Atomic data and modelling for fusion
The ADAS and ADAS-EU Project

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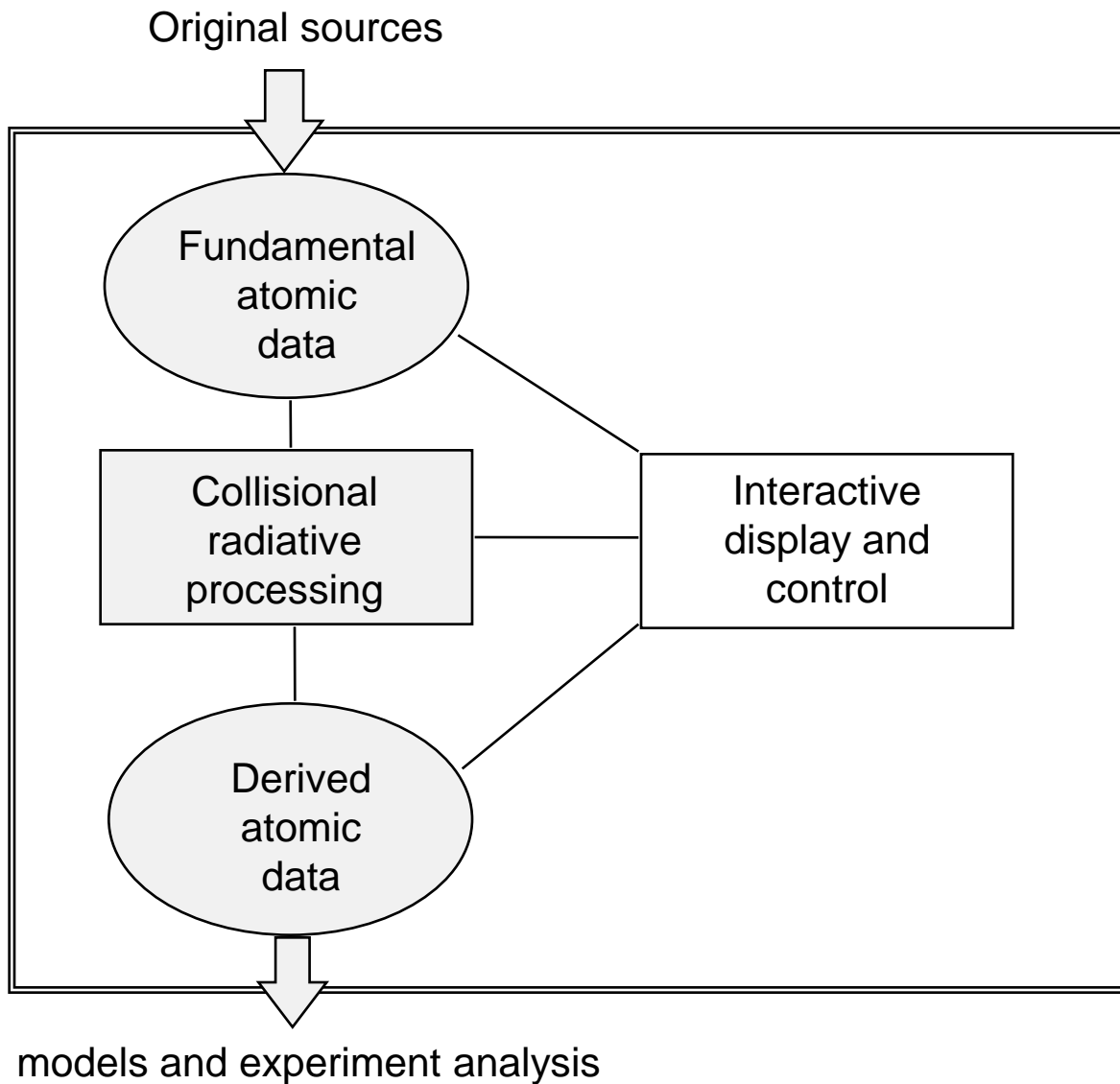
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The establishment of the ADAS Project

- Theoretical atomic physics support commenced at JET — 1984

- Centralised atomic data and coding under EDII, JET — 1985

- First IBM/TSO interactive ADAS release — 1989

- UNIX conversion preparatory study — 1993

- Start of ADAS project managed by Strathclyde University — 1993

- ADAS UNIX/IDL conversion — 1993/95

- 1st ADAS annual Workshop — 1995

- Start of ADAS project on going maintenance — 1996

- First non-voting university members (TUV) — 1997

ADAS modelling schematic

Original sources

Fundamental atomic data

Collisional radiative processing

Interactive display and control

Derived atomic data

models and experiment analysis

Atomic Data and Analysis Structure

- **ADAS Project**: origin in JET-ADAS, self-funded by subscription of participating laboratories.

  Membership:
  - EU Associated Labs.: JET, UKAEA Culham, IPP Garching/Greifswald, Fz-Juelich, CEA Cadarache, KTH Stockholm, CRPP Lausanne, CRFX Padua, TUW Vienna, FOM-Rijnhausen, NILPRP Bucharest, Rumania.
  - International Fusion: NIFS Japan, JAEA Japan, IPR India, BIRLA Jaipur India, SWIP China, IPP-CAS China, GA USA, Madison USA, ORNL USA, Univ. of Texas, USA, Univ. of Toronto Canada, Auburn University USA, Triniti/Kurchatov Russia, Princeton Univ. USA, NFRI Korea, ITER.
  - Other: Philips Research labs/ILT Aachen Germany, RAL Space Science UK, Catania Observatory/University Italy, Armagh Observatory Northern Ireland.

- **ADAS-EU**: European Union Framework 7 Support Action for fusion in Europe; Jan 2009 - Dec 2012; Univ. of Strathclyde research staff based full-time at fusion labs. in Europe - CCFE Culham/ JET Facility, IPP Garching, Fz-Juelich, CEA Cadarache/ITER. Extension to Sep 2013.

- **OPEN-ADAS**: open, web-based access to selected ADAS data, shared funding by IAEA A&M Data Unit and ADAS. A dissemination pathway for ADAS-EU. Upgrade 2013 by ADAS-EU.

- **EXTENDED-ADAS**: staff build and maintain shared analysis tools (eg CXSFIT, UTC) for fusion labs; support and prepare interfaces to primary fusion modelling codes; coordinate large scale developments for fundamental data generation.

ADAS overview and connections

http://www.adas.ac.uk

http://www.adas-fusion.eu
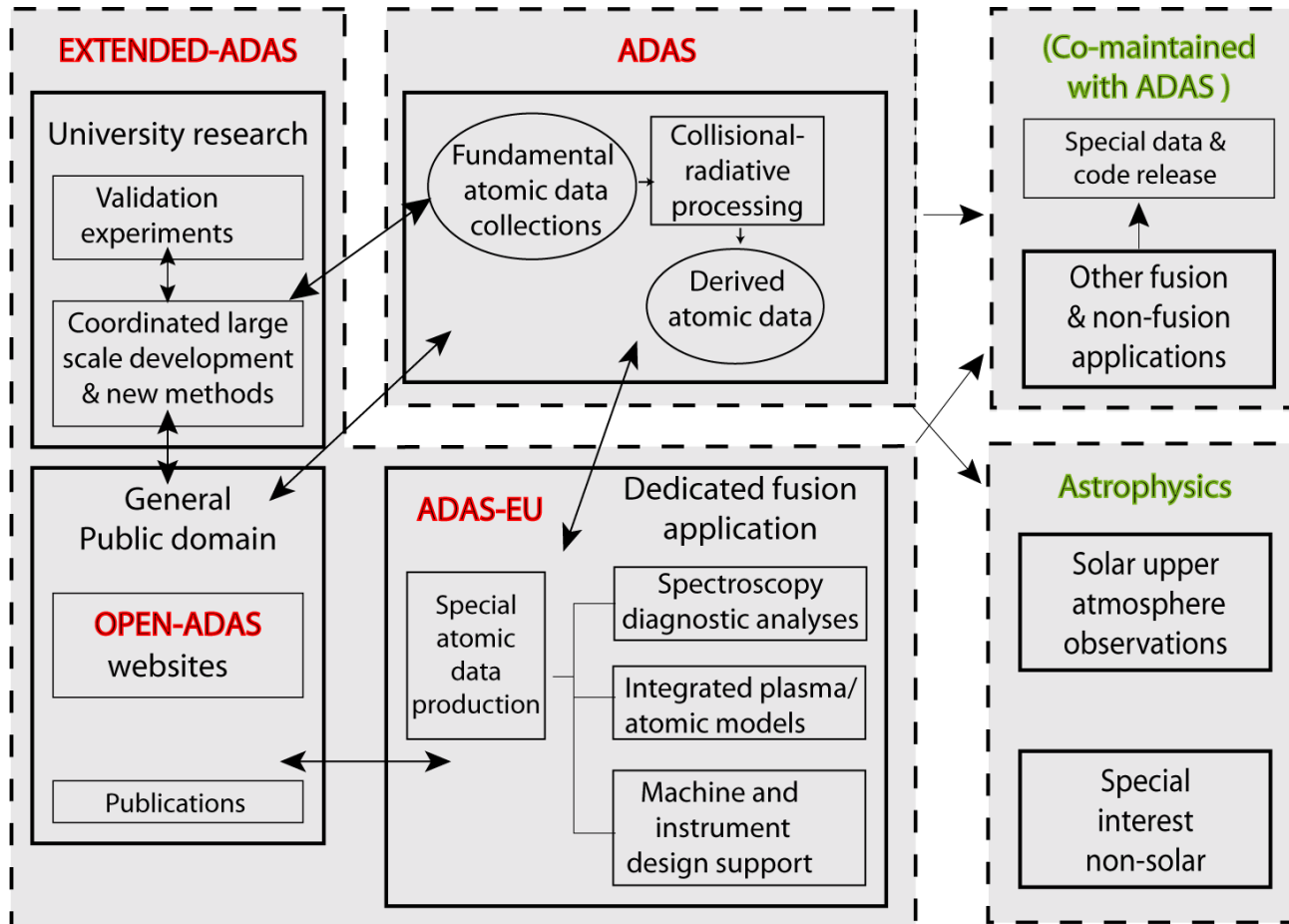
The character of ADAS

- ADAS is a reaction set database.

    - Comprises fundamental and derived data.

    - Associated with specific diagnostic or plasma model application purposes.

    - Reaction sets must be complete for a purpose, for example sufficient to support an excited population calculation for an ion.

    - ADAS implements its own *collisional-radiative* modelling to convert fundamental data to applied data.

    - The ADAS Project actively manages the procurement of fundamental data for its purposes.

http://www.adas.ac.uk

Fundamental and derived data

- Most spectroscopic diagnostic analysis of plasmas and most plasma models do not use fundamental reaction data directly.

- Derived data, combining the effects of perhaps many reactions through collisional-radiative models, are required, such as effective emission coefficients and effective recombination coefficients.

  - Plasma and atomic time constants determine the form of the derived coefficient data.
  - The derived data are, at minimum, functions of plasma Te and Ne.

- ADAS is quite prescriptive about the form and content of its fundamental and derived data – called ADAS data format numbers (adf<nn>).

- These formats are decided in advance with source producers and diagnosticians before substantive production.

Database

- Fundamental data, derived data, drivers etc. Currently ~ 18 Gbytes.

- There are ~ 55 different ADAS data formats.

- Some key ADFs and MDFs for general application

  - *ADF04* : specific ion data
  - *ADF11* : coll.-rad. ionis., recom. and related coefficients.
  - *ADF13* : ionisation per photon ratios
  - *ADF15* : emissivity coefficients
  - ADF40 : envelope feature photon emiss. Coefficients

  - *MDF00*: fundamental diatomic molecular constants
  - *MDF01*: rovibronic models
  - *MDF02*: fundamental cross-section data
  - *MDF04*: specific molecule data

Computational overview of ADAS

- The interactive user interface
  - ADAS series (9 series, ~85 programs)

- The fundamental and derived databases (~30,000 datasets)
  - ADAS data formats

- The application interface
  - ADAS Fortran subroutine (~1900) and IDL procedure (~1700) libraries
  - Data extraction procedures and subroutines by format: xxdata_<nn> , read_adf<nn>, xxdatm_<nn> , read_mdf<nn> .

- Offline-ADAS for large scale production
  - 6 large scale production packages: adas7#1, adas7#3, adas8#1, adas8#2, adas8#3, adas8#4 .

- Documentation

OPEN-ADAS

- Path for release of ADAS data and support software into the public domain.

- Development cost shared with ADAS and IAEA Vienna. Implemented by Allan Whiteford.

- Operational for five years. Resides on Strathclyde servers, mirrored at IAEA Vienna, who maintain statistics on usage.

- Major upgrade, supported by an ADAS-EU sub-contract, implemented by Allan Whiteford. New version released in Feb 2013.

http://open.adas.ac.uk

OPEN-ADAS

ADAS-EU: organisation

ADAS-EU: Organisation and Personnel

Governance Committee ⟶ **Director**
Prof. H. P. Summers

Appointees by :
ITER
UKAEA Culham Laboratory
IPP Garching
Fz Juelich
CEA Cadarache
IAEA Nucl. Data Section, Vienna

Special Advisor
Prof. R. K. Janev

Electron Working Party
Prof. N. R. Badnell

ADAS-EU Managers
Dr. M. G. O'Mullane[3]
Porf. N. R. Badnell[4]

Sub-contractors

ADAS-EU management staff location

CCFE Culham/JET-Facility
Univ. of Strathclyde

ADAS-EU staff placement laboratories

Fz Juelich
     Dr. F. Guzman (33%)
CEA Cadarache
     Dr. F. Guzman (67%)
IPP Garching
     Dr. L. Menchero (100%)
JET Facility
     Dr. A. Giunta (30%)

The ADAS-EU team

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Nigel Badnell

Francisco Guzman

Luis Menchero

ADAS-EU: physics theme support time chart

Figure 1   ADAS-EU: Physics theme and sub-theme support time chart

Theme	Code	Actions	2009	2010	2011	2012
Heavy element [1] spectroscopy and models	T1	applic.	Superstages & emissivities			Global scaling
		fund.	Baseline & emissivities [2]	Ionisation level 1	DR/GBPP level 1	Neutrals, level 2
		exploit. [3]	Heavy species in ITER studies	Tungsten spectral emission (ASDEX-U, JET)	Atomic model support of ITM for ITER	
Charge exchange spectroscopy	T2	applic.	CXSFIT shared analysis Parametric CXS	NEW-CHEAP shared analysis	CXS/UTC/transport link	
		fund.	Bundle-n & l-mix models	CTMC (improved) /CCAO/CCMC	Bundle-nl models for partially stripped receivers	
		exploit	CXS line fittiing extended to argon	Multi-line CXS region observation	Cross-linked CXS & passive diagnostic	
Beam stopping beam emission spectroscopy	T3	applic.	Li/Na beam analysis and database		Beam emission/beam stopping consistency	
		fund.	Li/Na beam database	Bundle-n & Stark GCR		
		exploit.	Li/Na beam edge parameter diagnosis		Beam emission exploitation for ITER	
Special features	T4	applic.	Integrated special feature fitting and display			
		fund.	Zeeman, soft-X-ray, Balmer series special features			
		exploit.	Fitting with spectral primitives	He-like soft X-ray line analysis	Balmer series/limit observations	
Diatomic spectra and coll-rad models	T5	applic.	H_2 isotopomer spectral simul.			
		fund.	H_2/H electr. & ion database	H_2/H vibronic/GCR populations		
		exploit.	Composite continuum emission studies	Integrated edge modelling		

Notes: (1) Sets of 3 to 5 work packages make up the scientific support of each theme. Each work package is sub-divided into tasks.

        (2) The completion of the sub-themes in the `applic.' and `fund.' categories mark science milestones. The sub-theme is an assembly of work package tasks.

        (3) `exploit' indicates the expected use by fusion plasma modellers and spectral diagnosticians on-site at European fusion laboratories, with which ADAS-EU staff will assist.

ADAS-EU: physics theme support time chart

Figure 9a: Theme 6: Medium weight element Generalised-Collisional-Radiative modelling

Work package	No.	Task	Task no.
AS/DW baseline lift to levels 1 and 2	27.	AUTOSTRUCTURE / Distorted Wave implementation in ls and ic coupling for ADAS adf04 production.	27-1
		AUTOSTRUCTURE / Distorted Wave mass production for medium weight elements.	27-2
GCR ionisation and recombination	28.	GCR ionisation fractionisation for metastables for level 1 and level 2 modelling.	28-1
		GCR dielectronic recombination for level 1 and level2 modelling using BBGP/adf04 type 6 and hybrid/adf09	28-2

ADAS-EU: sub-contract special studies

1. Univ. Autonoma, Madrid – Clara Illescas

   Charge exchange and ion impact data for fusion plasma spectroscopy: State-selective charge transfer and excitation for low/medium charge projectiles and neutral hydrogen targets

2. Univ. Vilnius, Lithuania (x2) - Pavel Bogdanovich

   Atomic structure and electron data for heavy element ions (1) configuration interaction and relativisitic/quasi-relativistic structure. (2) auger/cascade, multiple ionisation and shake-off. (3) production of configuration interaction, quasi-relativistic atomic structure and cross-sections for the adas database. (4) atomic structure interchange.

3. Univ. Giessen, Germany – Alfred Mueller, Stefan Schippers

   Electron impact cross-section data for fusion applications: Ionisation and recombination of heavy element ions

4. Tech. Univ. Vienna – Katherina Igenbergs

   Atomic data and models for neutral beam diagnostics. (1) lithium and sodium beam models and data.
   (2) CCAO calculations for H (n=1,2) targets.

5. Queen's Univ. Belfast – Allan Hibbert, Kathy Ramsbottom

   Electron collision cross-sections for heavy element ions : Pilot r-matrix calculations for tungsten – W^{+44} .

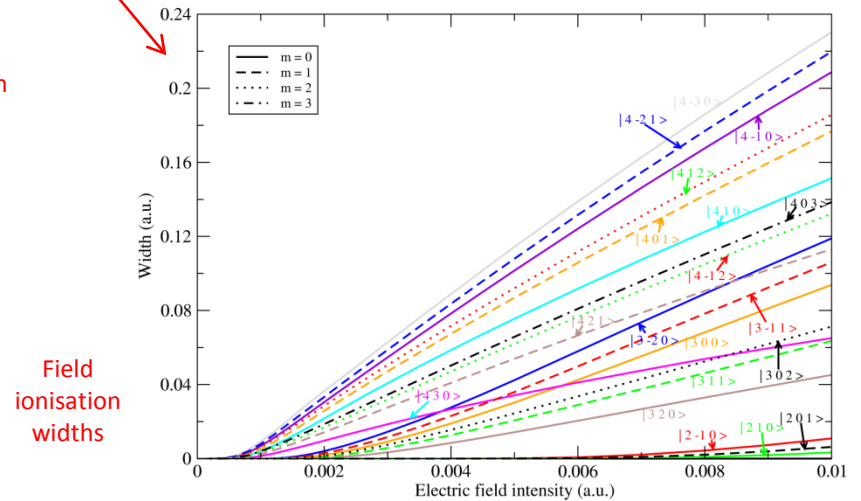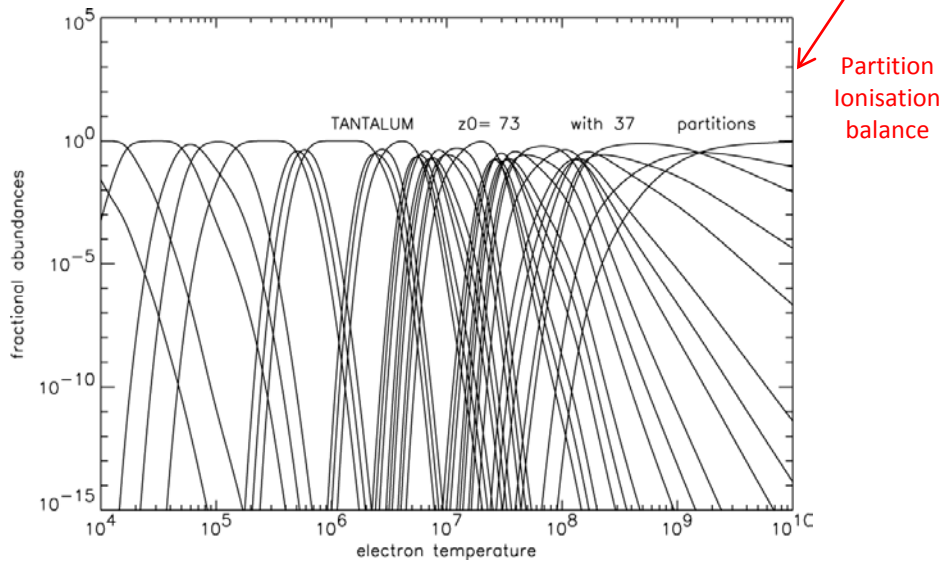6. Univ. Mons-Hainaut (x2) - Pascal Quinet, Patrick Palmeri

   Atomic structure and electron data for heavy element ions: (1) The tungsten ions W^{+0} to W^{+4} and adjacent element systems
   (2) The ions w+3 to w+5 and adjacent element neutral/near-neutral ions. Atomic structure mapping between codes

Natural partition

Zeroth-order wave-functions
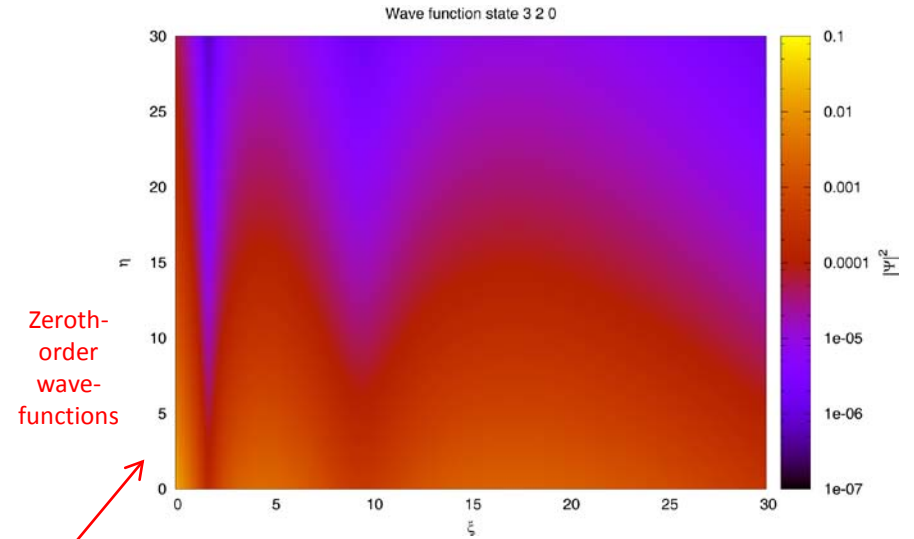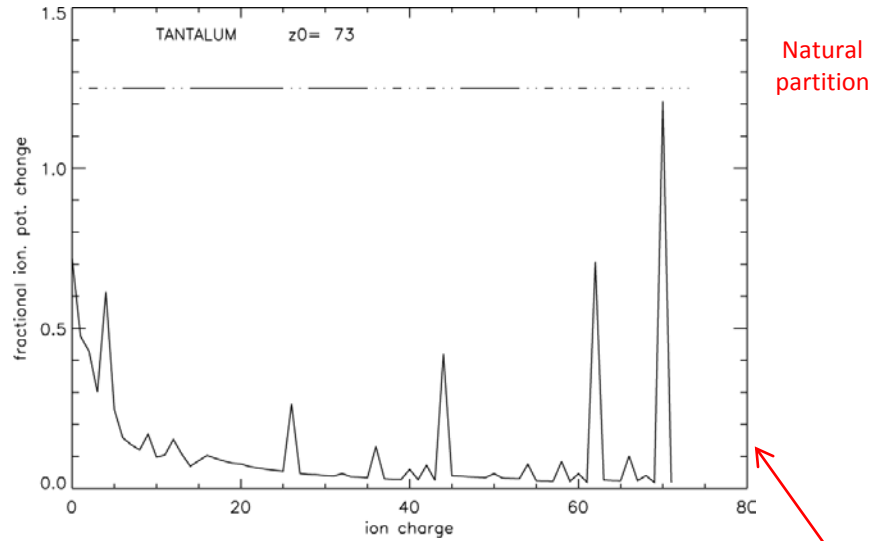
Superstages   **Stark modelling**

Partition Ionisation balance

Field ionisation widths

ADAS-EU: dissemination and knowledge transfer

- Courses: An intensive 1-2 week course on atomic modelling and using atomic data for fusion was presented annually.
  - 8-16 Oct 2009: IPP Garching
  - 7-15 Oct 2010: EFDA-JET Facility
  - 26-30 Mar 2012: RFX Padua
  - 26 Sep – 5 Oct 2012: CEA Cadarache

  Spawned additional courses: July 2010 Auburn USA, Dec 2010 ITER

- Visits: Six support visits/year to fusion laboratories in Europe.

- Collaborations: Small-scale sub-contracting to promote special studies for selective fundamental database improvement.

ADAS-EU: Modules

The ADAS-EU Euratom - Framework 7 Project of the European Community is sponsoring eight 3-day workshop/advanced training courses at fusion laboratories in Europe and in ITER participating countries outside Europe. The objectives are to examine atomic physics aspects of importance for participant laboratories, to inform by means of lectures and demonstrations about the principal advances made during the four years of ADAS-EU support, to explore the opportunities for new collaborative work on atomic physics with participants within the framework of the ADAS Project, cooperation with Europe and ITER.

There are eight modules available, each of duration 1.5 hours, comprising a lecture, demonstration and discussion.

1. Impurity atomic species in fusion plasma, their ionisation state and radiating characteristics - the ADAS approach.

2. Complex species in the core and edge of the fusion plasma. Describing and calculating their characteristics - the current state.

3. H2 molecular emission and collisional-radiative modelling.

4. Modelling and analysing special spectral features. A unified approach.

5. Charge exchange and beam emission spectroscopy. Modelling emitter populations and analysing spectra.

6. Advanced charge exchange plasma receiver and beam donor modelling – the current state.

1. Calculating fundamental atomic structure and electron impact cross-section data – Autostructure and R-Matrix .

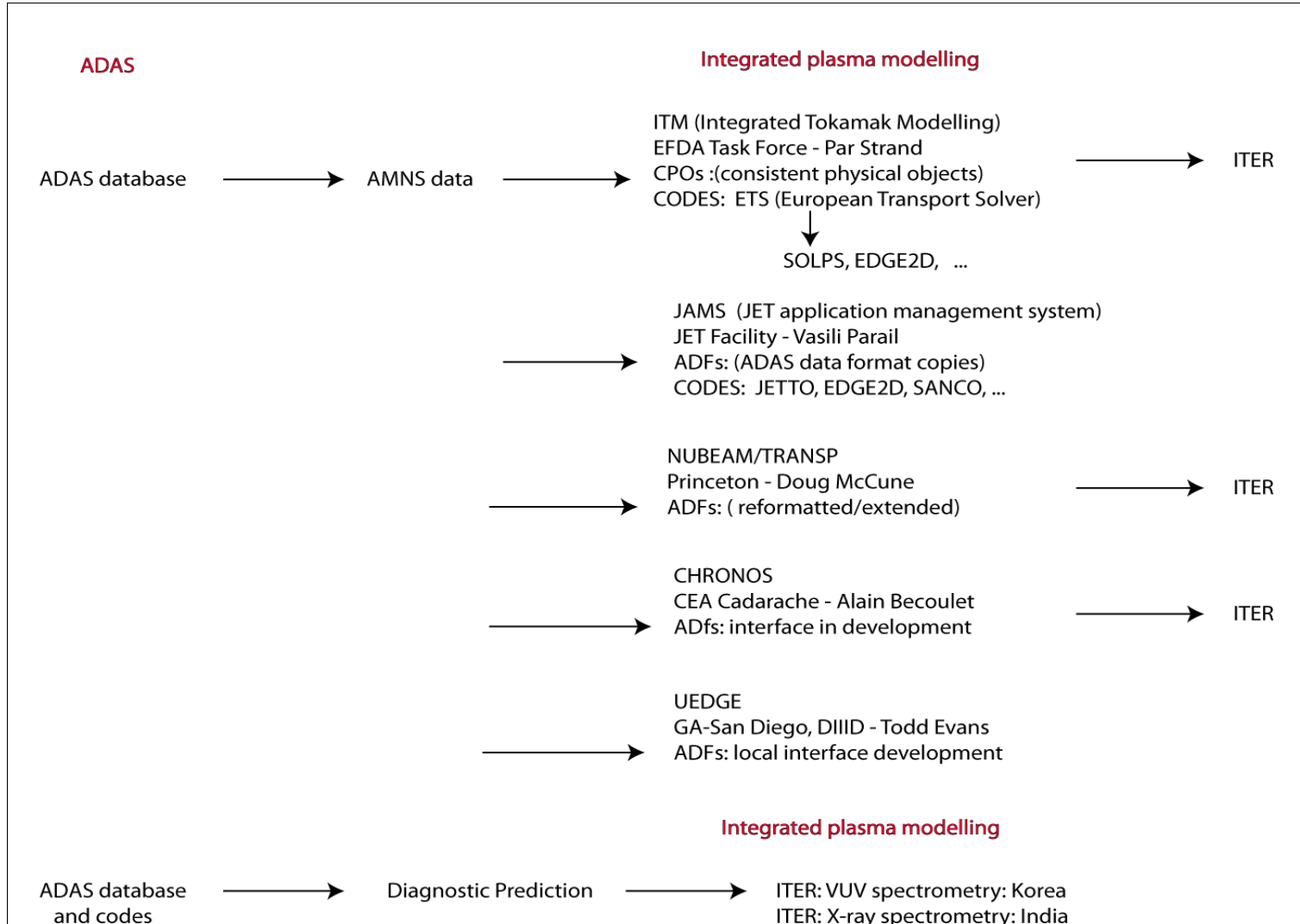2. Spectral diagnostics for special environments – the interface between fusion and astrophysics.

Extended ADAS: shared analysis tools

CXSFIT
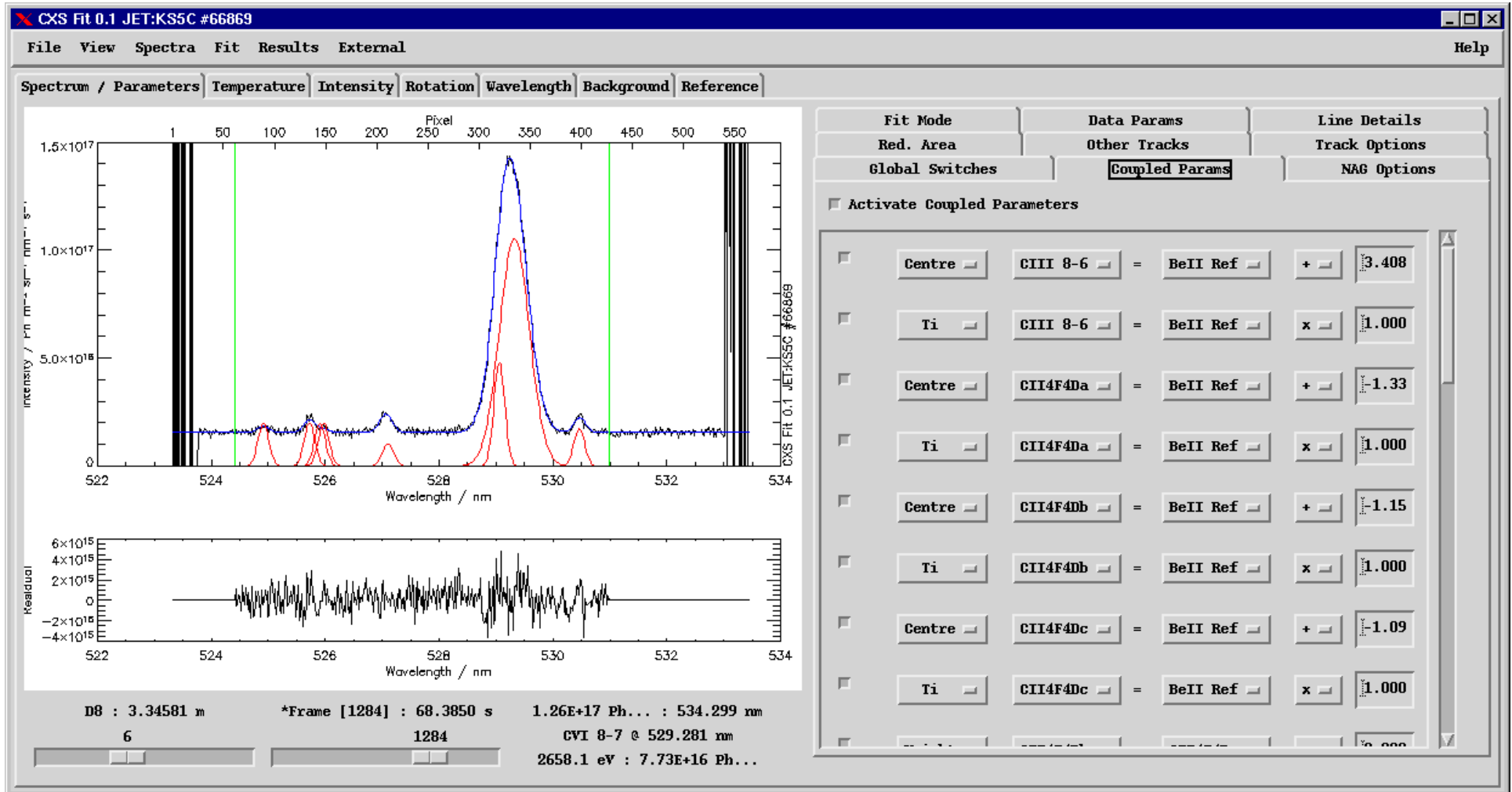
Extended ADAS: Interfacing to integrated plasma modelling

Complexity develops as ADAS data is adopted and linked into large scale modelling and analysis efforts.

Conclusions

1. A brief history of the ADAS Project has been given.

2. The ADAS-EU Project has allowed strong growth in the capabilities of ADAS for fusion.

3. Tomorrow a full day is assigned to presenting and demonstrating some of these capabilities.

4. The time available is such that only four of the eight modules can be presented. However, ADAS/ADAS-EU staff will be here through until the end of the week so hopefully there will be opportunity for supplementary demonstrations, questions and discussions.

5. A primary wish is progress to the establishment of relevant collaborations in the support of ITER.

6. The third day is devoted to discussions in this regard.