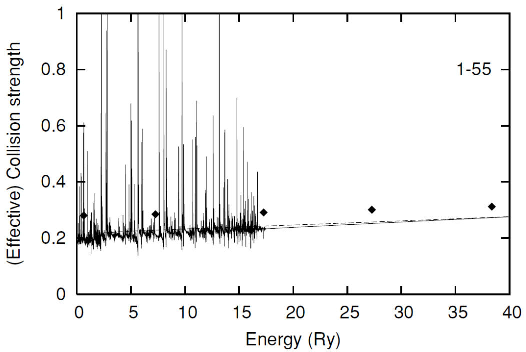
Site	Country	Official Contact	Technical Contact
Armagh Observatory	UK	Gerry Doyle	Gerry Doyle
Birla Institute of Technology	India	Ram Prakash	Ram Prakash
Centre de Recherches en Physique des Plasmas	Switzerland	Richard Pitts	Richard Pitts
Commissariat à l'énergie atomique Caderache	France	Rémy Guirlet	Rémy Guirlet
Consorzio RFX	Italy	Marco Valisa	Marco Valisa
FOM — Instituut voor Plasmafysica Rijnhuizen	**Netherlands**	**Manfred von Hellermann**	**Gerard van Rooij**
Forschungszentrum Jülich	Germany	Phillipe Mertens	Phillipe Mertens
General Atomics	USA	Todd Evans	Todd Evans
INAF — Osservatorio Astrofisico di Catania	Italy	Alessandro Lanzafame	Alessandro Lanzafame
Institute for Plasma Research	India	Parameswaran Vasu	Parameswaran Vasu
Japan Atomic Energy Agency	Japan	Hirtoka Kubo	Tomohide Nakano
JET	UK	Klaus-Dieter Zastrow	Martin O'Mullane
Kungliga Tekniska Högskolan	Sweden	Elisabeth Rachlew	Elisabeth Rachlew
Max-Planck-Institut für Plasmaphysik	Germany	Kurt Behringer	Thomas Pütterich
National Institute for Fusion Science	Japan	Takako Kato	Daiji Kato
Nat. Inst. for Laser, Plasma & Radiation Physics	Romania	Viorica Stancalie	Viorica Stancalie
Oak Ridge National Laboratory	USA	Dave Schultz	Predrag Krstic
Philips Research Lighting Division	Germany	Thomas Krücken	Thomas Krücken
Southwestern Institute of Physics	China	Xuru Duan	Xiaoyu Han
STFC Rutherford Appleton Laboratory	UK	Andrzej Fludra	Andrzej Fludra
UKAEA Fusion	UK	Klaus-Dieter Zastrow	Martin O'Mullane
University of Auburn	USA	Mitch Pindzola	Stuart Loch
University of Strathclyde	UK	Hugh Summers	Allan Whiteford
University of Toronto	Canada	Peter Stangeby	David Elder
University of Wisconsin	USA	Daniel Den Hartog	Daniel Den Hartog

What does ADAS do?

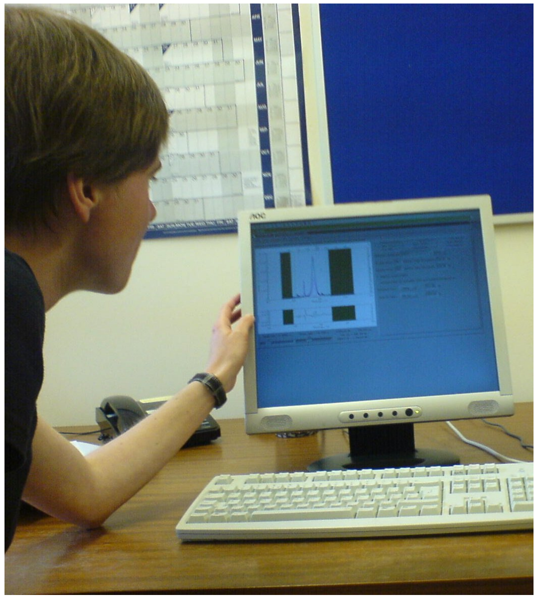


← Universities

Fusion labs →



← ADAS →
understands both of
these groups!



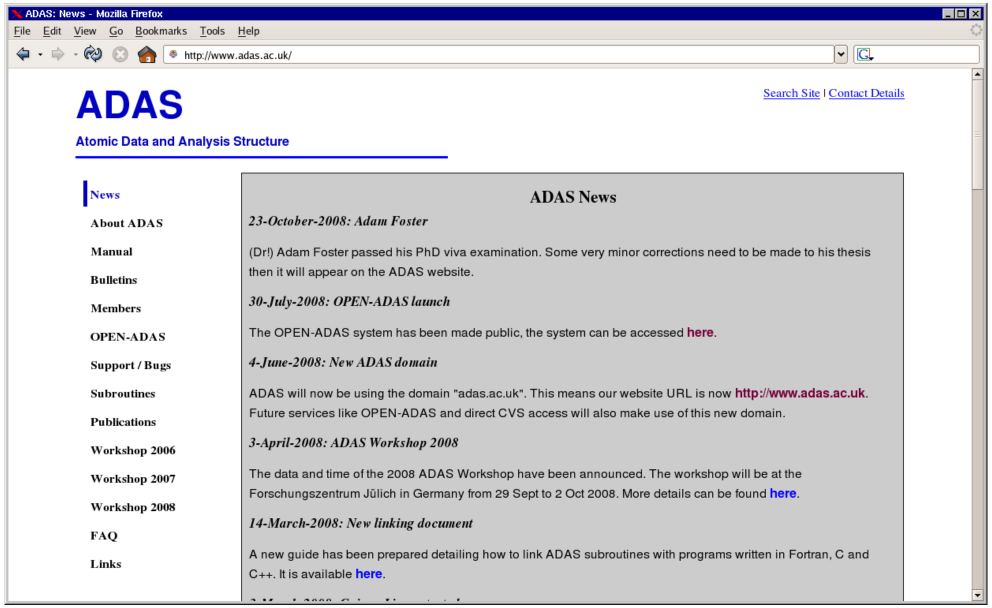
Yes, but what does it actually do?

- ADAS, as a computer system, is designed to:
  - provide codes which are easy to use,
  - provide subroutine libraries for inclusion in other codes,
  - allow direct access to diagnostically relevant data.

- ADAS, as an organisation:
  - provides guidance (training courses, visits etc.) on running codes,
  - gives recommendation on the best data to use,
  - assists in analysis and development of analysis tools and models.

ADAS brings people (diagnosticians, modellers and atomic physicists) together on the topic of atomic physics for magnetically confined fusion.

Parts of ADAS



http://www.adas.ac.uk

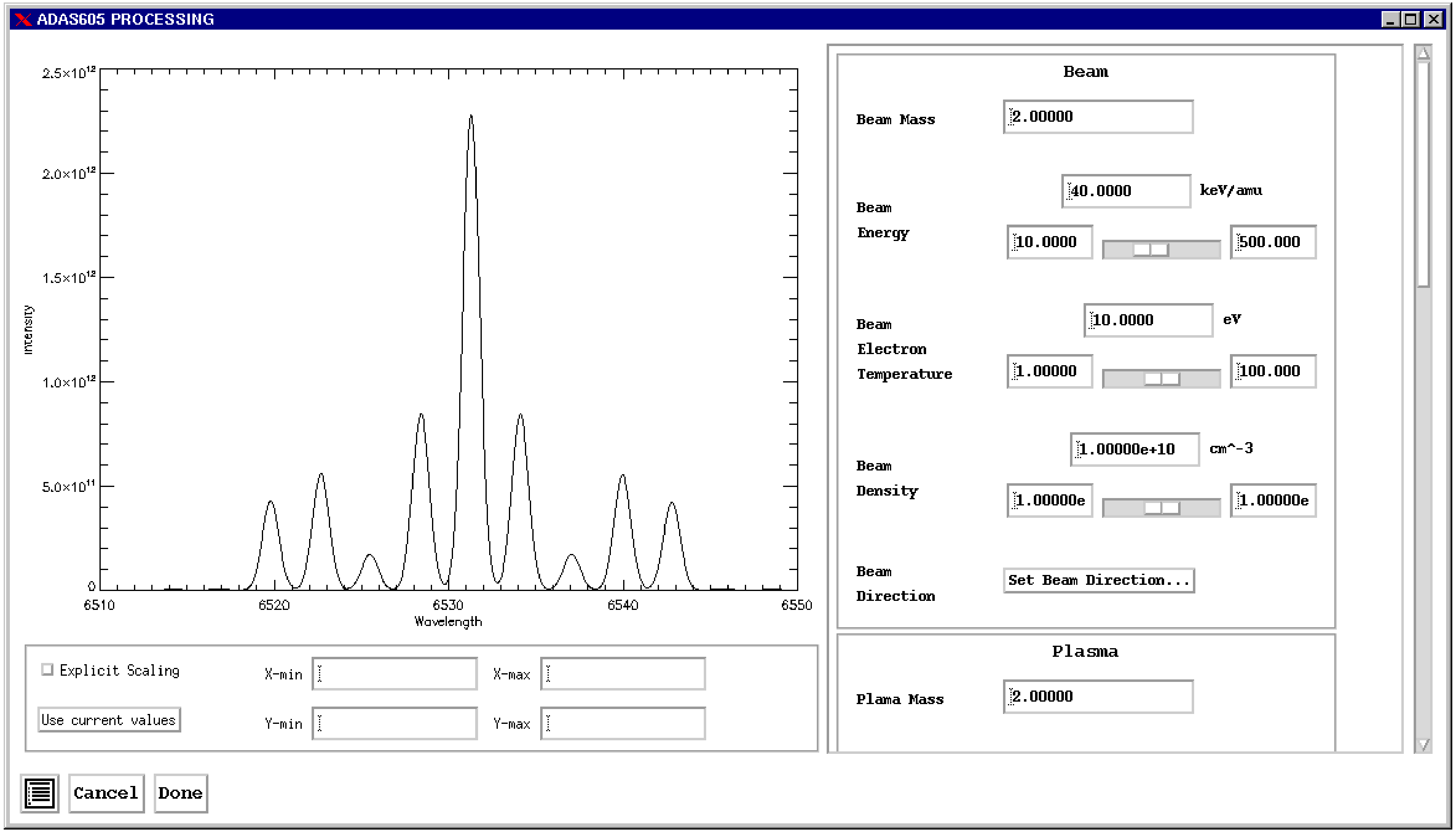
- Interactive ADAS
- The ADAS database
- Extended ADAS
- ADAS subroutine library
- ADAS Documentation (over 4000 pages!)
- Extended ADAS
- ADAS-EU

Interactive ADAS

- Interactive ADAS consists of around eighty distinct, but interlinked codes.
- There are eight distinct series covering different themes (e.g. series 3 covers beam related modelling and data).
- The interactive ADAS system allows:
  - generation of all ADAS *derived* atomic data files*,
  - generation of many of the ADAS *fundamental* atomic data files*,
  - interactive inspection of the data,
  - some plasma modelling capabilities.
- All interfaces are graphical and implemented in IDL.

* — distinction between derived and fundamental data will be discussed later.

Example: Displaying a Stark feature



Extended ADAS

- Covers a suite of codes which pass the *local atomic boundary*:
  - SANCO: $1\frac{1}{2}$-D impurity transport code,
  - UTC: Error propagating data analysis package for impurity transport,
  - FFS*: Generalised feature synthesis and fitting,
  - CXSFIT: Advanced spectral analysis of charge exchange measurements,
  - New-CHEAP*: Beam attenuation and modelling code for charge exchange.

- Very much tied to specific experimental analysis rather than applied atomic physics in the more general sense.

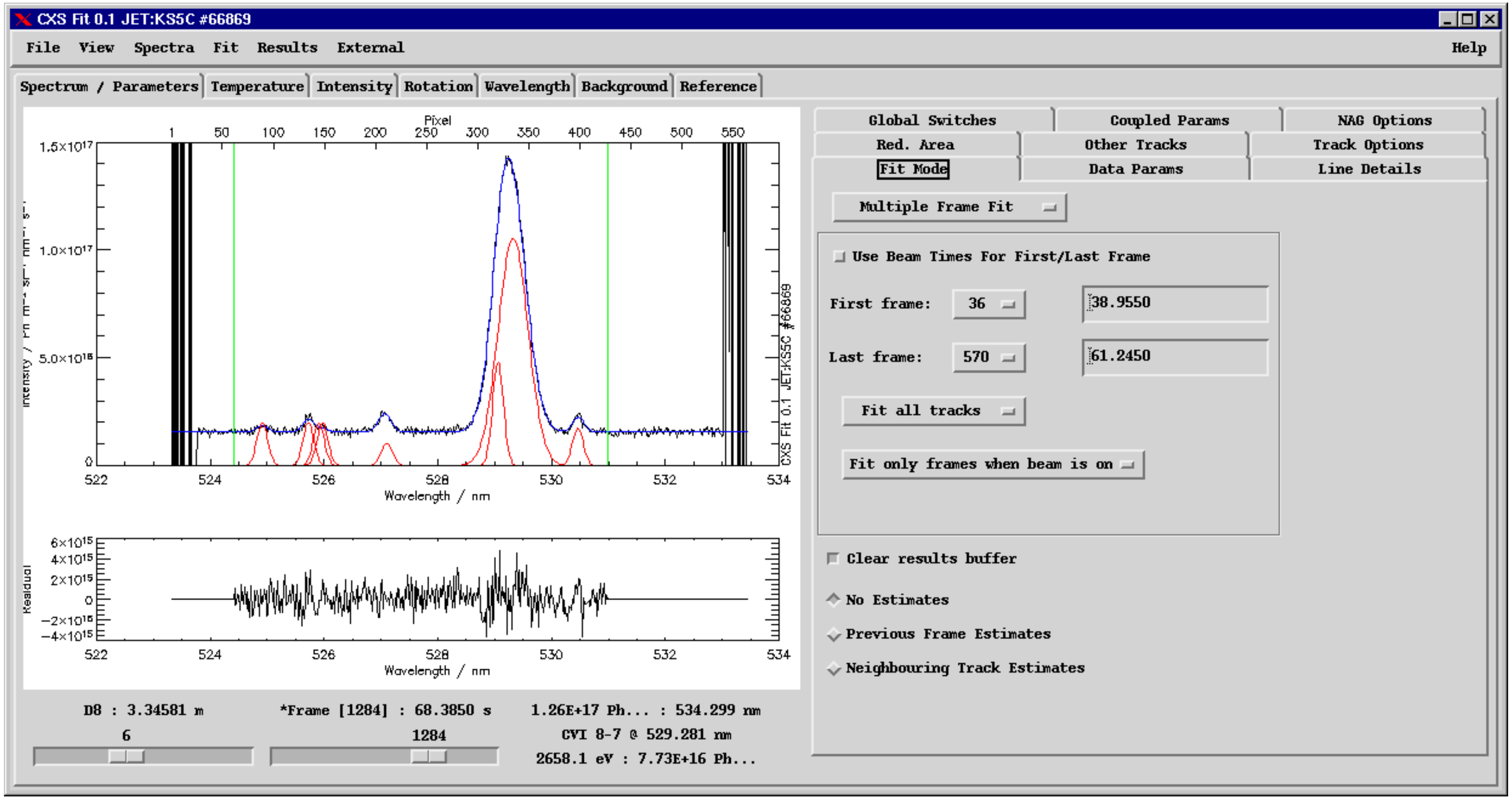
- Maintained and co-developed by the ADAS Project but not considered part of the core interactive ADAS series of programs.

* — early development/planning stage.

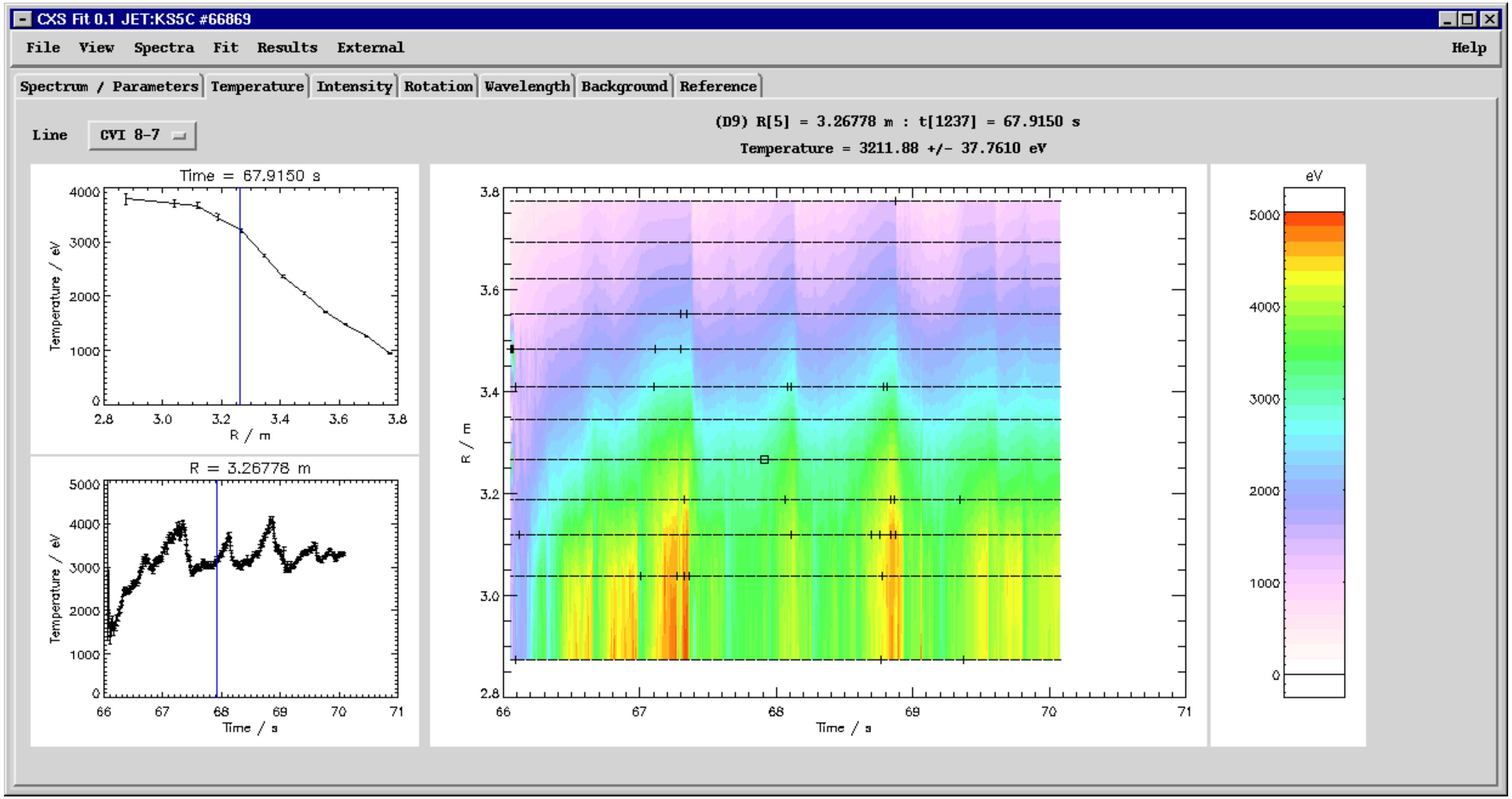
CXSFIT

- CXSFIT is a joint development between ADAS, FOM, Garching, Jülich and UKAEA to provide a universal interface to KS4FIT.
- Graphical user interface written in IDL.
- Contains all of the features present in the famous KS4FIT (**von Hellermann**).
- Provides visualisation of each fit and of the overall results.
- Almost all of the code is machine independent:
  - Machine specific reading/writing routines need to supplied.
  - We really do have an identical code running on AUG, JET and TEXTOR!

CXSFIT Graphical Interface (1/2)



CXSFIT Graphical Interface (2/2)



The ADAS database

- All data are strictly formatted according to ADF numbers
- Currently 50 distinct ADF numbers (some placeholders).
- Files all sit flat on a conventional UNIX filesystem.
- With release 2.13, 3.0GB of data in 20,103 distinct files.
- All data is stored as ASCII and in human readable file formats:
  - allows manual creation of datasets by users,
  - database has survived for > 20 years; ASCII was a good choice.
- We make a distinction between derived, fundamental and driver data.

Derived, fundamental and driver data

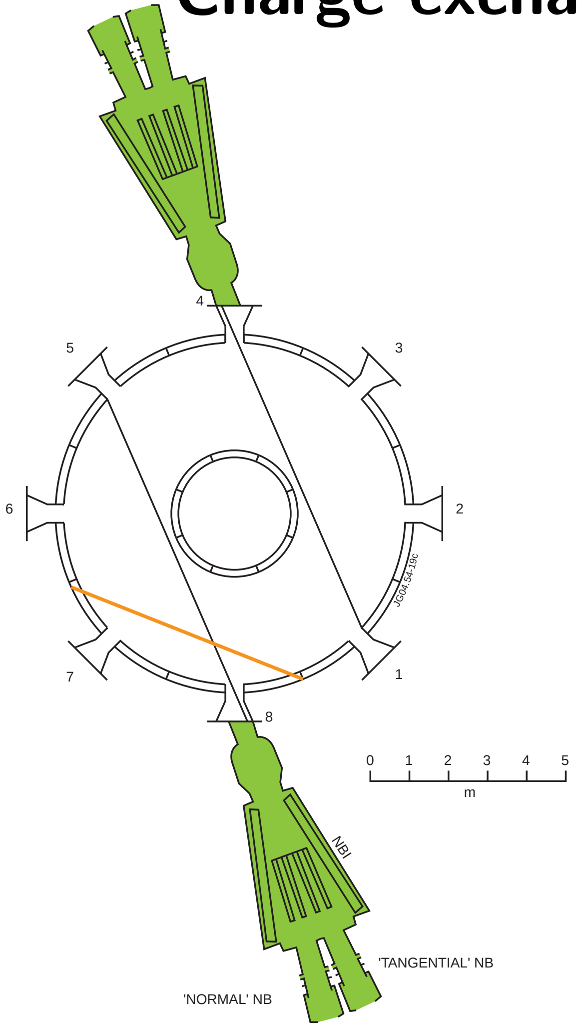
- **Fundamental data** are core atomic data necessary for modelling: A-values, cross sections, effective collision strengths etc.,
  - some generated in-house but many come from literature, data centres etc.
- **Derived data** are data tailored for modelling: effective emission coefficients, effective ionisation/recombination rates etc.,
  - most of these data are unique to ADAS and is one of the main differences between ADAS and other atomic databases (e.g. IAEA, ORNL, NIFS).
- **Driver data** allow complete regeneration of all ADAS derived data (and some fundamental data) in conjunction with the various ADAS codes,
  - completely unique to ADAS and of no general scientific interest.

Data highlights for beam studies

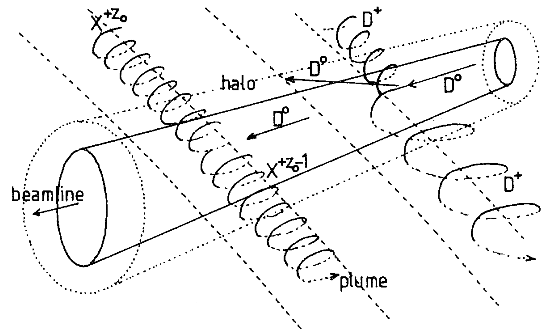
- ADF01 — Charge exchange cross sections:
  - fully n, nl or nlj resolved,
  - underpins all of the ADAS CX modelling.
- ADF12 — Charge exchange emission coefficients:
  - gives charge exchange emission as function of plasma and beam parameters,
  - fully density dependent modelling subsequent transitions after capture.
- ADF21 — Effective beam stopping/excitation coefficients
  - gives stopping coefficients for attenuation calculations,
  - split by impurity species.

Let's focus a bit on these charge exchange data and their application...

Charge exchange recombination spectroscopy



- Fast neutral particles in a beam undergo charge exchange with impurity ions which then emit light.



- A 'small' interaction volume between beam and background plasma.

The basis for a *localised* diagnostic.

Charge exchange emission modelling

Consider a typical charge exchange reaction for Carbon, naïvely we can say that:

$$\mathrm{H}^0 + \mathrm{C}^{6+} \rightarrow \mathrm{H}^+ + \mathrm{C}^{5+}\,(n=8) \rightarrow \mathrm{H}^+ + \mathrm{C}^{5+}\,(n=7) + h\nu\,(529.1nm)$$

but, of course, we can get the same emission from many possible routes, e.g.:

$$\mathrm{H}^0 + \mathrm{C}^{6+} \rightarrow \mathrm{C}^{5+}\,(n=9) \rightarrow \mathrm{C}^{5+}\,(n=8) + h\nu \rightarrow \mathrm{C}^{5+}\,(n=7) + h\nu\,(529.1nm)$$

$$\mathrm{H}^0 + \mathrm{C}^{6+} \rightarrow \mathrm{C}^{5+}\,(n=4) \rightarrow \mathrm{C}^{5+}\,(n=4) + e \rightarrow \mathrm{C}^{5+}\,(n=8) + e \quad ...$$

There are an infinite number of routes to go from an initial charge capture to an emission at 529.1nm!

ADAS data for charge exchange emission

- ADAS calculates these infinite routes using a collisional–radiative model and produces an ‘effective’ rate.

- These rates are tabulated in ADF12 files and called $\mathcal{QEF}$ data.

- For a given emission, they are tabulated as functions of:
  - beam energy (E),
  - electron temperature (T_e),
  - electron density (n_e).

- The emission is then simply:

$$I = \int_0^L n_i n_b \mathcal{QEF}\left(E, T_\mathrm{e}, n_\mathrm{e}\right) dl$$

Beam attenuation

A hydrogen beam is attenuated when an atom in the beam is ionised and this ion is then carried out of the beam and around the plasma. Naïvely we can say that:

$$\mathrm{H}^0 + \{e,p,i\} \rightarrow \mathrm{H}^+ + e + \{e,p,i\}$$

but, like the charge-exchange emission there are an infinite number of routes:

$$\{e,p,i\} + \mathrm{H}^0 \rightarrow \{e,p,i\} + \mathrm{H}^0\,(n=4) \begin{array}{l} \nearrow \quad \mathrm{H}^0\,(n=4) + \{e,p,i\} \rightarrow \mathrm{H}^+ + e \\ \searrow \quad \mathrm{H}^0\,(n=4) \rightarrow \mathrm{H}^0\,(n=3) + h\nu \end{array}$$

$$\swarrow$$

$$\{e,p,i\} + \mathrm{H}^0\,(n=3) \rightarrow \mathrm{H}^+ + e$$

ADAS data for beam attenuation

- Like the charge-exchange emission, ADAS calculates these infinite routes using a collisional–radiative model and produces an 'effective' rate.

- These rates are tabulated in ADF21 files and called $\mathcal{BMS}$ data.

- For two impurity species (say C and Be) the differential equation modelling attenuation is then something like:

$$\frac{dn_b}{dt} = -\left(\begin{array}{cl} & n_{\rm H}\mathcal{BMS}_H\left(E, T_{\rm e}, n_{\rm e}\right) \\ + & n_{\rm C}\mathcal{BMS}_C\left(E, T_{\rm e}, n_{\rm e}\right) \\ + & n_{\rm Be}\mathcal{BMS}_{\rm Be}\left(E, T_{\rm e}, n_{\rm e}\right) \end{array} \right) n_b$$

- Slightly more complicated due to charge neutrality and normalising with respect to $n_{\rm e}$ but the key feature is that all of the **intrinsic** atomic modelling is done by ADAS leaving the user to do the **extrinsic** plasma/beam modelling.

Beam emission and beam attenuation in a plasma model

- We want to determine the impurity concentrations.

- To go from an emission measure to an impurity concentrations we need to use:

$$I = \int_0^L n_i n_b \mathcal{QEF}\left(E, T_{\rm e}, n_{\rm e}\right) dl$$

- This requires us to know the beam concentration but to determine the beam concentration we need to solve:

$$\frac{dn_b}{dt} = -\mathcal{BMS}\left(E, T_{\rm e}, n_{\rm e}\right) n_i n_b$$

- which requires us to know the impurity concentration!

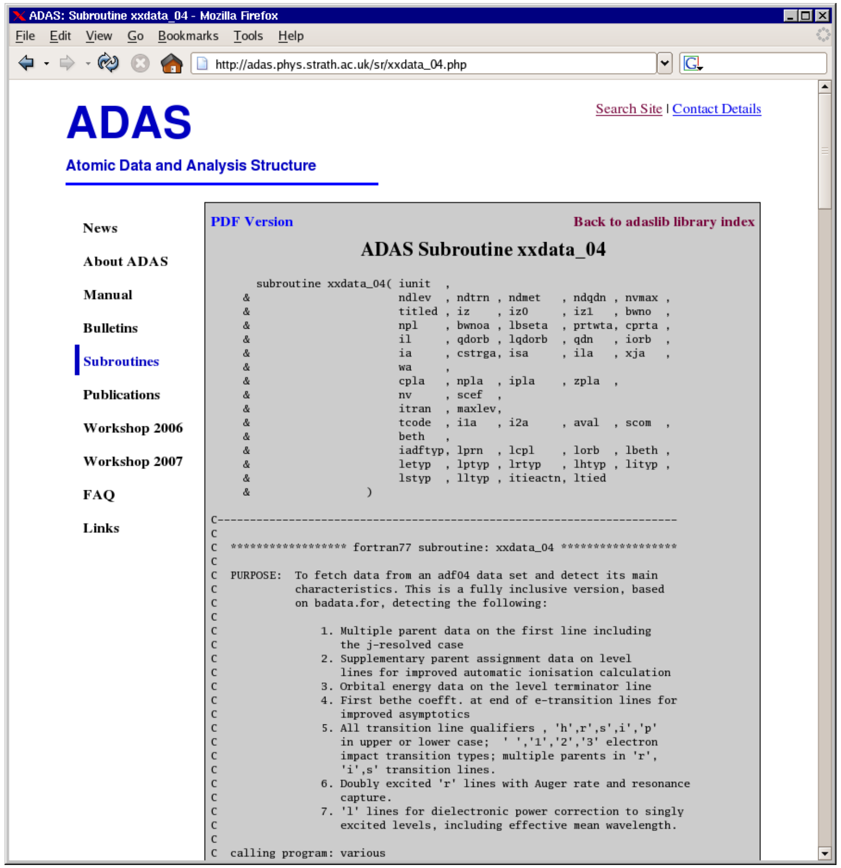
CHEAP

- The solution to this problem is the **CH**arge **E**xchange **A**nalysis **P**ackage.
- Development led by von Hellermann at JET.
- There is now a certain degree of splitting:
  - JET uses a code called ‘CHEAP’ written in Fortran.
  - TEXTOR uses a code called ‘CHEAP’ written in Matlab.
  - ASDEX-Upgrade uses a code called ‘CHEAP’ written in IDL.
- The ADAS Project has undertaken to help Manfred and others rationalise these versions under a current working title of ‘New-CHEAP’.
- We expect to have a working code in the next year to eighteen months.

CHEAP is built upon being able to call ADAS modules as subroutines

Callable ADAS

- ADAS Comes with a Fortran library of over 750 routines:
  - all documented in ~ 1500 page appendix to the user manual,
  - also documented on-line.

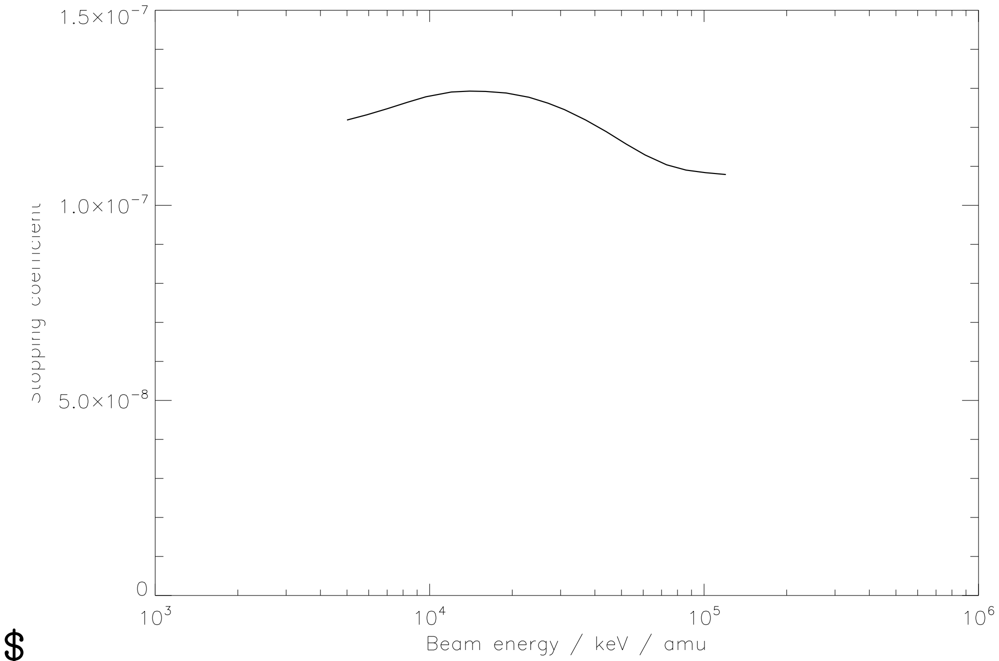


- Also comes with extensive IDL library:
  - far easier to use for interactive work at the command line,
  - self documenting; almost all routines accept a '`/help`' keyword.

Partial/planned support for C, C++, Matlab, Perl and Python access.

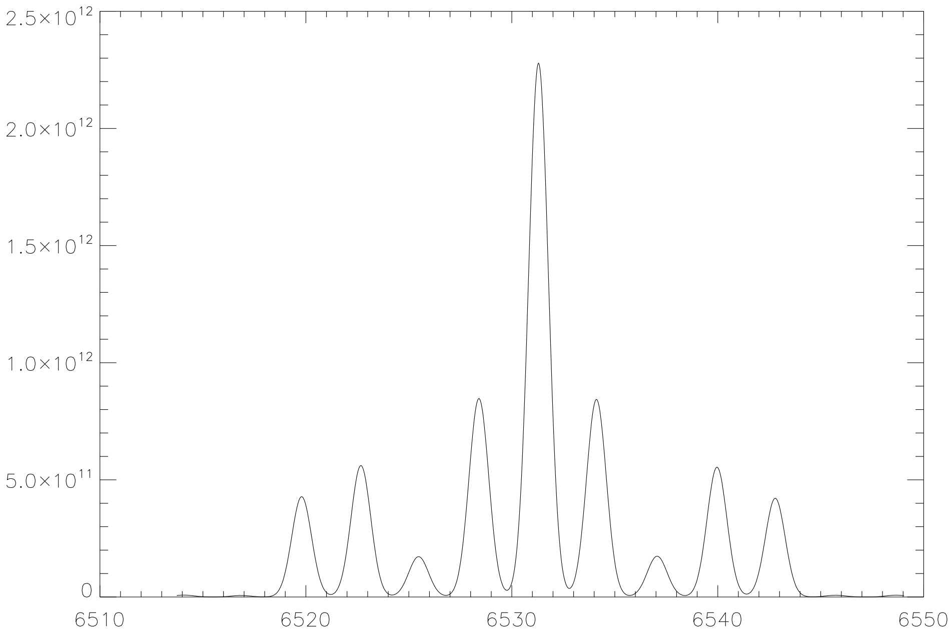
Reading beam attenuation coefficients

```
files=[ '/home/adas/adas/adf21/bms97#h/bms97#h_h1.dat' , $
        '/home/adas/adas/adf21/bms97#h/bms97#h_c6.dat' , $
        '/home/adas/adas/adf21/bms97#h/bms97#h_be4.dat'  ]

fraction=[0.96,0.03,0.01]

temp = fltarr(80)+2000
dens = fltarr(80)+1e13
ener = [ 5000, 5900, 7000, 8300, $
          9700,12000,14000,16000, $
         19000,23000,27000,31000, $
         37000,44000,52000,61000, $
         73000,86000,101000,120000]

read_adf21,files=files,data=data, $
           fraction=fraction,te=temp,dens=dens,energy=ener
plot,ener,data,/xlog,ytitle='Stopping coefficient', $
                     xtitle='Beam energy / keV / amu'
```



Producing a stark feature

```
pars=afg('stark',/parameters)
pars.broaden=1
res=afg('stark',calculate=pars)
plot,res.wv,res.intensity
```

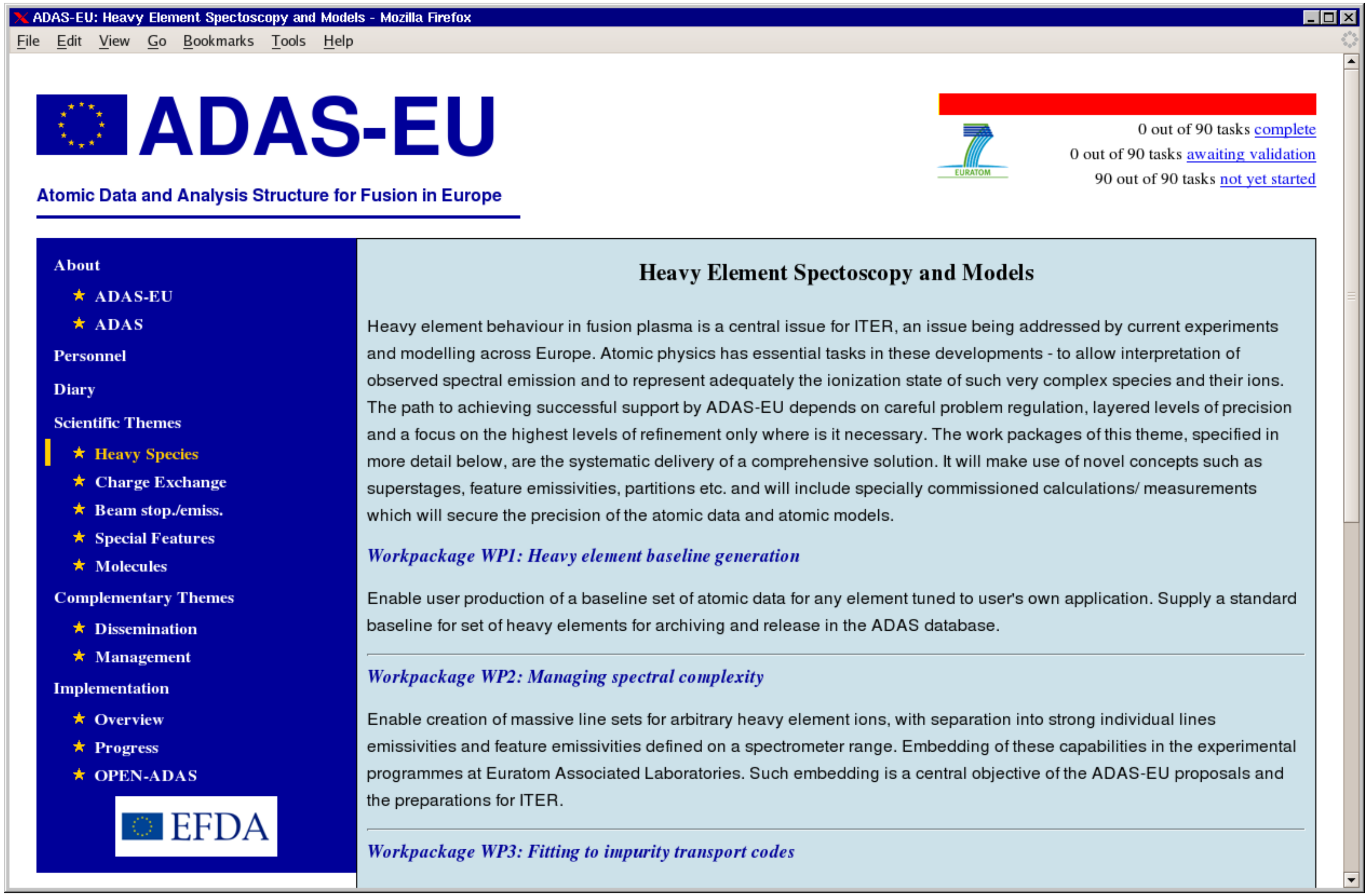


BEAM_MASS	FLOAT	2.00000
BEAM_ENERGY	FLOAT	40.0000
BEAM_TE	FLOAT	10.0000
BEAM_DENSITY	FLOAT	1.00000e+10
PLASMA_MASS	FLOAT	2.00000
PLASMA_TE	FLOAT	4440.00
PLASMA_DENSITY	FLOAT	2.50000e+13
PLASMA_ZEFF	FLOAT	2.00000
BEAM_DC_X	FLOAT	0.00000
BEAM_DC_Y	FLOAT	0.00000
BEAM_DC_Z	FLOAT	1.00000
BFIELD_VALUE	FLOAT	3.39150
BFIELD_DC_X	FLOAT	0.788000
BFIELD_DC_Y	FLOAT	0.00530000
BFIELD_DC_Z	FLOAT	0.615200
EFIELD_VALUE	FLOAT	0.00000
EFIELD_DC_X	FLOAT	1.00000
EFIELD_DC_Y	FLOAT	0.00000
EFIELD_DC_Z	FLOAT	0.00000
OBS_DC_X	FLOAT	0.870100
OBS_DC_Y	FLOAT	-0.0470000
OBS_DC_Z	FLOAT	0.490500
OBS_SIGMA	FLOAT	0.510000
OBS_PI	FLOAT	1.00000
BROADEN	INT	1

ADAS-EU: ADAS for Fusion in Europe

- Recently awarded Euratom FP7 Grant.
- Funding for four years to cover five main themes:
  - Heavy element spectroscopy and models,
  - Charge exchange spectroscopy,
  - Beam stopping and beam emission spectroscopy,
  - Special features,
  - Diatomic spectra and collisional-radiative models.
- Will employ two new people and provide part-funding for existing people.
- We note specifically that ADAS is still an international collaboration and project: ADAS-EU is a complementary project focusing on Europe. This will not lead to less support for the existing ADAS Project members.

ADAS-EU Website: `http://www.adas-fusion.eu`



Some thoughts on software and atomic physics for ITER

- When diagnostics or models disagree it is not helpful if they have different underlying atomic physics.
- ADAS has shown that it's possible (and, indeed, typical for ADAS members) to have consistency across diagnostics and models in a given fusion lab. Indeed, this consistency extends to a consistency across ADAS-member labs.
- It's been more recently shown (i.e. CXSFIT) that it's really possible to have identical* analysis codes running across different machines.
- ITER represents a unique challenge with so many people coming together from different labs. Careful thought has to be given to any atomic physics or analysis software which is being built-in to diagnostic packages.

* I really mean **identical** — not just 'the same' in the sense that everyone has something which they call EFIT.

Summary

- Some beam-specific examples:
  - CXSFIT
  - Stark feature
  - Using data in your own codes
  - Need for derived data
  - New-CHEAP
- Mentioned ADAS-EU — hopefully some of you will visit the website:
  - `http://www.adas-fusion.eu`
- Touched on moving forward towards ITER.

The 2009 ADAS Workshop will be held in conjunction with IPP Garching from 4th – 7th October 2009 just outside Munich (Ringberg Castle).