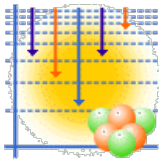
Outstanding issues in ENSDF codes & a possible way of going forward: progress report



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Introduction

- since 2007 the maintenance & upgrade of most ENSDF analysis codes is very limited, exception BrICC, avetools, BrICCMixing that are developed and maintained by T. Kibedi at ANU
  - ✓ **danger**: different centers (people) will use their own codes – non-uniformity (different physics/assumptions, different treatment of uncertainties) – introducing *un*intentional errors - affect the quality of the evaluations
  - ✓ **opportunity:** to revitalize the old fortran codes, improve some of the programs - > new codes could have significant impact on the quality and production time of ENSDF evaluations, especially when new people are involved
- frank discussion at the last NSDD meeting -> it is not about issues with *fortran* at all-> due credit to Vivian for the follow up

Observations from recent ICTP WS…

- new evaluators are confused by most of the programs
  - ✓ no manuals on how to install and run them
  - ✓ no descriptions on what a code actually does – what are the assumptions, how uncertainties are treated, auxiliary files information, etc. – no policy information (or perhaps it is somewhere there …)
- people run computers that operate different OS – the programs need to operate on Windows, Linux and Mac OS – lost 2 days at the recent ICTP WS to get this done …
- some of the codes need auxiliary input data, e.g. *radmas.dat mednew.dat* (used by *radlist)* for example – those files are also not maintained and updates are not provided

Requirements for the new programs

- need to run on different OS –Windows, Linux and Mac
- need to have a manual on how to be installed, what is the physics and computational structure, what assumptions were made and how the uncertainties are treated – similar to *BrICC* & *radlist*
- need to be rigorously tested before officially distributed – creation of test samples (benchmarks)?
- dissemination – several (independent) repositories, e.g. IAEA, NNDC, others …
- coordination – need to avoid duplication of effort
- priorities – start with the most urgent ones and continue with the rest as time permits

Why python?

- object-oriented – just like C, C++,Java, modern Fortran, etc.
- multi-platform – Mac OS X, Linux, Windows …
- a lot of stuff already developed for science and engineering …

uncertainties

Overview User Guide Uncertainties in arrays Technical Guide

SciPy.org Sponsored By ENTHOUGHT

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SciPy (pronounced "Sigh Pie") is a Python-based ecosystem of open-source software for mathematics, science, and engineering. In particular, these are some of the core packages:

NumPy
Base N-dimensional array package

SciPy library
Fundamental library for scientific computing

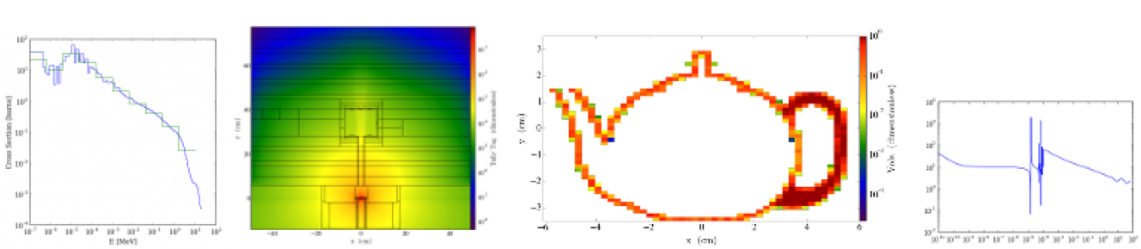
Matplotlib
Comprehensive 2D Plotting

ractive

Sympy
Symbolic mathematics

pandas
Data structures & analysis

PyNE: The Nuclear Engineering Toolkit



What about uncertainties?

http://pythonhosted.org/uncertainties/

uncertainties

Overview User Guide Uncertainties in arrays Technical Guide

```
>>> x = ufloat(0.20, 0.01)  # x = 0.20+/-0.01
```

```
>>> from uncertainties import ufloat_fromstr
>>> x = ufloat_fromstr("0.20+/-0.01")
>>> x = ufloat_fromstr("(2+/-0.1)e-01")  # Factored exponent
>>> x = ufloat_fromstr("0.20(1)")  # Short-hand notation
>>> x = ufloat_fromstr("20(1)e-2")  # Exponent notation
>>> x = ufloat_fromstr(u"0.20±0.01")  # Pretty-print form
>>> x = ufloat_fromstr("0.20")  # Automatic uncertainty of +/-1 on last digit
```

An example with ruler

$$\tau_{sp}(XL) = \frac{\hbar \cdot L[(2L+1)!!]^2}{2(L+1)\cdot R^{2L}} \left(\frac{3+L}{3}\right)^2 \left(\frac{\hbar c}{E_\gamma}\right)^{2L+1} \cdot \begin{cases} 1/e^2 & \text{for X} \equiv \text{E.} \\ R^2/(40\cdot\mu_N^2) & \text{for X} \equiv \text{M.} \end{cases}$$

for 50.4 (10) keV E1 transition in ^{246}Cm

```
246CM  L 1179.66   13 8-                1.12 S    24                          C
246CM2 L %IT=100
246CM  cL T$From Z009ShAA
246CM  G 50.4      10   0.46 7 M1                          51.2   10
```

ruler: $T_{1/2W}(E1)$ = **1.35** (**19**) ns – **14.1%**

fgk: $T_{1/2W}(E1)$ = **1.35** (**8**) ns – **5.9%**

```
EG=50.4 10
        WEISSKOPF SINGLE-PARTICLE HALF-LIFES (SEC), INCLUDES UNCERTAINTY IN EG
        ORDER     ELECTRIC                MAGNETIC
          1       1.35E-12        19      1.72E-10        24
          2       1.9E-5          5       0.0024          6
          3       4.1E2           13      5.2E4           16
          4       1.3E10          5       1.7E12          7
          5       6.E17           3       7.E19           4
```

it is a 2 lines of code:

x = ufloat(50.4,1.0)

Result = Weisskopf ('E1',A,x)

it does it right!

$T_{1/2W}(E1) = f = \text{const}/E\gamma^3 = a/x^3$

by hand: $\Delta f = 3*1.35*1.0/50.4 = 0.08$

Priority 1: ruler

- this program calculates the strength (in Weisskopf units) of a particular gamma-ray transition and compare to RUL
- links the lifetime of a particular level with the matrix element connecting the initial and final state:

$$\Gamma \propto |<\psi_1 | M | \psi_2>|^2$$

$$|M|^2(\sigma\lambda) = \Gamma_\gamma \cdot \frac{\lambda \cdot [(2\lambda+1)!!]^2}{2 \cdot (\lambda+1) \cdot R^{2\lambda}} \cdot \left(\frac{3+\lambda}{3}\right)^2 \cdot \left(\frac{\hbar c}{E_\gamma}\right)^{2\lambda+1} \cdot \begin{cases} 1/e^2 & \text{for } \sigma \\ R^2/(40 \cdot \mu_N^2) & \text{for } \sigma \end{cases}$$

$$\Gamma_\gamma^k = \frac{\hbar \cdot ln\,2}{T_{1/2,\gamma}^k} = \frac{\hbar \cdot ln\,2}{T_{1/2}^{exp}} \cdot \frac{I_\gamma^k}{\sum_{j=1}^{N} I_\gamma^j \cdot (1+\alpha_T^j)} \cdot BR$$

- uses $T_{1/2}$, BR, Eγ, Iγ, Mult., δ and α_T and their uncertainties
- this program is 'sick' & **MUST** be replaced – issues with non-symmetric uncertainties and low-energy Eγ - wrong results already disseminated through *Nuclear Data Sheets* and ensdf

New ruler - what to consider?

- if all quantities have symmetric uncertainties or ~ or no uncertainties – it is a piece of cake – perhaps 2 days work …
- but what about the following scenarios:
  - ✓ **T1/2** +a/-b and/or **BR** +a/-b? – it is not so difficult!
  - ✓ **Mult.** is given as *M1,E2* or *M1+E2* with no MR or *E0+M1+E2* – note that BrICC is giving you automatically an ICC value with assumed MR, which is not folded into calculation of the transition strength by ruler?
  - ✓ **RI** is a limit, e.g. < 10 or >10?
  - ✓ **MR** is missing for a mixed transition, **MR** +a/-b, or MR is a limit, e.g. **MR** > -2 or MR < 0.5
- what about if all of the above happen **simultaneously** …?

New ruler - what to consider? - cont.

- should automatically check for deviations from RUL and give warnings – don't need to run the program twice
  - ✓ B. Singh proposed some time ago several changes to RUL – where they implemented?
- shall we extend it to treat K-forbidden transitions?

Status

- T. Kibedi (ANU): working on a new version of the ruler code – investigating implementation of a MC module to treat non-symmetric uncertainties
- F.G. Kondev (ANL): working on a stand-alone version
- ensdf-formatted benchmark file with numerous examples is under preparation
- new manual is under preparation
- to be completed by the NSDD meeting in Vienna

Alphad - hindrance in α decay

- treating non-symmetric T1/2 and BR - HF should be non-symmetric – very useful for heavy elements – especially when spectroscopy using a few events is invoked

PRL 111, 112502 (2013) PHYSICAL REVIEW LETTERS week ending 13 SEPTEMBER 2013

Spectroscopy of Element 115 Decay Chains

D. Rudolph,[1,*] U. Forsberg,[1] P. Golubev,[1] L. G. Sarmiento,[1] A. Yakushev,[2] L.-L. Andersson,[3] A. Di Nitto,[4]

- **alphad** does not treat the non-symmetric uncertainties – it is very easy to implement!!! **fmtchk** needs to be modified in order to allow non-symmetric HF

Question: **who** (nndc/iaea), **when** (tomorrow, this year, in ten years or never?); do we (usndp & nsdd) have capabilities to promptly address issues with the computer codes?

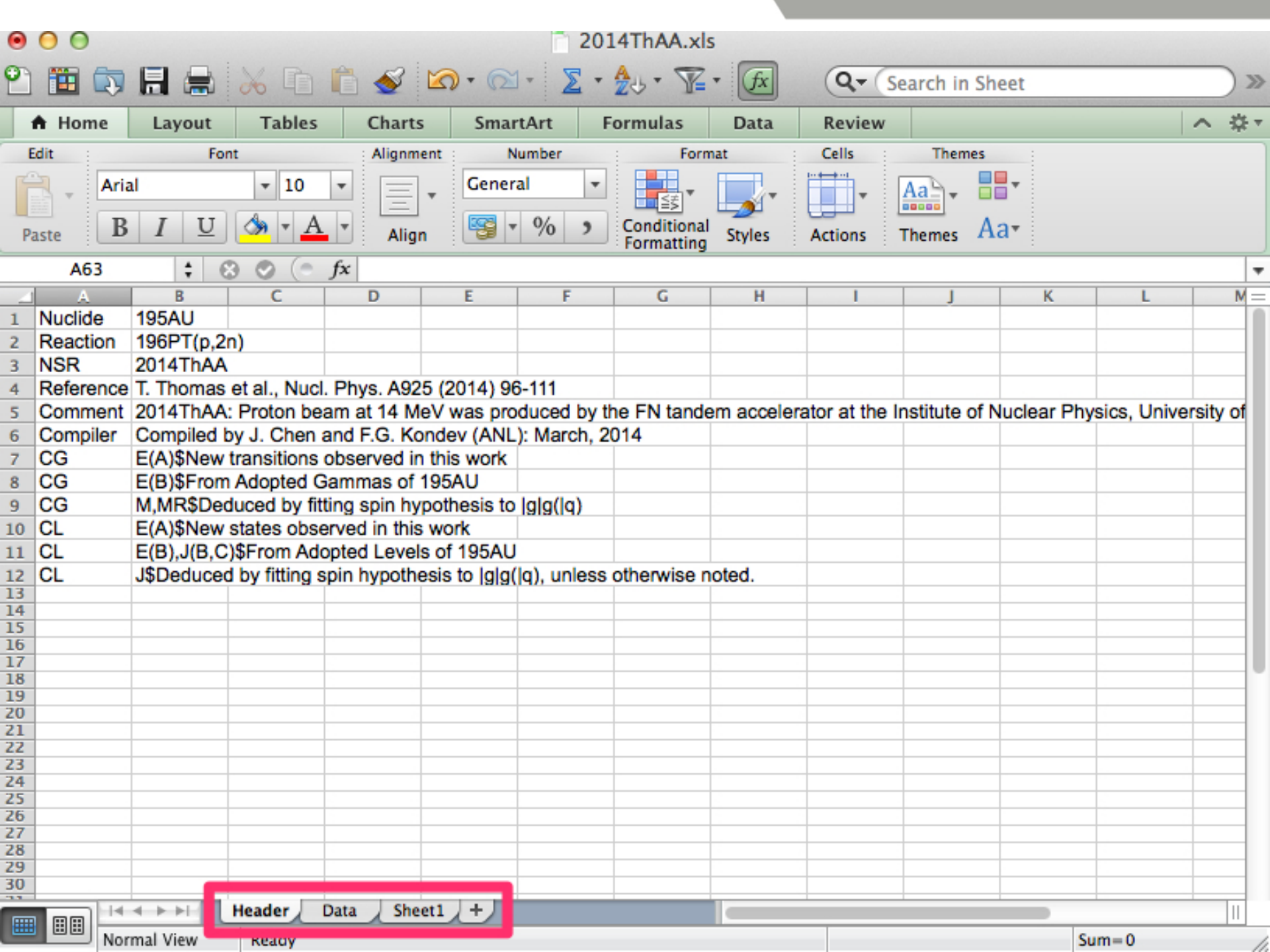
Data compilation tool - xls2ens

- physicist can prepare an ensdf-formatted file from the original publication via MS Excel spreadsheet
  - ✓ allows to use MS Excel flexibility to compute, manipulate, plot data before exporting into an ensdf-formatted file
- similar to what was developed some time ago at McMaster
- written in python by J. Chen and F.G. Kondev - it can run on Mac OSX, Linux, and Windows
- short notes on how to run it are available

external package needed: **xlrd**

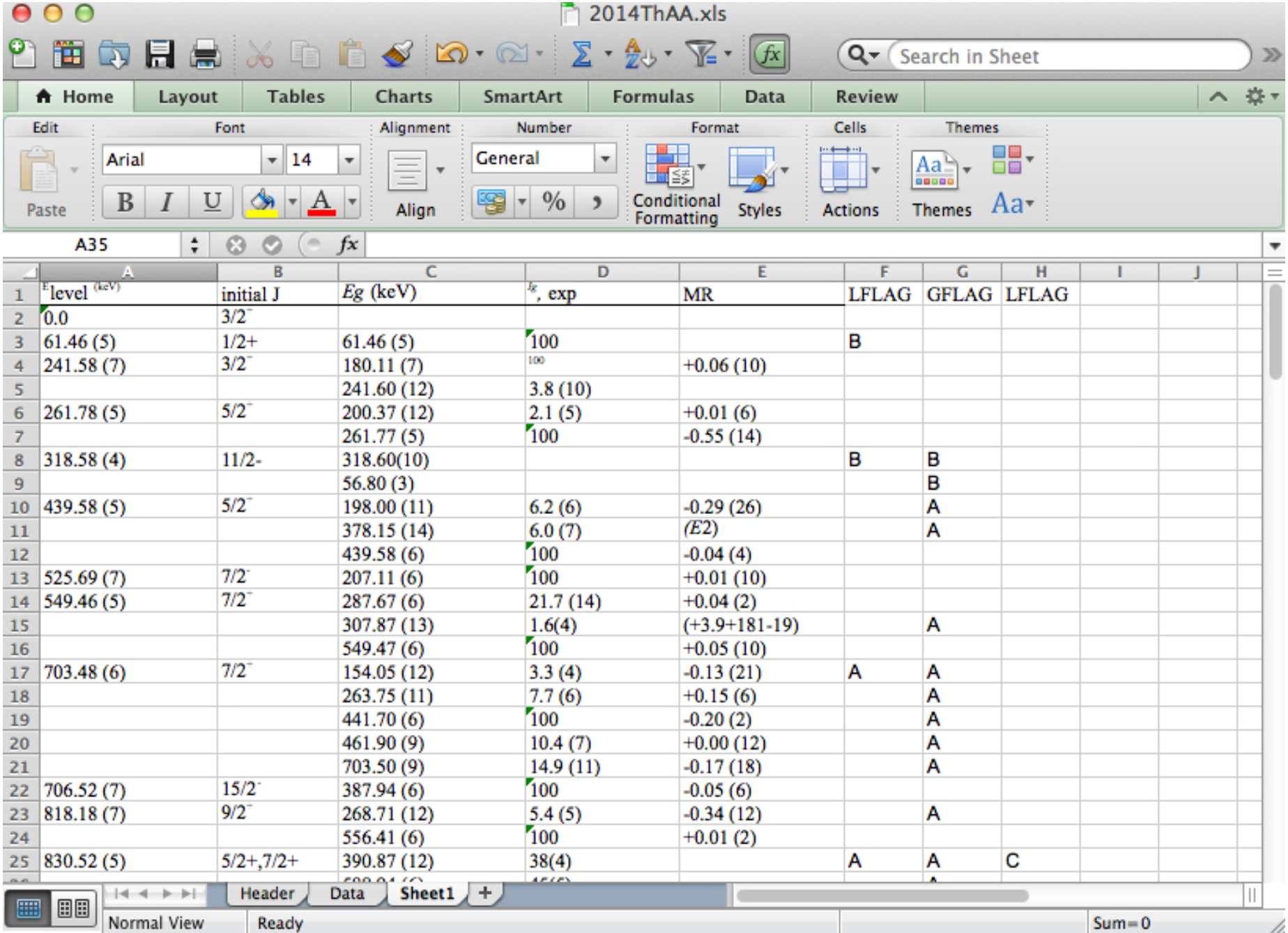
http://www.python-excel.org

from xlrd import * → the only line needed in your code



	A	B
1	Nuclide	195AU
2	Reaction	196PT(p,2n)
3	NSR	2014ThAA
4	Reference	T. Thomas et al., Nucl. Phys. A925 (2014) 96-111
5	Comment	2014ThAA: Proton beam at 14 MeV was produced by the FN tandem accelerator at the Institute of Nuclear Physics, University of
6	Compiler	Compiled by J. Chen and F.G. Kondev (ANL): March, 2014
7	CG	E(A)$New transitions observed in this work
8	CG	E(B)$From Adopted Gammas of 195AU
9	CG	M,MR$Deduced by fitting spin hypothesis to |g|g(|q)
10	CL	E(A)$New states observed in this work
11	CL	E(B),J(B,C)$From Adopted Levels of 195AU
12	CL	J$Deduced by fitting spin hypothesis to |g|g(|q), unless otherwise noted.

work directly on the pdf file: pdfminer or xpdf or scanning into an xls file



2014ThAA.xls

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A35

	A	B	C	D	E	F	G	H	I	J
1	E_{level} (keV)	initial J	*Eg* (keV)	I_g, exp	MR	LFLAG	GFLAG	LFLAG		
2	0.0	3/2⁻								
3	61.46 (5)	1/2+	61.46 (5)	100		B				
4	241.58 (7)	3/2⁻	180.11 (7)	100	+0.06 (10)					
5			241.60 (12)	3.8 (10)						
6	261.78 (5)	5/2⁻	200.37 (12)	2.1 (5)	+0.01 (6)					
7			261.77 (5)	100	-0.55 (14)					
8	318.58 (4)	11/2-	318.60(10)			B	B			
9			56.80 (3)				B			
10	439.58 (5)	5/2⁻	198.00 (11)	6.2 (6)	-0.29 (26)		A			
11			378.15 (14)	6.0 (7)	*(E2)*		A			
12			439.58 (6)	100	-0.04 (4)					
13	525.69 (7)	7/2⁻	207.11 (6)	100	+0.01 (10)					
14	549.46 (5)	7/2⁻	287.67 (6)	21.7 (14)	+0.04 (2)					
15			307.87 (13)	1.6(4)	(+3.9+181-19)		A			
16			549.47 (6)	100	+0.05 (10)					
17	703.48 (6)	7/2⁻	154.05 (12)	3.3 (4)	-0.13 (21)	A	A			
18			263.75 (11)	7.7 (6)	+0.15 (6)		A			
19			441.70 (6)	100	-0.20 (2)		A			
20			461.90 (9)	10.4 (7)	+0.00 (12)		A			
21			703.50 (9)	14.9 (11)	-0.17 (18)		A			
22	706.52 (7)	15/2⁻	387.94 (6)	100	-0.05 (6)					
23	818.18 (7)	9/2⁻	268.71 (12)	5.4 (5)	-0.34 (12)		A			
24			556.41 (6)	100	+0.01 (2)					
25	830.52 (5)	5/2+,7/2+	390.87 (12)	38(4)		A	A	C		

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A40 | 988.34 (12)

	A	B	C	D	E	F	G	H	I	J	K	L
1	EL	JPI	EG	RI	MUL	MR	LFLAG	GFLAG				
2	0.0	3/2-										
3	61.46 (5)	1/2+	61.46 (5)	100			B					
4	241.58 (7)	3/2-	180.11 (7)	100	M1+E2	+0.06 (10)						
5			241.60 (12)	3.8 (10)								
6	261.78 (5)	5/2-	200.37 (12)	2.1 (5)	M1(+E2)	+0.01 (6)						
7			261.77 (5)	100	M1+E2	-0.55 (14)						
8	318.58 (4)	11/2-	318.60(10)				B	B				
9			56.80 (3)					B				
10	439.58 (5)	5/2-	198.00 (11)	6.2 (6)	M1+E2	-0.29 (26)		A				
11			378.15 (14)	6.0 (7)	(E2)			A				
12			439.58 (6)	100	M1(+E2)	-0.04 (4)						
13	525.69 (7)	7/2-	207.11 (6)	100	M1(+E2)	+0.01 (10)						
14	549.46 (5)	7/2-	287.67 (6)	21.7 (14)	M1+E2	+0.04 (2)						
15			307.87 (13)	1.6(4)	(M1+E2)			A				
16			549.47 (6)	100	M1(+E2)	+0.05 (10)						
17	703.48 (6)	7/2-	154.05 (12)	3.3 (4)	M1(+E2)	-0.13 (21)	A	A				
18			263.75 (11)	7.7 (6)	M1+E2	+0.15 (6)		A				
19			441.70 (6)	100	M1+E2	-0.20 (2)		A				
20			461.90 (9)	10.4 (7)	M1(+E2)	+0.00 (12)		A				
21			703.50 (9)	14.9 (11)	M1(+E2)	-0.17 (18)		A				
22	706.52 (7)	15/2-	387.94 (6)	100	M1(+E2)	-0.05 (6)						
23	818.18 (7)	9/2-	268.71 (12)	5.4 (5)	M1+E2	-0.34 (12)		A				
24			556.41 (6)	100	M1(+E2)	+0.01 (2)						
25	830.52 (5)	5/2,7/2+	390.87 (12)	38(4)			A	A				

```
195AU    196PT(P,2NG)                    2014ThAA
195AU C  Compiled (unevaluated) dataset from 2014ThAA:
195AU2c  T. Thomas et al., Nucl. Phys. A925 (2014) 96-111
195AU c  Compiled by J. Chen and F.G. Kondev (ANL): April 15, 2014
195AU C  2014ThAA: Proton beam at 14 MeV was produced by the ^FN tandem
195AU2C  accelerator of the Institute of Nuclear Physics, University of Cologne
195AU3C  and impinged on a 1.1 mg/cm{+2} thick 196Pt target, enriched up to
195AU4C  96.1%. |g rays were detected with the ^HORUS Spectrometer consisting of
195AU5C  10 HPGe detectors. Measured E|g, I|g, |g(|q), |g|g(|q). Deduced levels,
195AU6C  J|p, branching and mixing ratios. Comparisons with ^IBFM calculations.
195AU CG E(A)$|g-ray transition observed for the first time in 2014ThAA
195AU CG E(B),M(D)$From Adopted Gammas of 195AU in ^ENSDF
195AU CG RI$Relative photon branching from each level
195AU CG M,MR$From |g|g(|q) in 2014ThAA, unless otherwise stated
195AU CL E$From a least-squares fit to E|g
195AU CL E(A)$Levels observed for the first time in 2014ThAA
195AU CL J(C)$From Adopted Levels of 195AU in ^ENSDF
195AU CL J$From the deduced |g-ray transition multipolarities and the observed
195AU2CL decay pattern, unless otherwise stated
195AU PN                                                              6
195AU  L 0.0         3/2+                                            C
195AU  L 61.45      41/2+                                            C
195AU  G 61.46     5 100
195AU  L 241.56     43/2+
195AU  G 180.11    7 100.0     M1+E2     +0.06   10
195AU CG MR$second solution in the |g|g(|q) analysis (2014ThAA) gives
195AU2cG |d=-1.86 71, but it is inconsistent with that deduced from the ICC
195AU3cG data, as presented in ENSDF
195AU  G 241.60    123.8     10
195AU  L 261.75     35/2+
195AU  G 200.37    122.1     5 E2(+M3)   +0.01   4
195AU  G 261.77    5 100       M1+E2     -0.55   14
195AU  L 318.54     411/2-                                          C
```

Some programs wont need an update at all …

Additional Slides

Current status – is this correct?

Analysis Codes

Code	Function		Version No./Date	FORTRAN					Documentation
				ANS[a]	DVF[b]	VMS[c]	UNX[d] Linux	UNX[d] UNIX	
ALPHAD	Calculates α R_0's, HF's and theoretical $T_{½}(α)$'s		2.0a 20061106	X	X		X		No (See "Read Me" file)
Brlcc	Calculates internal conversion coefficients, internal electron-positron pair formation coefficients, and E0 electronic form factors.		2.0b 20070112		X[e]		X[ef]	X[eg]	Yes
DELTA	Analyzes angular correlation data.		1.01 19930415	X	X	X	X[h]		LUNFD/(NFFR-3048) 1-27
GABS	Calculates absolute $ΔI_γ$'s.		9.2 20010207	X	X	X	X[h]		Yes
GTOL	Determines level energies from a least-squares fit to $E_γ$'s & feedings.		7.2e 20060701	X	X		X		BNL-NCS-23375/R LUNFD/(NFFR-3049) 1-27
HSICC	Interpolates internal conversion coefficients		11.13f 20011009	X	X	X	X[h]		Nucl. Data **A4**, 1 Nucl. Data Tables **A6**, 235 Nucl. Data Tables **A9**, 119 BNL-NCS-23375/R (1977)
LOGFT	Calculates log *ft*.		7.2a 20010220	X	X	X	X[h]		Nucl. Data Tables **A10**, 206 BNL-NCS-23375/R (1977)
NSDFLIB	Support subprograms for many codes	FORTRAN7	1.5d 19990628						No
		FORTRAN9	1.7a 20120612		X		X		Yes
PANDORA	Physics check of ENSDF data sets. Aids with adopted gammas & XREF.		7.1 20120517		X		X		Yes
RadList	Calculates atomic & nuclear radiations. Checks energy balance.		5.5 19881005	X	X	X			BNL-NCS-52142
RULER	Calculates reduced transition probabilities.		3.2a 20070806	X	X		X		Yes

a ANSI-standard FORTRAN 95, except as noted
b Compaq/Digital Visual Fortran (Win9x/ME/NT/2000/XP)
c OpenVMS Fortran, except as noted
d Lahey/Fujitsu FORTRAN 95, except as noted
e Only executables are available
f INTEL FORTRAN 90
g Digital FORTRAN 90
h Linux GNU f77 Fortran

???