The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

2028-8

Joint ICTP/IAEA Workshop on Atomic and Molecular Data for Fusion

20 - 30 April 2009

Atomic Molecular and Particle-Surface Interaction
Web Databases and Data Exchange
Lecture 3 - Numerical Data

Denis HUMBERT

IAEA, Div. of Physical & Chemical Science
Dept. of Nuclear Sciences & App. A-1400
Vienna
Austria

Atomic, molecular and particle-surface interaction web databases and data exchange

Lecture 3
Numerical Data

ICTP Workshop on Atomic and Molecular Data for Fusion Energy Research

Trieste, 20-30 April 2009

Denis Humbert

Content

1. **Atomic and Molecular Data Unit of the IAEA**

2. **Bibliographic data**

3. **Numerical data**
   - Data quality
   - Data centres
   - Web numerical databases
   - ALADDIN
   - A search engine: GENIE
   - Web calculation tools

4. **Data exchange**

Numerical Data for Fusion Energy Research

- Data Centres with on line numerical data
  - NIST http://physics.nist.gov/PhysRefData
  - CAMDB http://www.camdb.ac.cn/e/
  - NIFS http://amdata.nifs.ac.jp/
  - IAEA http://www-amdis.iaea.org
  - KAERI http://amods.kaeri.re.kr
  - OPEN-ADAS http://open.adas.ac.uk
- Astrophysics web sites
- Other web sites

Database definition

- Origin: computer science, but broadened to popular use even to non-electronic data collections.
- Possible definition: database is a collection of records stored in a computer in a systematic way, so that a computer program can consult it to answer questions
- A database implies:
  - Schema: definition of the different objects (tables and relations between tables)
  - Database model: the relational model is the most common one
  - Database management system (DBMS) to manage and query the data.

Quality Assurance

- Traceability: source of the reference, how, where and when
  - Type of publication: refereed paper, lab report…
  - Year of publication / production
- Nature of the organisation originally reporting the data, authors

- Nature of the data provider: data centre, research lab…
- A system for error reporting on the part of users

- Evaluated data, recommended data from a well-know organisation
- Accuracy, error bars
- Type of data: raw data (tables), fitting function, interpolation…
- Nature of the method used
  - Experimental / theoretical / compilation
  - Detailed information on the method: what theory, what code, what experiment and diagnostic…

Data Quality: a traceability example

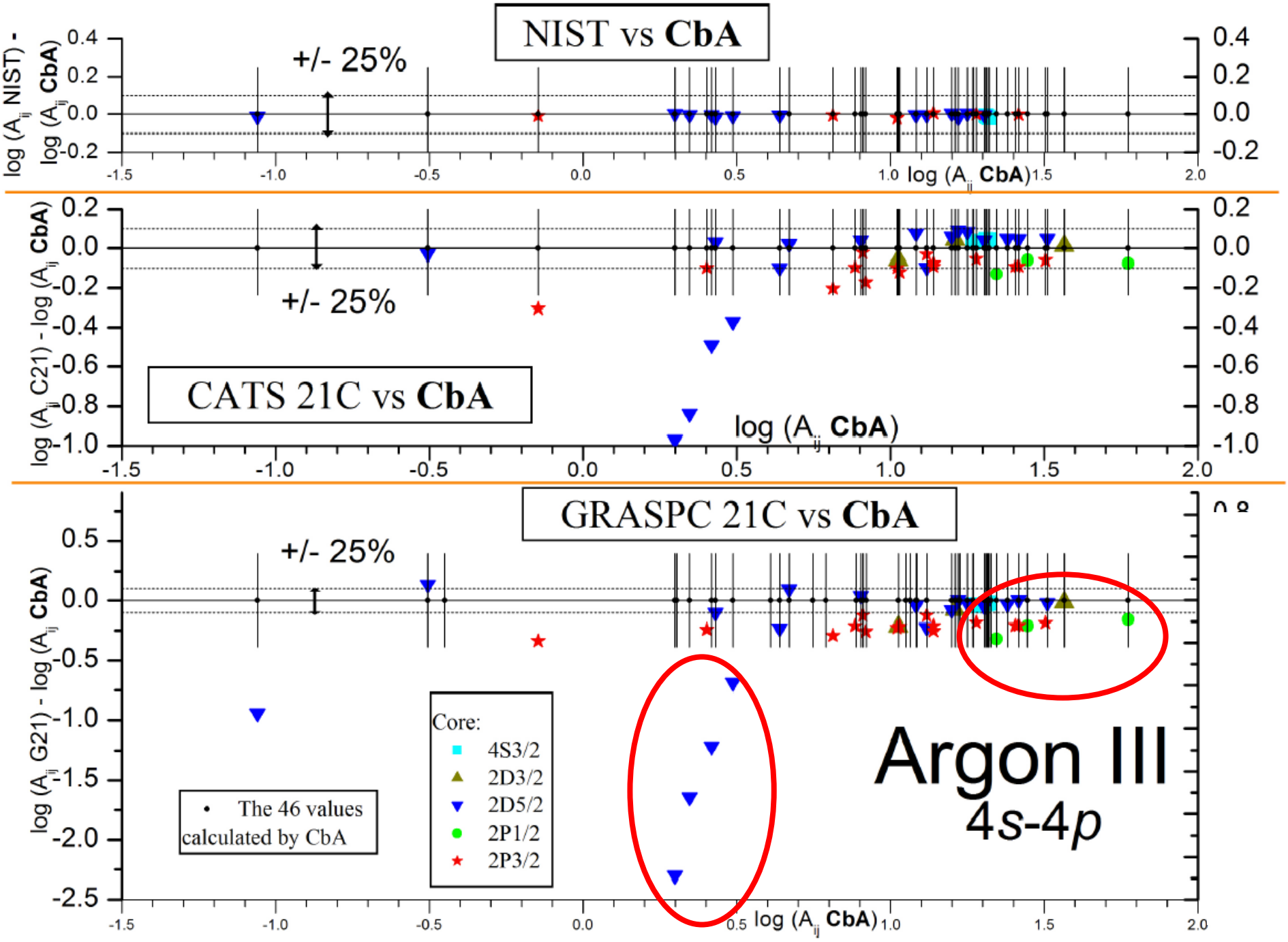
Radiative transitions of Ar III 4s-4p

Evaluation of ~ 70 levels

Data sources:

- CbA: Coulomb Approximation
- NIST
- CATS code
- GRASP code

⟹ comparison of the transition probabilities


NIST vs CbA
+/- 25%
log (A_ij NIST) - log (A_ij CbA)
log (A_ij CbA)
CATS 21C vs CbA
+/- 25%
log (A_ij C21) - log (A_ij CbA)
log (A_ij CbA)
GRASPC 21C vs CbA
+/- 25%
log (A_ij G21) - log (A_ij CbA)
log (A_ij CbA)
Core:
4S3/2
2D3/2
2D5/2
2P1/2
2P3/2
• The 46 values calculated by CbA
Argon III
4s-4p

Ar III 4s-4p transitions

4S3/2

C icm-1	C jcm-1	Ang CATS	AijCATS	NIST icm-1	NIST icm-1	Ang NIST	TERM i	TERM j	AijCbA	NIST	GRPB	GRPC
173950.	203780.	3352.330	22.59	174378.490	204569.950	3312.195	5.S2.0	5.P1.0	20.41	20.00	18.70	19.06
173950.	203850.	3344.482	22.74	174378.490	204655.780	3302.806	5.S2.0	5.P2.0	20.59	20.00	18.89	19.33
173950.	203970.	3331.113	23.03	174378.490	204803.340	3286.787	5.S2.0	5.P3.0	20.89	20.00	19.31	19.91
173950.	208630.	2883.506	.02	174378.490	209126.150	2877.892	5.S2.0	3.P1.0			.04	.05
173950.	208650.	2881.844	.05	174378.490	209150.880	2875.845	5.S2.0	3.P2.0			.08	.10
173950.	208650.	2881.844		174378.490	209165.600	2874.628	5.S2.0	3.P0.0				
180000.	203780.	4205.214	.01	180678.310	204569.950	4185.564	3.S1.0	5.P1.0			.02	.01
180000.	203850.	4192.872	.02	180678.310	204655.780	4170.582	3.S1.0	5.P2.0			.03	.02
180000.	203970.	4171.882		180678.310	204803.340	4145.073	3.S1.0	5.P3.0				
180000.	208630.	3492.840	19.98	180678.310	209126.150	3515.205	3.S1.0	3.P1.0	18.51		17.98	16.98
180000.	208650.	3490.401	19.93	180678.310	209150.880	3512.152	3.S1.0	3.P2.0	18.56		17.88	16.80
180000.	208650.	3490.401	20.03	180678.310	209165.600	3510.338	3.S1.0	3.P0.0	18.59		18.08	17.13

2D3/2

C icm-1	C jcm-1	Ang CATS	AijCATS	NIST icm-1	NIST icm-1	Ang NIST	TERM i	TERM j	AijCbA	NIST	GRPB	GRPC
199670.	224260.	4066.694	9.27	199763.410	223663.150	4184.146	1.D2.0	1.P1.0	10.59		7.33	6.44
199670.	226960.	3664.346	17.91	199763.410	227244.160	3638.911	1.D2.0	1.F3.0	16.24		14.22	13.59
199670.	235380.	2800.336	37.77	199763.410	236064.620	2754.729	1.D2.0	1.D2.0	36.66		33.90	35.33

2D5/2

C icm-1	C jcm-1	Ang CATS	AijCATS	NIST icm-1	NIST icm-1	Ang NIST	TERM i	TERM j	Aij CbA	NIST	GRPB	GRPC
196630.	225050.	3518.649	.85	196590.630	225149.210	3501.575	3.D1.0	3.D2.0	2.62	2.60	.19	.16
196630.	225130.	3508.772	10.46	196590.630	225156.590	3500.670	3.D1.0	3.D1.0	13.12	13.00	8.11	7.87
196630.	225250.	3494.060		196590.630	225404.110	3470.598	3.D1.0	3.D3.0				
196630.	225950.	3410.641	20.52	196590.630	226357.010	3359.495	3.D1.0	3.F2.0	16.64	16.00	16.59	16.79
196630.	226070.	3396.739		196590.630	226504.160	3342.969	3.D1.0	3.F3.0				
196630.	226190.	3382.950		196590.630	226646.670	3327.118	3.D1.0	3.F4.0				
196630.	231100.	2901.073	.29	196590.630	231342.160	2877.571	3.D1.0	3.P2.0			.41	.43
196630.	231260.	2887.670	8.78	196590.630	231627.360	2854.148	3.D1.0	3.P1.0	8.01		8.10	8.79
196630.	231330.	2881.844	36.25	196590.630	231754.830	2843.802	3.D1.0	3.P0.0	32.36		28.07	30.95
196660.	225050.	3522.367	14.39	196615.210	225149.210	3504.591	3.D2.0	3.D2.0	12.11	12.00	11.46	11.10
196660.	225130.	3512.469	3.48	196615.210	225156.590	3503.685	3.D2.0	3.D1.0	4.36	4.30	2.66	2.57
196660.	225250.	3497.726	.21	196615.210	225404.110	3473.561	3.D2.0	3.D3.0	1.99	2.00		.01
196660.	225950.	3414.135	1.31	196615.210	226357.010	3362.271	3.D2.0	3.F2.0	3.07	3.00	.60	.63
196660.	226070.	3400.204	21.59	196615.210	226504.160	3345.718	3.D2.0	3.F3.0	17.83	18.00	16.68	16.97
196660.	226190.	3386.387		196615.210	226646.670	3329.841	3.D2.0	3.F4.0				
196660.	231100.	2903.600	4.94	196615.210	231342.160	2879.608	3.D2.0	3.P2.0	4.68		5.39	5.86

Ar III 4s-4p transitions, contd.

196720.	225250.	3505.082	18.19	196680.840	225404.110	3481.498	3.D3.0	3.D3.0	15.82	16.00	13.69	13.19
196720.	225950.	3421.143		196680.840	226357.010	3369.707	3.D3.0	3.F2.0	.09	.09	.01	.01
196720.	226070.	3407.155	.32	196680.840	226504.160	3353.081	3.D3.0	3.F3.0	2.22	2.20	.04	.05
196720.	226190.	3393.281	22.15	196680.840	226646.670	3337.134	3.D3.0	3.F4.0	20.23	20.00	17.55	18.10
196720.	231100.	2908.668	29.10	196680.840	231342.160	2885.060	3.D3.0	3.P2.0	26.11		24.15	26.36
196720.	231260.	2895.194		196680.840	231627.360	2861.515	3.D3.0	3.P1.0				
196720.	231330.	2889.338		196680.840	231754.830	2851.116	3.D3.0	3.P0.0				

2P1/2

C icm-1	C jcm-1	Ang CATS	AijCATS	NIST icm-1	NIST icm-1	Ang NIST	TERM i	TERM j	AijCbA	NIST	GRPB	GRPC
213980.	241910.	3580.380	16.44	211063.760	241807.180	3252.729	1.P1.0	1.P1.0	22.05		11.09	10.64
213980.	244710.	3254.149	24.30	211063.760	244358.070	3003.516	1.P1.0	1.D2.0	27.90		16.20	17.21
213980.	252960.	2565.418	49.93	211063.760	255107.830	2270.453	1.P1.0	1.S0.0	59.28		42.00	41.41

2P3/2

C icm-1	C jcm-1	Ang CATS	AijCATS	NIST icm-1	NIST icm-1	Ang NIST	TERM i	TERM j	AijCbA	NIST	GRPB	GRPC
211200.	239630.	3517.411	12.17	207233.000	239194.040	3128.809	3.P2.0	3.S1.0	13.09		9.82	9.82
211200.	240370.	3428.180	.36	207233.000	240152.010	3037.758	3.P2.0	3.D1.0	.71	.70	.34	.33
211200.	240450.	3418.803	4.07	207233.000	240258.460	3027.967	3.P2.0	3.D2.0	6.50	6.40	3.38	3.33
211200.	240480.	3415.301	21.15	207233.000	240292.370	3024.861	3.P2.0	3.D3.0	26.06	26.00	16.02	16.26
211200.	243130.	3131.851		207233.000	242924.570	2801.782	3.P2.0	3.P0.0				
211200.	243250.	3120.125	11.20	207233.000	243147.060	2784.425	3.P2.0	3.P1.0	13.83		6.80	7.72
211200.	243410.	3104.626	20.65	207233.000	243425.790	2762.981	3.P2.0	3.P2.0	25.46		14.16	15.83
211110.	239630.	3506.311	6.16	207532.320	239194.040	3158.388	3.P1.0	3.S1.0	7.67		4.75	4.74
211110.	240370.	3417.635	8.36	207532.320	240152.010	3065.633	3.P1.0	3.D1.0	10.47	10.00	6.27	6.24
211110.	240450.	3408.316	16.78	207532.320	240258.460	3055.661	3.P1.0	3.D2.0	19.04	19.00	12.32	12.48
211110.	240480.	3404.835		207532.320	240292.370	3052.498	3.P1.0	3.D3.0				
211110.	243130.	3123.048	27.84	207532.320	242924.570	2825.477	3.P1.0	3.P0.0	31.93		18.43	20.84
211110.	243250.	3111.388	7.73	207532.320	243147.060	2807.826	3.P1.0	3.P1.0	8.13		5.45	6.10
211110.	243410.	3095.975	5.59	207532.320	243425.790	2786.022	3.P1.0	3.P2.0	8.31		4.09	4.61
211070.	239630.	3501.401	2.02	207674.190	239194.040	3172.604	3.P0.0	3.S1.0	2.53		1.45	1.45
211070.	240370.	3412.969	11.63	207674.190	240152.010	3079.024	3.P0.0	3.D1.0	13.81	14.00	8.47	8.52
211070.	240450.	3403.676		207674.190	240258.460	3068.966	3.P0.0	3.D2.0				
211070.	240480.	3400.204		207674.190	240292.370	3065.775	3.P0.0	3.D3.0				
211070.	243130.	3119.152		207674.190	242924.570	2836.849	3.P0.0	3.P0.0				
211070.	243250.	3107.520	8.12	207674.190	243147.060	2819.056	3.P0.0	3.P1.0	10.73		5.78	6.52
211070.	243410.	3092.146		207674.190	243425.790	2797.077	3.P0.0	3.P2.0				

Ar III 4s-4p transitions, contd.

levels		A_{ij}				$\log_{CbA} - \log_{GRASP}$	$\log_{CATS} - \log_{GRASP}$
i	j	CbA	NIST	GRASP	CATS		
$^2P_{1/2}$							
$^1D_2$	$^1P_1$	22.05		11.09	16.44	.30	.17
$^1D_2$	$^1F_3$	27.9		16.2	24.3	.24	.17
$^1D_2$	$^1D_2$	59.28		42.00	49.93	.15	.07
$^2D_{5/2}$							
$^3D_2$	$^3D_3$	1.99	2.00	.01	.21	2.3	1.3
$^3D_3$	$^3F_3$	2.22	2.20	.05	.32	1.7	.49
$^3D_1$	$^3D_2$	2.62	2.60	.16	.85	1.2	.72
$^3D_3$	$^3D_2$	2.7	2.6	2.14	2.89	.10	.13

NIST ASD

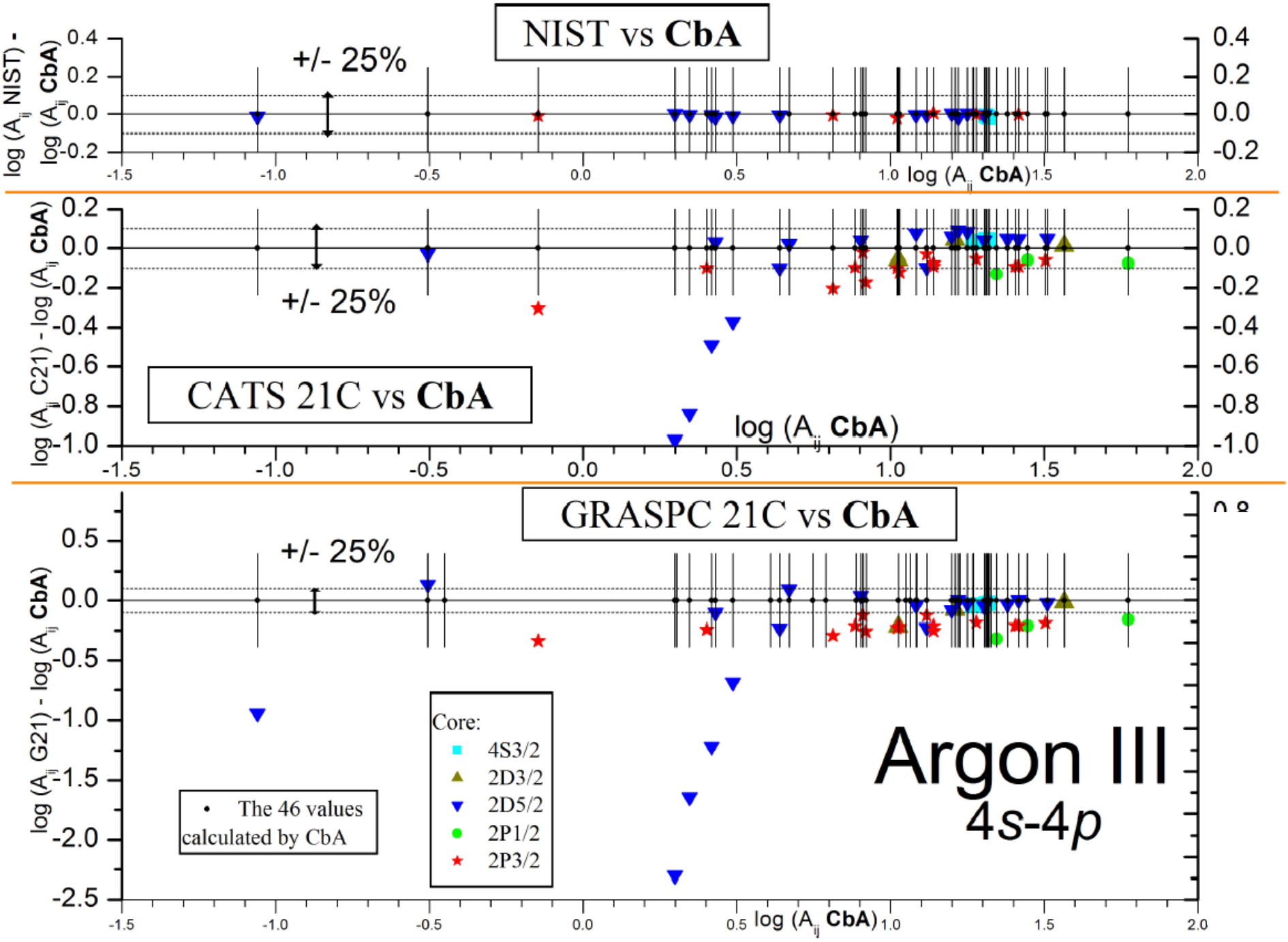
NIST Traceability

Sources

- **367**. J. C. Boyce, Phys. Rev. **48**, 396 (1935)
- **373**. T. L. De Bruin, Zeeman Verhandelingen, (The Hague, 1935) p.415
- **372**. T. L. De Bruin, Proc. Roy. Acad. Amsterdam **36**, 727 (1933)
- **375**. T. L. De Bruin, Proc. Roy. Acad. Amsterdam **40**, 339 (1937)

Methods

- **ca**. Coulomb approximation
- **ls**. The transition probability for this line was calculated from the multiplet value assuming a pure LS-coupling


NIST vs CbA
+/- 25%
log (A_ij NIST) - log (A_ij CbA)
log (A_ij CbA)
CATS 21C vs CbA
+/- 25%
log (A_ij C21) - log (A_ij CbA)
log (A_ij CbA)
GRASPC 21C vs CbA
+/- 25%
log (A_ij G21) - log (A_ij CbA)
log (A_ij CbA)
• The 46 values calculated by CbA
Core:
4S3/2
2D3/2
2D5/2
2P1/2
2P3/2
Argon III
4s-4p

Spectroscopic Data
Atoms and Molecules Properties

- Atomic Spectrocopy: waves lengths, energy levels, transition probabilities → **GENIE**
  - ASD, NIST, Atomic spectra http://physics.nist.gov/PhysRefData/ASD
  - SPECTR-W^3 http://spectr-w3.snz.ru
  - Kurucz's CD-ROM
  - http://cfa-www.harvard.edu/amdata/ampdata/kurucz23/sekur.html
  - Atomic Line List v.2.04 http://www.pa.uky.edu/~peter/atomic
  - TOPbase and TIPbase http://cdsweb.u-strasbg.fr/OP.htx
  - Kelly Atomic Line Database
    - http://cfa-www.harvard.edu/amdata/ampdata/kelly/kelly.html
  - MCHF/MCDHF Collection http://atoms.vuse.vanderbilt.edu
  - CAMDB http://www.camdb.ac.cn/e/

- Molecular spectroscopy
  - NIST Molecular Spectra Db http://physics.nist.gov/PhysRefData/MolSpec/
  - CDMS: http://www.astro.uni-koeln.de/cgi-bin/cdmssearch
  - NIST Chemistry Webbook http://webbook.nist.gov/chemistry/
  - Finding Chemical Spectra and Spectral Data, University of Texas, Austin
  - http://www.lib.utexas.edu/chem/info/spectra.html
  - HITRAN: ftp download free of charge, registration required
    http://www.cfa.harvard.edu/hitran/
  - Ionization potentials, CAMDB http://www.camdb.ac.cn/e/

Collisional Data

- IAEA ALADDIN http://www-amdis.iaea.org/ALADDIN
- Atomic and Molecular Data, NIST
  http://physics.nist.gov/PhysRefData/contents-misc.html
- CAMDB http://www.camdb.ac.cn/e/
  - Electron impact ionization, excitation
  - Dielectronic recombination
  - Photon ionization, auto ionization
  - Ion molecules collisions
- AMDIS NIFS http://dbshino.nifs.ac.jp
  Rate coefficients, cross sections
  - Atomic data: excitation, ionization, recombination
  - Molecular data
- KAERI, total and differential cross sections by electron impact
  http://amods.kaeri.re.kr/impact/IMPACT.html
- OPEN-ADAS http://open.adas.ac.uk/
- Kyoto Univ. http://toshi3.nucleng.kyoto-u.ac.jp:5560/isqlplus
  - Charge exchange cross sections
  - Ion-atom and ion-molecule collisions
- BASECOL http://basecol.obspm.fr/

Particle Surface Interactions

- IAEA ALADDIN
  http://www-amdis.iaea.org/AL1/surface.html
- NIFS AMDIS, TRIM.SP data from W. Eckstein
  http://amdata.nifs.ac.jp/DB/Eckstein

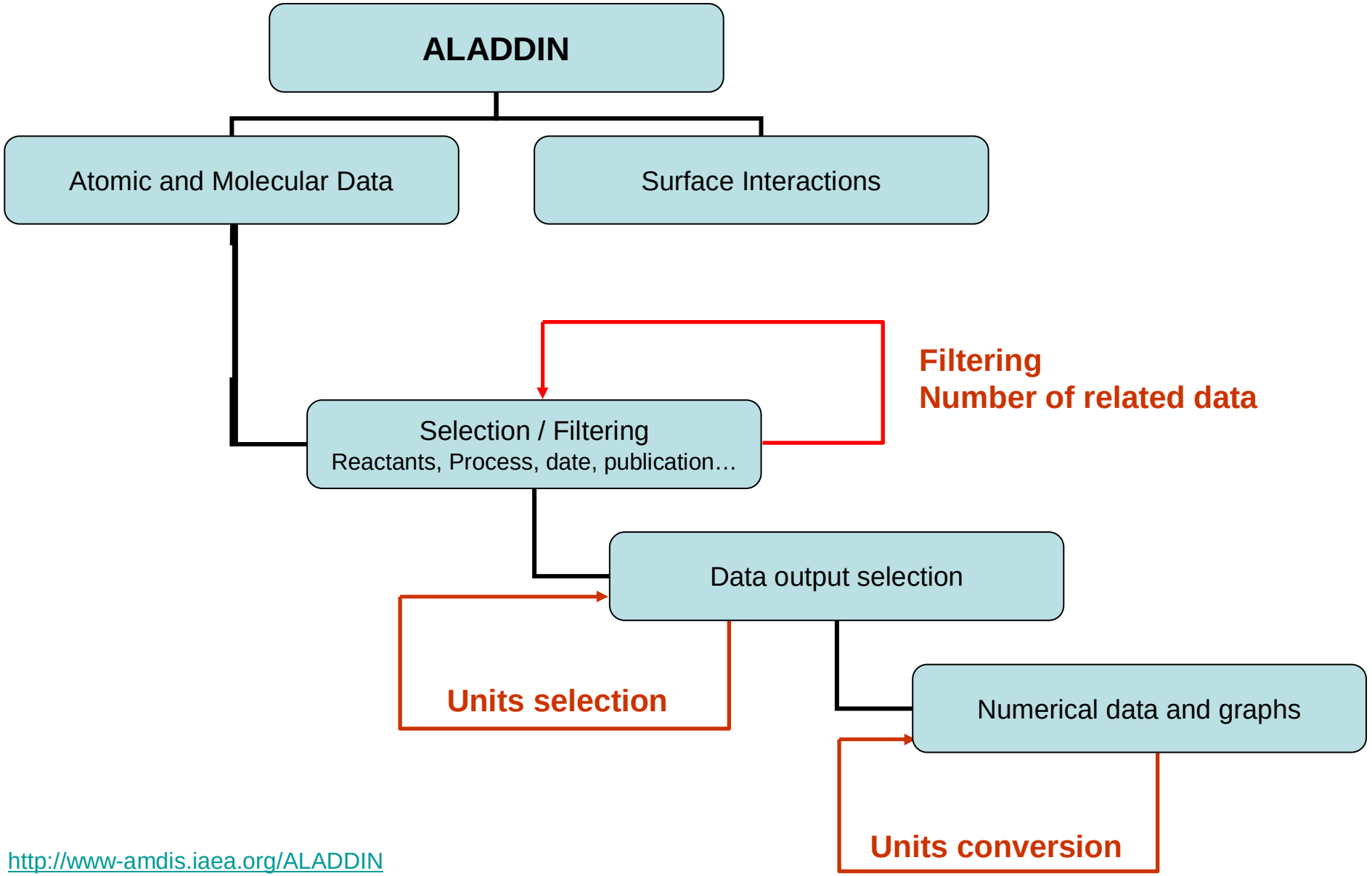
ALADDIN

Domain

- Atomic and molecular collisions (8500 data)
- Particle surface interactions (2600 data)

Search criteria (atomic and molecular data)

- process and category of processes
- 1 or 2 reactants, including possible ionization and quantum state
- 1 product, including possible ionization and quantum state
- data quantity: cross sections, rate coefficients differential cross sections
- data type: experimental, theoretical, derived
- data accuracy
- Bibliography: publication, author, date



http://www-amdis.iaea.org/ALADDIN

OPEN-ADAS

ADAS is an interconnected set of computer codes and data collections for modelling:

- Radiating properties of ions and atoms in plasmas
- Analysis and interpretation of spectral measurements

Database scope: data for fusion and astrophysical application

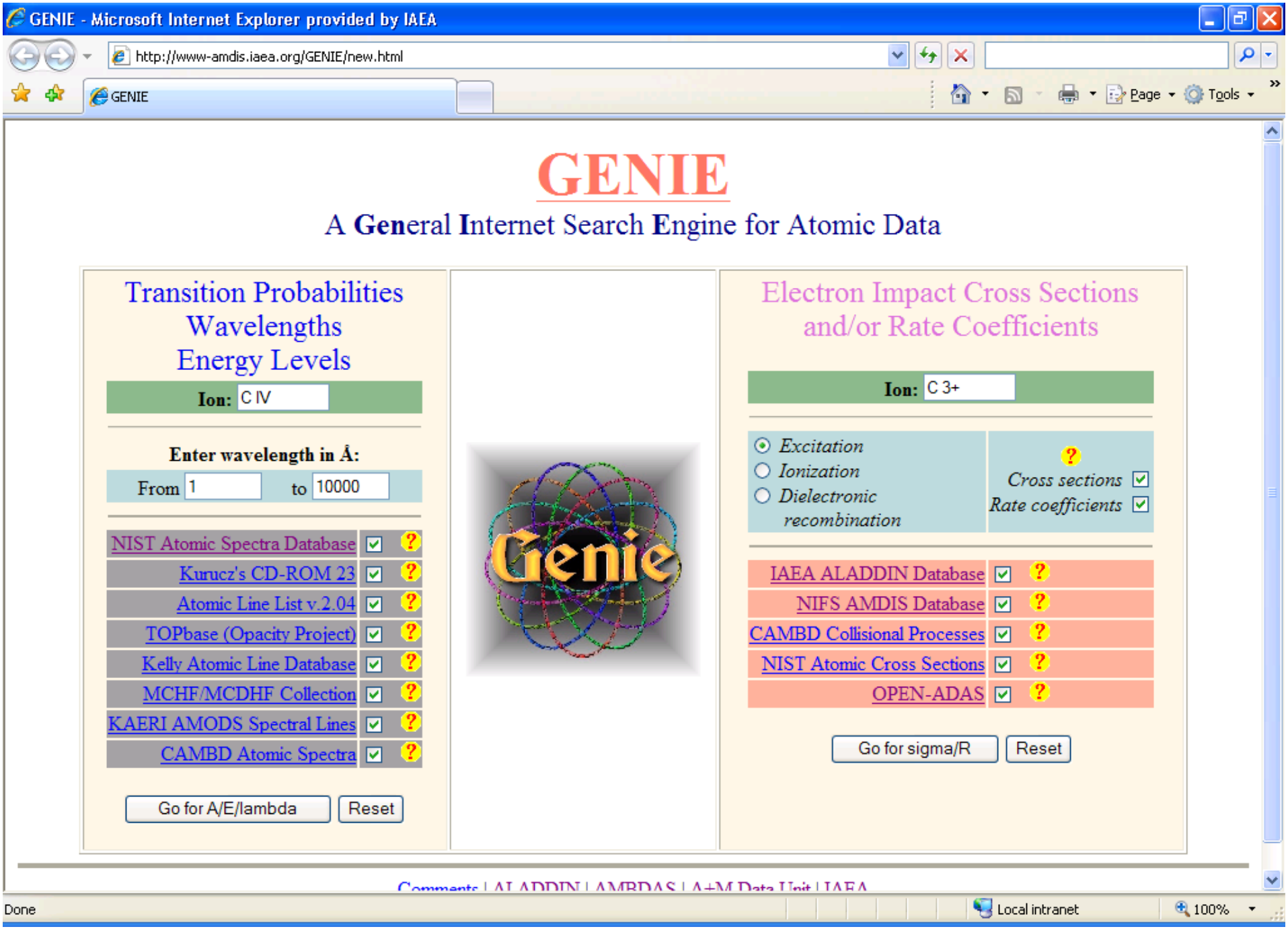
ADAS accessible to members (fee), not WWW access

OPEN-ADAS

Free WWW access to ADAS data

http://open.adas.ac.uk

Search Engine


GENIE - Microsoft Internet Explorer provided by IAEA
http://www-amdis.iaea.org/GENIE/new.html
GENIE
Page
Tools
GENIE
A General Internet Search Engine for Atomic Data
Transition Probabilities
Wavelengths
Energy Levels
Ion: C IV
Enter wavelength in Å:
From 1 to 10000
NIST Atomic Spectra Database
Kurucz's CD-ROM 23
Atomic Line List v.2.04
TOPbase (Opacity Project)
Kelly Atomic Line Database
MCHF/MCDHF Collection
KAERI AMODS Spectral Lines
CAMBD Atomic Spectra
Go for A/E/lambda
Reset
Genie
Electron Impact Cross Sections
and/or Rate Coefficients
Ion: C 3+
Excitation
Ionization
Dielectronic recombination
Cross sections
Rate coefficients
IAEA ALADDIN Database
NIFS AMDIS Database
CAMBD Collisional Processes
NIST Atomic Cross Sections
OPEN-ADAS
Go for sigma/R
Reset
Comments | ALADDIN | AMBDAS | A+M Data Unit | IAEA
Done
Local intranet
100%

GENIE

General Internet Search Engine

- http://www-amdis.iaea.org/GENIE/

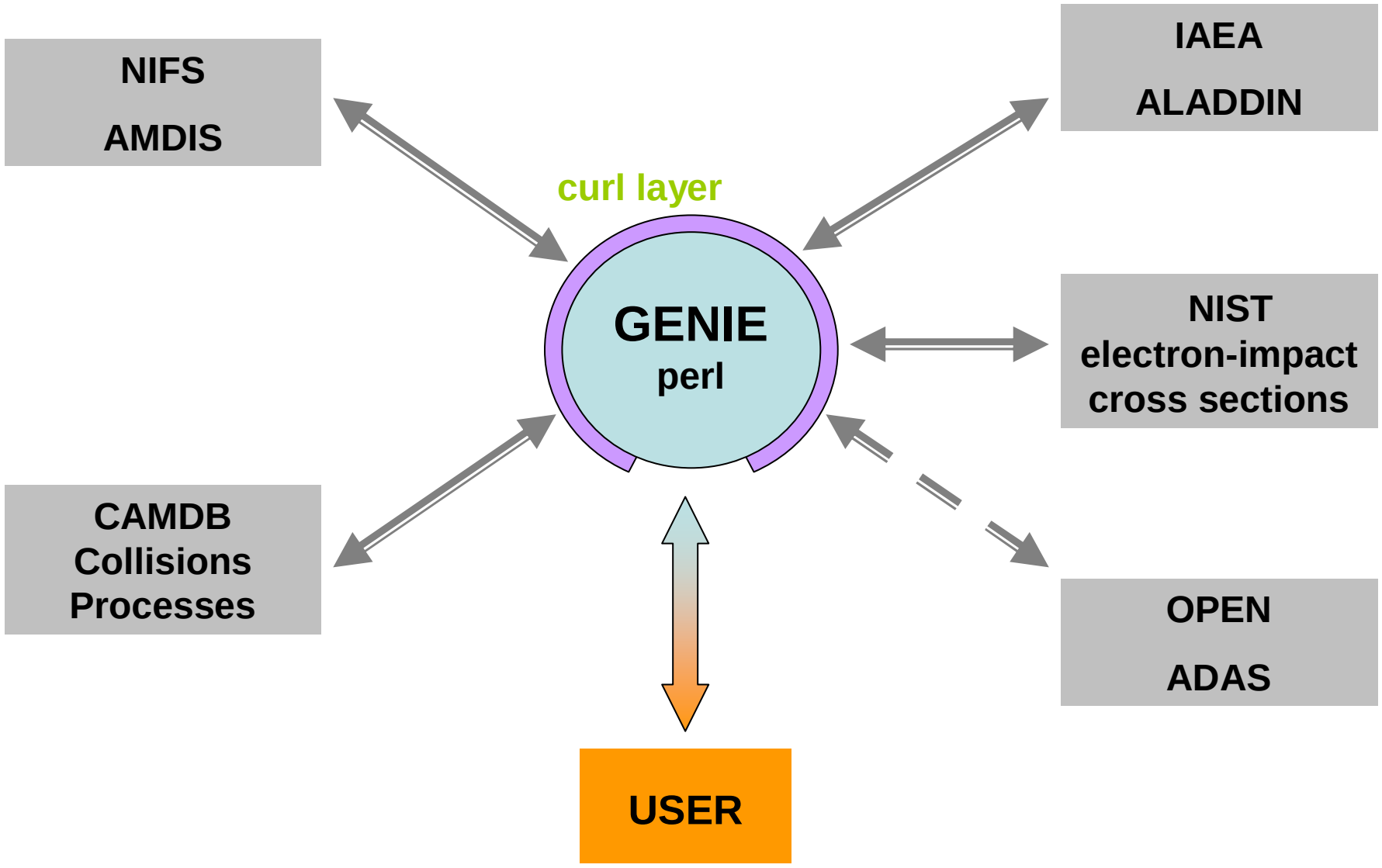
Spectroscopic data

- Oscillator strengths, transition probabilities and energy levels
- 8 databases

Electronic Collisions

- Electronic ionisation, excitation and dielectronic recombination cross-sections and rate coefficients
- 4 databases (+1 with OPEN-ADAS in test)

Excitation, Ionization and DR Cross Sections



Web calculation tools

IAEA

- Cross sections of bare nuclei on hydrogenic ions:
  http://www-amdis.iaea.org/HEAVY/
- Average approximation for electron impact excitation of atomic ions:
  http://www-amdis.iaea.org/AAEXCITE
- Results from collisional radiative calculations of plasmas are available, as carried out with the Los Alamos modeling codes:
  http://www-amdis.iaea.org/RATES/

LANL

- Los Alamos atomic physics codes: an interface is available to run several Los Alamos atomic physics codes to calculate atomic structure and electron impact excitation, as well as ionization processes
  http://aphysics2.lanl.gov/tempweb/lanl/

Conclusion

Available data

	Atoms	Molecules
AM Spectroscopy	xxx	x
AM Collisions	xx	x
Particle surface interactions	x	

Need for better data access and data exchange

- Development of new web calculation tools
- Search engines for AM/PSI data
- Development of new standards?

Exercises

1. Using NIST ASD, http://physics.nist.gov/PhysRefData/ASD, find the major oxygen atomic lines in the range of 150 to 230 nm. Compare with your results obtained using the LANL code.

2. Using GENIE, htpp://www-amdis.iaea.org/GENIE, find the cross sections for the $1s^2 \rightarrow 1s2p\ ^1P$ transition in C^{+4}