ADAS operations and release 2.11

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12th October 2007

Contents

- Current ADAS computational requirements.
- Current size of ADAS and ADAS sites.
- ADAS visits.
- Major additions.
- New website.
- Documentation with focus on Fortran library documentation.
- Data status and direct CVS access.
- Questions (both from and to me).

Computational requirements

- Usual to create an ADAS account:
  - username of 'adas' and home directory of `/home/adas`,
  - exact setup varies according to network implementation at each site.
- ADAS requires the following software:
  - IDL,
  - FORTRAN compiler,
  - C compiler,
  - csh,
  - Perl,
  - CVS.

Size of ADAS and distribution

- Hard disk requirements are just over 3.0GB but we would request at least a 3.5GB disk quota.
- 422,967 lines of FORTRAN and 400,776 lines of IDL
- Some Perl, Matlab, csh and PHP.
- 2.8GB of data in 19,158 distinct files.
- Even at maximum compression (i.e. `gzip -9`) ADAS won't fit on a CD.
- Release 2.12 will be distributed from next week.

Current and supported platforms

- PC-based linux systems:
  - now our preferred platform,
  - support for and experience with g77 and Portland Group compilers,
  - IDL licenses are 40% cheaper!
- Sun and DEC systems are becoming few and far between.
- gfortran seems to work fine.
- ifort stopped being free (at version 10) so we've given up on it.
- Other systems are supported but not recommended.

Current ADAS sites

Site	Country	Platform	IDL	Contact
Auburn	USA	Linux	6.3	Stuart Loch
Caderache	France	Linux⋆	6.0	Rémy Guirlet
Catania	Italy	Linux	6.0	Alessandro Lanzafame
FOM	The Netherlands	Linux	?.?	Manfred von Hellermann
Garching	Germany	Sun	ALL	Thomas Pütterich
GA	USA	Linux	6.0	Todd Evans
IPR	India	Linux	5.4	Parameswaran Vasu
JAERI	Japan	DEC	5.4	Tomohide Nakano
JET	England	Linux	6.3	Martin O'Mullane
Jülich	Germany	Linux	6.1	Phillipe Mertens
Lausanne	Switzerland	Linux	5.5	Richard Pitts
NIFS	Japan	Linux	5.4	Daiji Kato
ORNL	USA	Linux	6.3	Predrag Krstic
Padua	Italy	Linux	5.6	Marco Valisa
Philips	Germany	Linux	5.6	Thomas Krücken
RAL	England	Linux⋆	5.4	Andrzej Fludra
Stockholm	Sweden	Linux	6.0	Elisabeth Rachlew
Strathclyde	Scotland	Linux	6.4	Allan Whiteford
SWIP	China	Linux	?.?	Xuru Duan
Toronto	Canada	Linux	6.1	David Elder
UKAEA	England	Linux	6.1	Martin O'Mullane
Wisconsin	USA	Linux	5.4	Daniel Den Hartog

ADAS visits Oct 2006 – Oct 2007

Hugh Summers	Martin O'Mullane	Allan Whiteford
IPP-Garching	FZ-Jülich	IAEA
CEA	IPP-Garching	FZ-Jülich
FZ-Jülich	CEA	IPP-Garching
Catania	NIFS	NIFS
		Catania

(Oct 2005 – Oct 2006:

Hugh Summers	Martin O'Mullane	Allan Whiteford
IPP-Garching	IAEA	JAEA
IPR	IPP-Garching	NIFS
JAEA	Auburn	IPP-Garching
NIFS	GA	
SWIP	Madison	

)

Planned visits

Hugh Summers	Martin O'Mullane	Allan Whiteford
KTH	ORNL	KTH
IPR	GA	SWIP
FOM	Auburn	JAEA
Padua	Wisconsin	NIFS
CEA / ITER	CEA / ITER	Padua

Major additions since last year

- Documentation of subroutines (discussed later in this talk).
- Superstage and flexible partitioning infrastructure:
  - Update to numerous reading/writing routines,
  - ADAS408 now gives out ZCD, YCD and ECD.
- LS and IC resolved adf00 files for H, He, Li, Be, B, C, N, F, Ne and Ar.
- Major (but backward compatible) changes to adf12 data format.
- Routines to do arbitrary charge exchange (talk of Foster).
- Update of all W ionisation potentials (from Kramida and Reader).

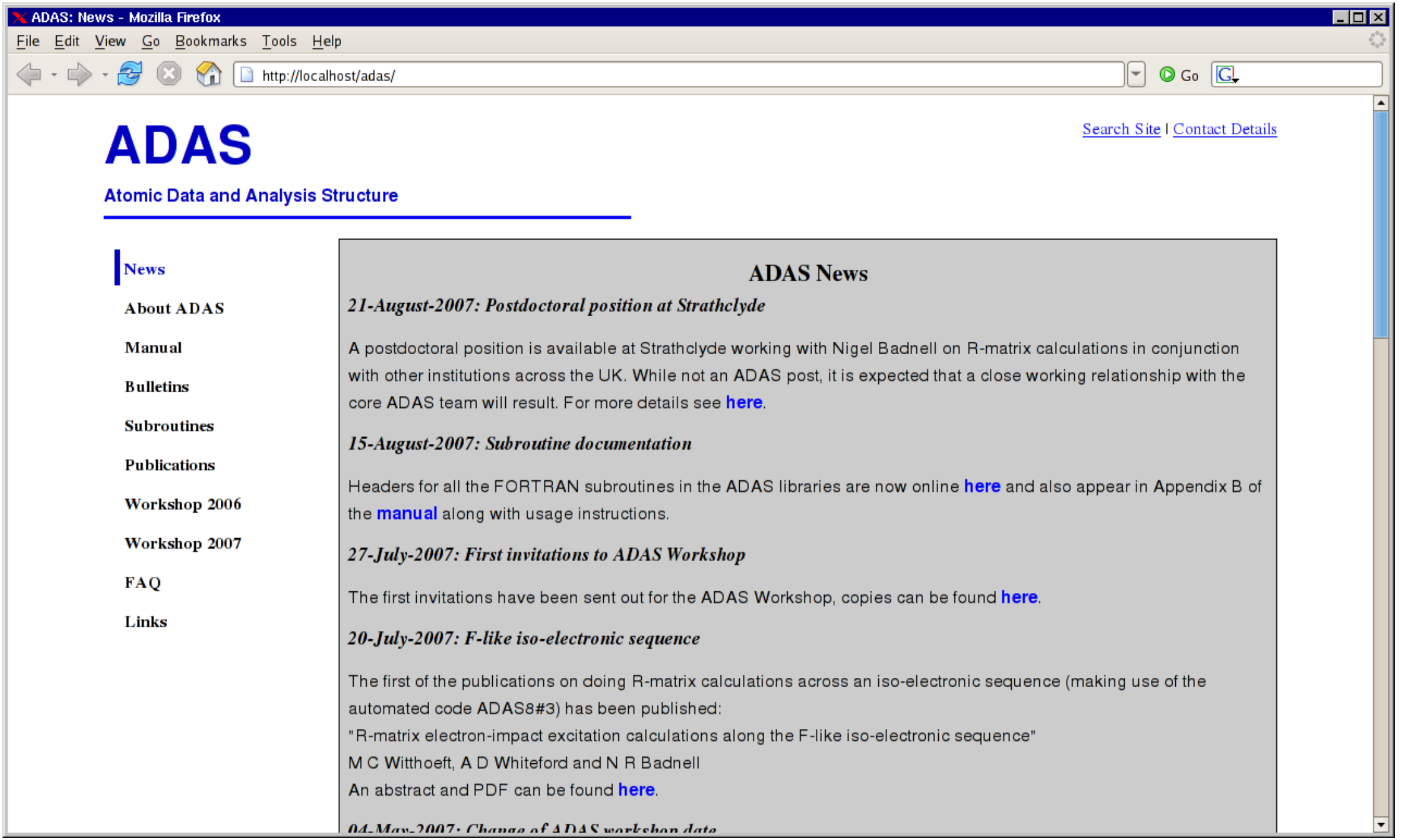
Upcoming major additions

- F-like excitation sequence data.
- H-like, He-like and Li-like iso-electronic sequence data.
- Mg-like RR and DR sequence.
- SFF system for special features (discussed by Meigs).
- Balmer series modelling code (ADAS217).
- Automated GCR program (discussed previously by O'Mullane)

Website — `http://adas.phys.strath.ac.uk`

- At this session last year, comment was made that the ADAS website was poor.
- New website was written and launched in January 2007 (Martin and Allan were at the top of a hill in Japan — lots of work was done in the evening).
- Implemented using PHP5 on an Apache 2 daemon serving out "XHTML 1.0 Transitional" with rendering controlled via CSS2 (whatever that all means!).
- Contains ADAS manual in PDF format along with other information.
- Full text search available (but Google can do it faster!).
- Theme, colours and layout are very similar to OPEN-ADAS site — perhaps too similar: could cause confusion.

Some pictures...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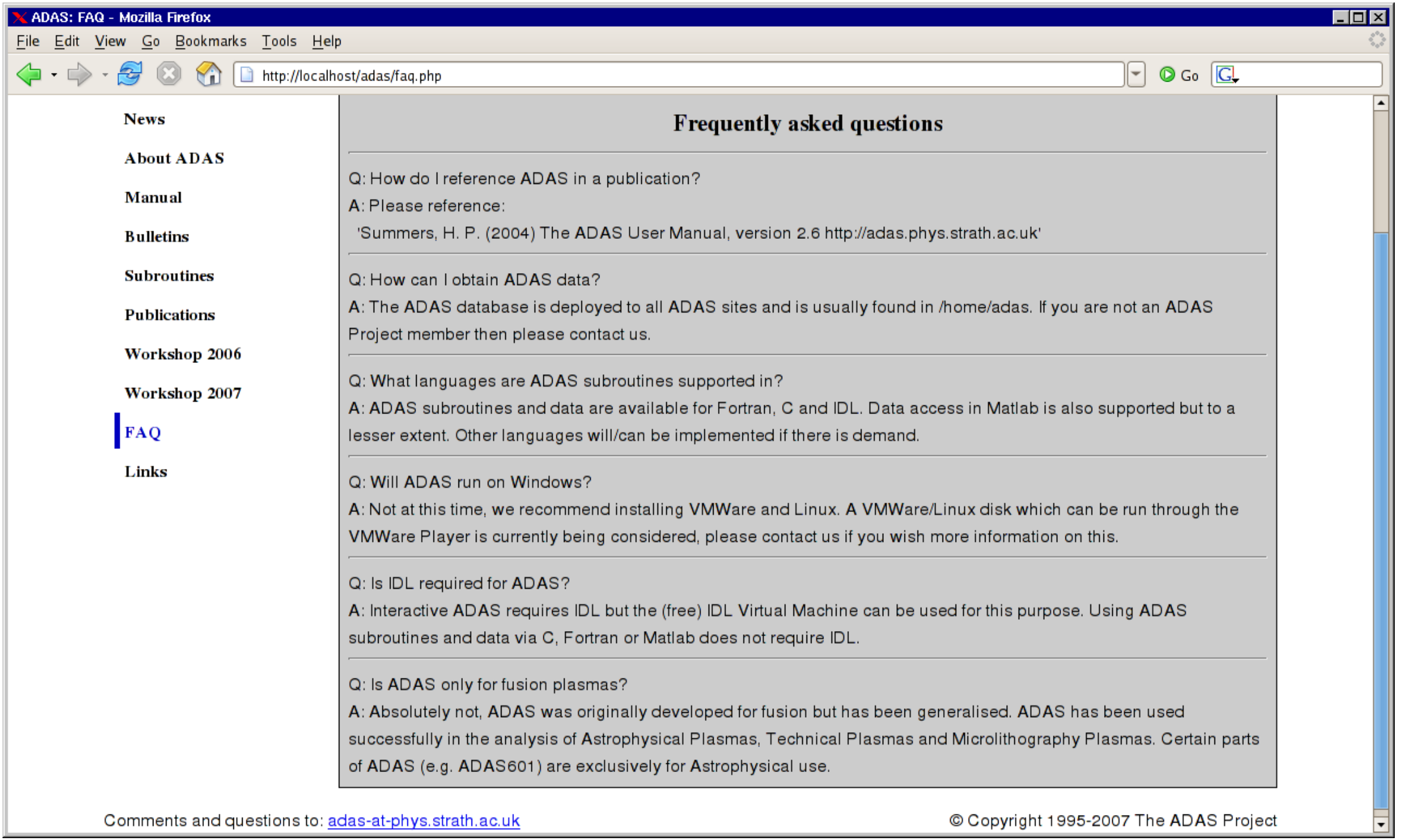
News
About ADAS
Manual
Bulletins
Subroutines
Publications
Workshop 2006
Workshop 2007
FAQ
Links
ADAS News
21-August-2007: Postdoctoral position at Strathclyde
A postdoctoral position is available at Strathclyde working with Nigel Badnell on R-matrix calculations in conjunction with other institutions across the UK. While not an ADAS post, it is expected that a close working relationship with the core ADAS team will result. For more details see here.
15-August-2007: Subroutine documentation
Headers for all the FORTRAN subroutines in the ADAS libraries are now online here and also appear in Appendix B of the manual along with usage instructions.
27-July-2007: First invitations to ADAS Workshop
The first invitations have been sent out for the ADAS Workshop, copies can be found here.
20-July-2007: F-like iso-electronic sequence
The first of the publications on doing R-matrix calculations across an iso-electronic sequence (making use of the automated code ADAS8#3) has been published:
"R-matrix electron-impact excitation calculations along the F-like iso-electronic sequence"
M C Witthoeft, A D Whiteford and N R Badnell
An abstract and PDF can be found here.


ADAS: Docmentation - Mozilla Firefox
File Edit View Go Bookmarks Tools Help
http://localhost/adas/manual.php
Go
Manual
Bulletins
Subroutines
Publications
Workshop 2006
Workshop 2007
FAQ
Links
Introductory Material
Table of Contents
Introduction
ADAS Series 1 - Atomic Data Entry and Verification
Introduction to Series 1
ADAS101: Electron Impact Excitation Cross Section - Graphing and Rate Evaluation
ADAS102: Electron Impact Excitation Rate - Graphing and Interpolation
ADAS103: Dielectronic Recombination - Graphing and Interpolation
ADAS105: Electron Impact Ionisation Cross Section - Graphing and Rate Evaluation
ADAS106: Electron Impact Ionisation Rate - Graphing and Interpolation
ADAS108: Electron Impact Excitation of Neutrals and Molecules. - Graphing and Rate Evaluation
ADAS Series 2 - General Z Data and Population Processing
Introduction to Series 2
ADAS201: Specific Z Excitation File - Graph and Fit Coefficient
ADAS202: General Z Recom./Ionis. File - Extraction from General Z File
ADAS203: General Z Excitation File - Extraction from General Z File
ADAS204: Specific Z Recom./Ionis. File - Process ACD,SCD and Population
ADAS205: Specific Z Excitation File - Process Meta./Excit. Population
ADAS206: Specific Z Excitation File - Process Line/Total Power
ADAS207: Meta./Excit. Population File - Process Line Emissivities
ADAS208: Specific Z Excitation File - Advanced Population Processing
ADAS209: General Level Bundling File - Process Effective Collision Strengths
ADAS210: General Level Unbundling File - Process Effective Collision Strengths
ADAS211: Radiative Recombination - Process for Specific Ion File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http://localhost/adas/faq.php
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News
About ADAS
Manual
Bulletins
Subroutines
Publications
Workshop 2006
Workshop 2007
FAQ
Links
Frequently asked questions
Q: How do I reference ADAS in a publication?
A: Please reference:
'Summers, H. P. (2004) The ADAS User Manual, version 2.6 http://adas.phys.strath.ac.uk'
Q: How can I obtain ADAS data?
A: The ADAS database is deployed to all ADAS sites and is usually found in /home/adas. If you are not an ADAS Project member then please contact us.
Q: What languages are ADAS subroutines supported in?
A: ADAS subroutines and data are available for Fortran, C and IDL. Data access in Matlab is also supported but to a lesser extent. Other languages will/can be implemented if there is demand.
Q: Will ADAS run on Windows?
A: Not at this time, we recommend installing VMWare and Linux. A VMWare/Linux disk which can be run through the VMWare Player is currently being considered, please contact us if you wish more information on this.
Q: Is IDL required for ADAS?
A: Interactive ADAS requires IDL but the (free) IDL Virtual Machine can be used for this purpose. Using ADAS subroutines and data via C, Fortran or Matlab does not require IDL.
Q: Is ADAS only for fusion plasmas?
A: Absolutely not, ADAS was originally developed for fusion but has been generalised. ADAS has been used successfully in the analysis of Astrophysical Plasmas, Technical Plasmas and Microlithography Plasmas. Certain parts of ADAS (e.g. ADAS601) are exclusively for Astrophysical use.
Comments and questions to: adas-at-phys.strath.ac.uk
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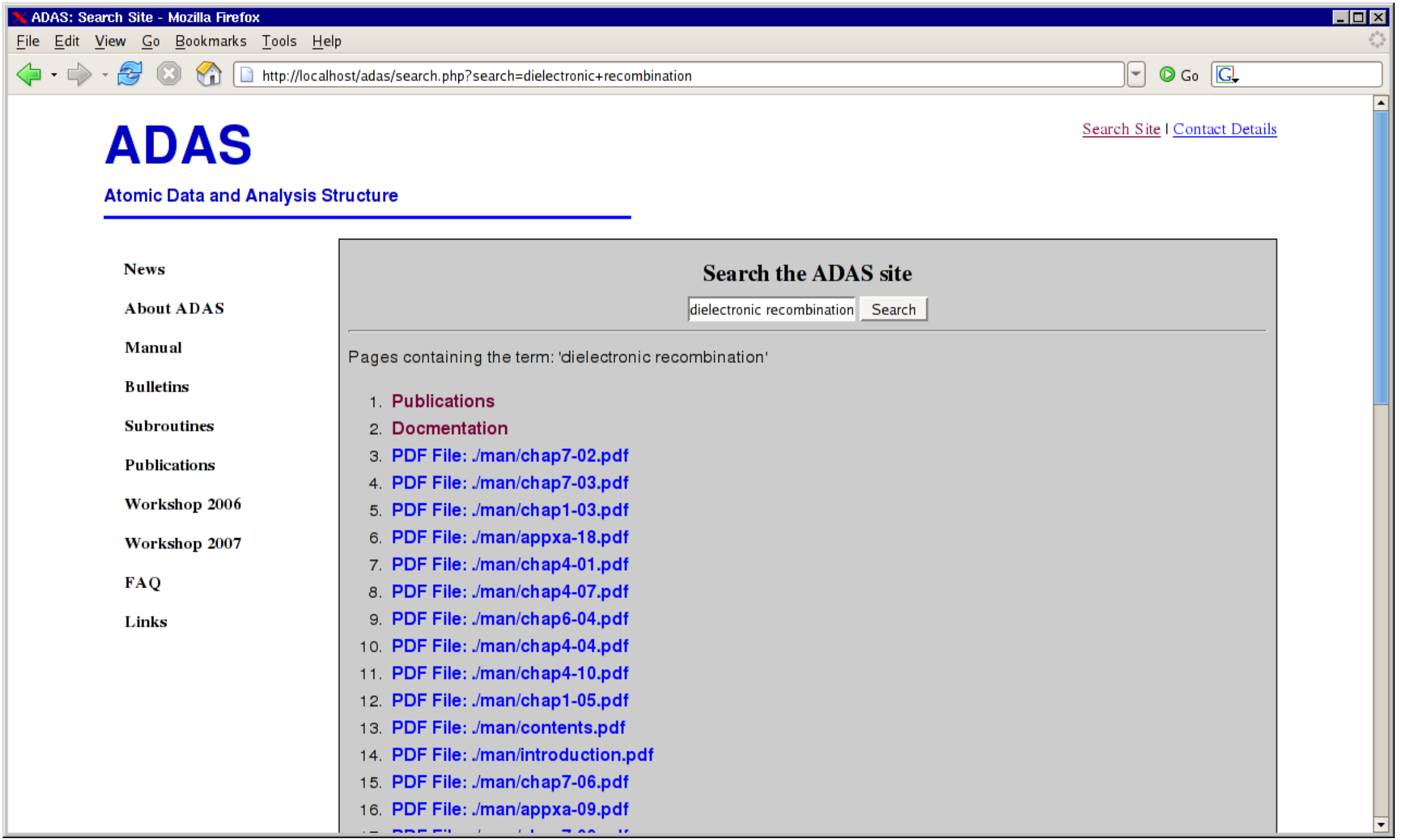
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News
About ADAS
Manual
Bulletins
Subroutines
Publications
Workshop 2006
Workshop 2007
FAQ
Links
Search the ADAS site
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Pages containing the term: 'dielectronic recombination'
1. Publications
2. Docmentation
3. PDF File: ./man/chap7-02.pdf
4. PDF File: ./man/chap7-03.pdf
5. PDF File: ./man/chap1-03.pdf
6. PDF File: ./man/appxa-18.pdf
7. PDF File: ./man/chap4-01.pdf
8. PDF File: ./man/chap4-07.pdf
9. PDF File: ./man/chap6-04.pdf
10. PDF File: ./man/chap4-04.pdf
11. PDF File: ./man/chap4-10.pdf
12. PDF File: ./man/chap1-05.pdf
13. PDF File: ./man/contents.pdf
14. PDF File: ./man/introduction.pdf
15. PDF File: ./man/chap7-06.pdf
16. PDF File: ./man/appxa-09.pdf

Documentation

- Bulletins are issued with every release, all of the ADAS bulletins are available at all ADAS sites under the directory `/.../adas/docs/bulletins`.

- CXSFIT manual has been written and will be published as an internal report.

- GCR Paper I is available for people who haven't yet read it (twice):
  - 'Ionization state, excited populations and emission of impurites in dynamic finite density plasmas. I:
    The generalized collisional–radiative model for light elements'
    Summers H P, Dickson W J, O'Mullane M G, Badnell N R, Whiteford A D, Brooks D H, Lang J, Loch S D and Griffin D C
    Plasma Phys. Contr. Fusion **48** 263 (February 2006)

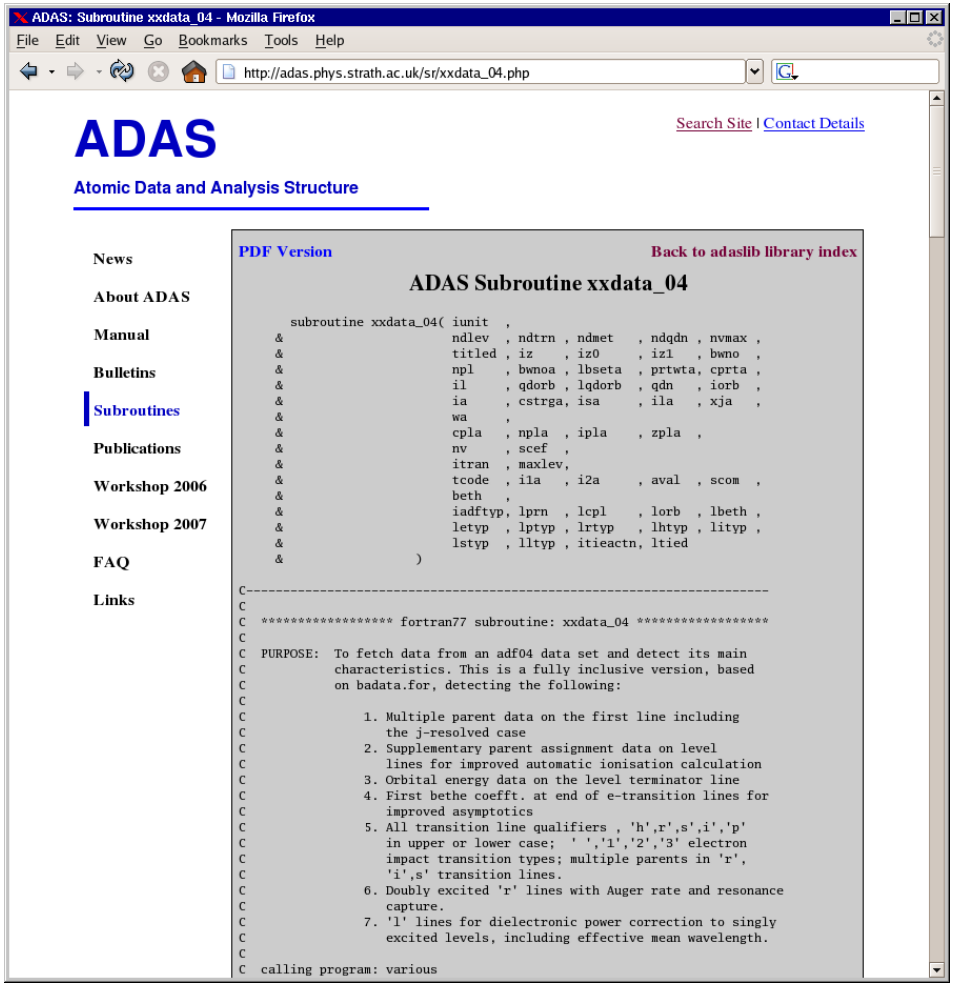
- Made it on to the PPCF list of top 25 downloads for 2006!

Subroutine documentation

- We now have a > 1500 page manual documenting every subroutine in our linkable Fortran libraries.
  - Shows subroutines description and precise specification of inputs and outputs
  - Block of fortran statements for dimensioning (convenient for copying).
  - Full revision history included.
  - Examples of calling from C and Fortran included.
  - Contents section by ADAS series and index by name.
- Documentation is automatically generated by a Perl program.
- Almost every subroutine has been (tediously) inspected by hand.
- IDL is partially self-documenting (via `/help`) keyword but we plan to have a parallel IDL document available in the next year.

On-line subroutine documentation

- Also available on-line
- Full text search available
- Can be viewed in browser
- Individual (typically 2-3 page) PDF files can be downloaded
- Indexed by Google — first hit for "burgess general program" is ADAS library.



Data Status

- Data status is no longer the definitive source of ADAS data.
- Interim recommendations and reminders:
  - ADF11 and ADF15 files are categorised according to the year a method was introduced. '96' data is currently the best (GCR) and should be used where available.
  - ADF04 files are categorised according to the year they were produced so a general recommendation is not always possible.
- From early next year, recommended data searching system will be OPEN-ADAS or derived from OPEN-ADAS.
- Possibility of a more interactive non-web based searching solution at each ADAS site depending on demand.

Direct CVS access

- Possible to have indirect read-only access to parts of ADAS CVS respository:
  - `export CVSROOT=`
    `:pserver:username@adascvs.phys.strath.ac.uk:/work/adascvs`
  - `cvs checkout adf11`
  - `cvs checkout xxdata_11`
- Login required: contact us for a username/password.
- Not actually a 'real' CVS repository but looks like one.
- Virtual-modules are self-contained (so duplication of files across modules).
- Still beta but tested with standard UNIX CVS and Windows CVS.

Questions

- Are there any languages people are **actually** using which we don't support?
- Should we make offline-ADAS easier to compile/use or is it ok as it is?
- Bootable DVD with interactive ADAS?
- VMware-style virtual machine distribution of ADAS?
- Is there any call for the XML tag files from OPEN-ADAS and/or a MySQL database to be made available on local machines?