ENSDF analysis and utility codes I

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Heavy Ion Accelerator Facility, ANU Canberra

NEC 14UD tandem electrostatic accelerator commissioned 1975

HV: up to 15.85 MV

Max beam on target: ~1 μA

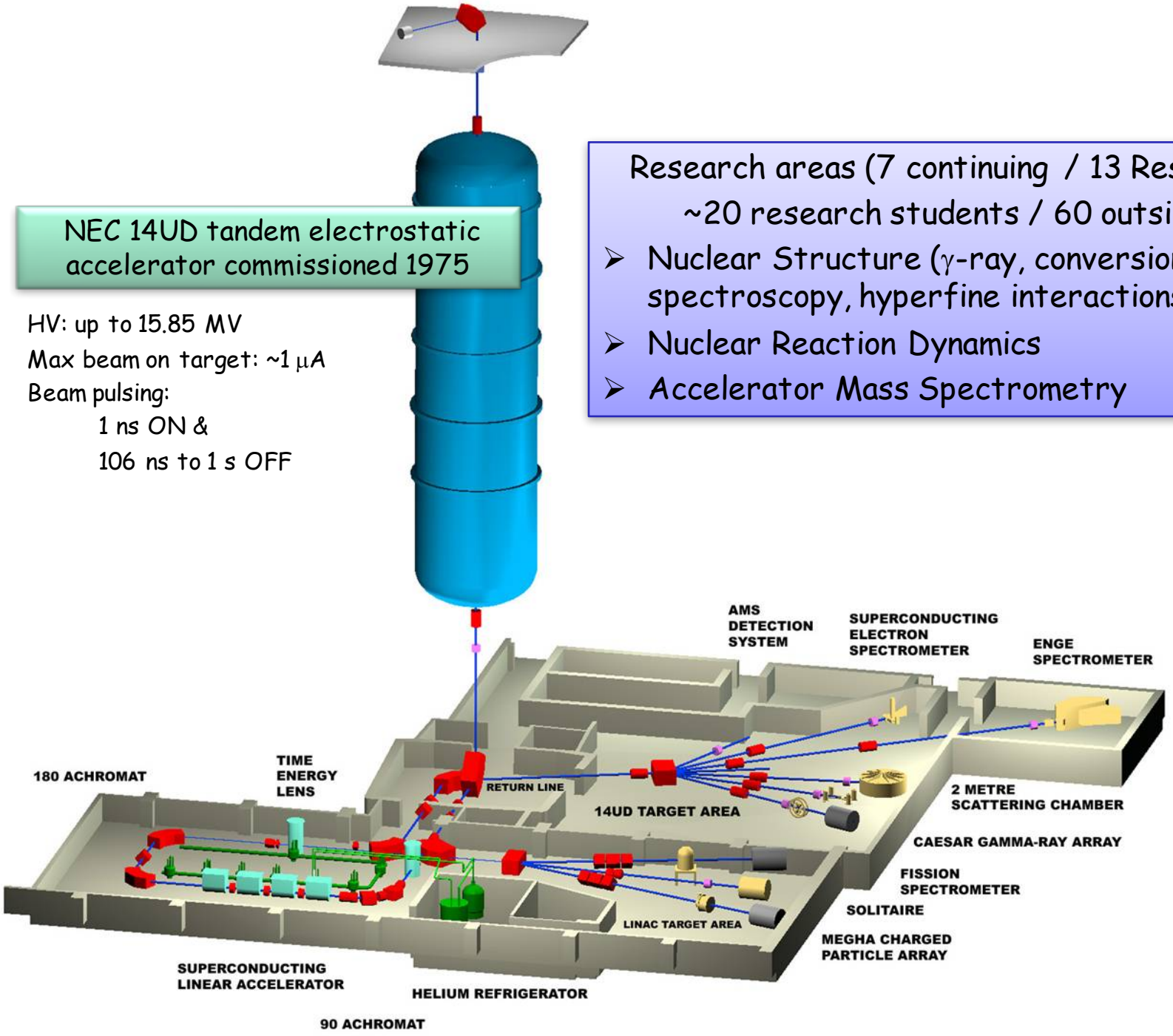
Beam pulsing:

1 ns ON &

106 ns to 1 s OFF

Research areas (7 continuing / 13 Researchers / ~20 research students / 60 outside users)

- Nuclear Structure (γ-ray, conversion electron spectroscopy, hyperfine interactions)
- Nuclear Reaction Dynamics
- Accelerator Mass Spectrometry



ENSDF files & editors

- ENSDF: 80 character/line (record or card) ASCII (American Standard Code for Information Interchange) file (Jag Tuli`s talk on ENSD format)
- 17 record types: Identification, Normalization, Parent, Q-value, Level, Alpha, Beta, EC+beta+, Gamma, Reference, Cross reference, Delayed Particle, Product normalisation, Special record, History, Atomic Relaxation, End records
- Fixed length fields: VALUE UNIT UNC
- Value is given as ASCII string to preserve accuracy reported in the original paper
- Uncertainty: symmetric, asymmetric, limits, data came from systematics (More on Friday)
- No ENSDF editor available yet for all platforms

  See talks next Tuesday by

  -- Elisabeth McCutchan on EVP (Windows)

  -- Viktor Zerkin on web based ENSDF editor

Redit (Windows)
Sergey Lisin (PNPI)

```
174TM     174ER B- DECAY                    1991BE04,1989CH05          99NDS     199908
174TM   H TYP=UPD$AUT=Tibor Kibedi$CUT=1-Sep-2015$
174TM   H TYP=FUL$AUT=E. BROWNE, HUO JUNDE$CIT=NDS 87, 15 (1999)$CUT=1-Nov-1998
174TM   c Activity produced by bombarding natural tungsten target with {+176}Yb
174TM  2c (E=1.5 GeV) projectiles (1989Ch05) and {+186}W target with {+136}Xe
174TM  3c (E=1.577 GeV) projectiles (1991Be04). Mass separated {+174}Er.
174TM  4c Measured |b(+-), |g-ray energies and intensities, coincidences, Tm
174TM  5c K-x rays (1991Be04,1989Ch05).
174TM   c {+174}Er decay scheme is based on 1991Be04. Direct |b{+-} population
174TM  2c to levels at 767 and 773 from {+174}Er (J|p=0+) is inconsistent with
174TM  3c |g-ray decay from these levels to (+174)Tm (J|p=4-) g.s., which
174TM  4c suggests the existence of a a very low-energy level with J|<2
174TM  5c (1991Be04). But 2006Ch10 exclude this conclusion.
174TM   c Measured E|b|~1.3 MeV (1989Ch05).
174TM  cG E,RI$From 1991Be04.
174TM  cG M$From adopted gammas
174TM  cL T$From adopted levels. Other: 3.3 M 2 (1989Ch05), 3.1 M 3 (1991Be04)
174TM  CL J$ From adopted levels
174TM  DG CC$FROM BrIcc v2.3b (16-Dec-2014) 2008Ki07, "Frozen Orbitals" appr.
174TM  CG MR$IF NO VALUE GIVEN IT WAS ASSUMED MR=1.00 FOR E2/M1,
174TM 2CG MR=1.00 FOR E3/M2 AND MR=0.10 FOR THE OTHER MULTIPOLARITIES
174ER   P 0.0                0+              3.2 M      2                1.92E3     30
174TM   N 0.114           7                1.0
174TM  cN NR$Assuming no |b{+-} population to levels at 58.5 keV and below, and
174TM 2cN using I|g(71.7|g + 100.4|g + 130.4|g + 708.6|g + 714.4 + 766.5|g
174TM 3CN + 773.4|g)=100%.
174TM  PN                                                                        3
174TM   L 0.0                4-              5.4 M      1
174TM   L 58.53           17 (2-)
174TM   G 58.5             2  45       LT  (E2)                    25.6       6
174TMS  G LC=19.6 5$MC=4.81 11
174TMS  G NC=1.091 24$OC=0.124 3$PC=0.0001396 22
174TM  cG $Observed only in a coincidence experiment (1989Ch05). Not observed
174TM 2cG by 1991Be04 (I|g|<45, estimated from K| x ray intensities).
174TM   L 100.40           20 3-
174TM   G 100.4            2  100           M1                       3.07
174TMS  G KC=2.57 4$LC=0.389 6$MC=0.0867 14
174TMS  G NC=0.0203 3$OC=0.00291 5$PC=0.0001577 24
174TM  cG $EKC=1.7 {I3} (1991Be04) suggests M1+E2 with MR=1.1 {I+7-4}, which
174TM 2cG disagrees with 2005Ch67 and 2006Ch10
174TM  CG $Other: E|g=100.4 {I2}, I|g=100 {I1} (1989Ch05)
```

ENSDF codes - typical workflow

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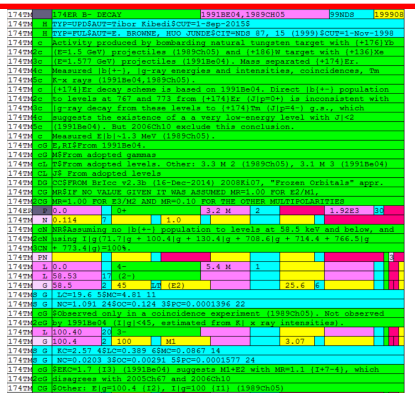
Input: ENSDF file

ENSDF code

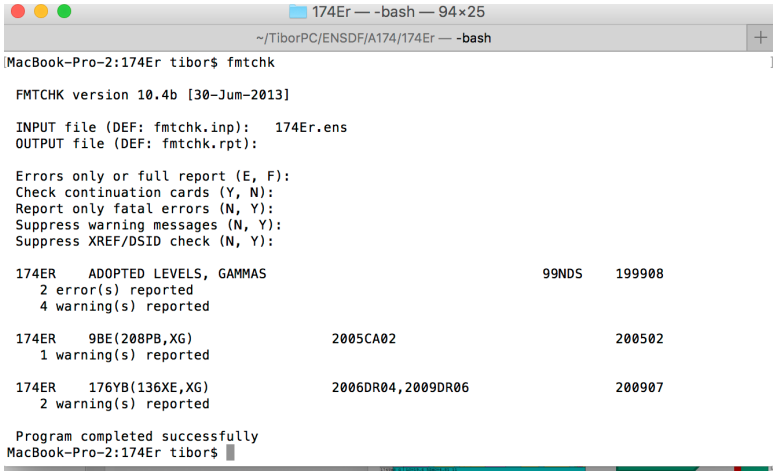
- Calculation of level energies, level feeding, conversion coefficients, normalization factors,…
- Format and physics checking

New ENSDF file

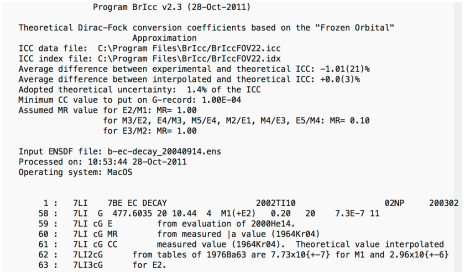


Most codes running from terminal/command

- Interactive : fmtchk<cr>
- Command line: fmtchk [ENSDF-file]<cr>



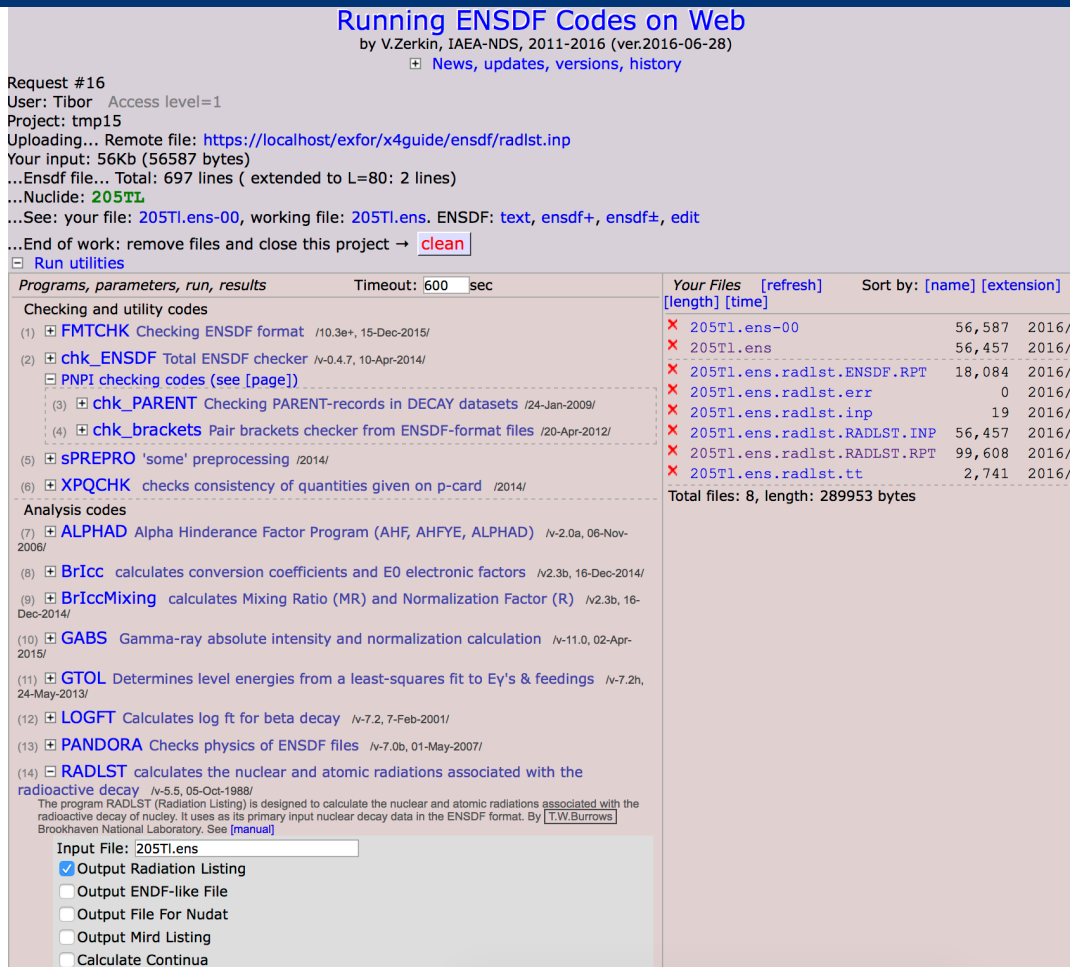
Calculation report file



NOTE: Some codes use special input files

Running ENSDF codes on the web

- ENSDF file uploaded to IAEA server
- No local program installation is required
- See Viktor Zerkin`s talk on next Tuesday



Platforms, programming languages & compilers

- Supported platforms: Windows, Linux and MacOS
- Programming languages: FORTRAN 77, FORTRAN 95, Java, Python
- FORTRAN compilers
  - GFORTRAN: freely available at https://gcc.gnu.org/wiki/GFortran
    - Windows users download the "MinGW native windows" binary packages using the MinGW installation manager; add "C:\MinGW\bin" to the path
    - Linux and MacOS users follow the instructions on the https://gcc.gnu.org/wiki/GFortranBinaries
  - Intel FORTRAN: not free; USD ~400 (academic) at https://software.intel.com/en-us/fortran-compilers
    - Free student licenses at:

      https://software.intel.com/en-us/qualify-for-free-software/student
    - Windows: integrated with MS Visual Studio
    - Linux & MacOS: use makefiles
  - 👉 Optional exercise: compile FMTCHK using GFORTRAN

Obtaining ENSDF codes

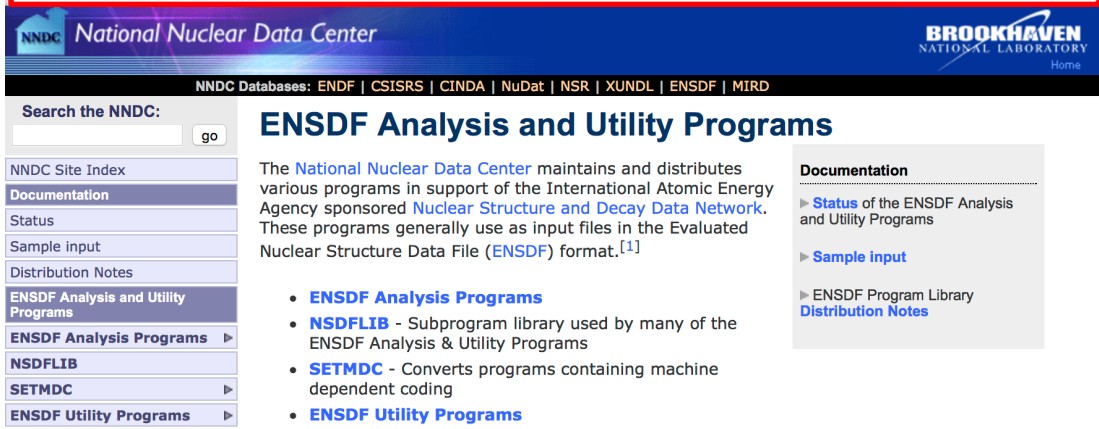
- Source codes

Looking the source code could be helpful to resolve problems!

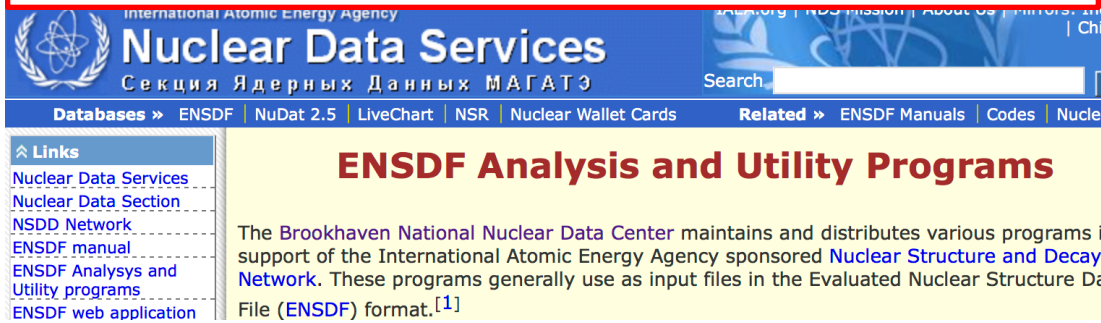
Error messages not always sufficiently clear

- Executables for Windows/Linux/MacOS
- ReadMe files / pdf manuals
- Sample input & output files

http://www.nndc.bnl.gov/nndcscr/ensdf_pgm/



https://www-nds.iaea.org/public/ensdf_pgm/

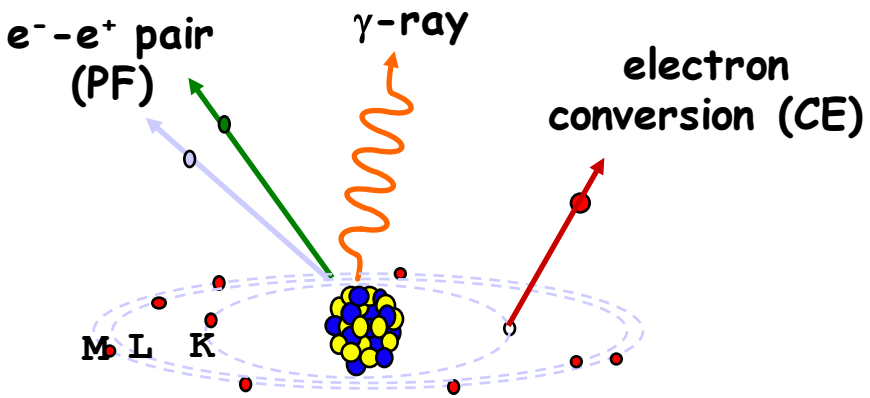


ENSDF Analysis codes - ALPHAD

For alpha decay calculates the theoretical $T_{1/2}(\alpha)$'s and R_o's to deduce the hindrance factor.

- Hindrance factor: $T_{1/2}(exp)/T_{1/2}(calc)$; typically between 1 and 3E4
- Theoretical α-decay half life derived from a simple model. Alpha particle contained inside the nucleus by a potential barrier at $r=R_o$
- R_o can be specified in the ENSDF input file; use the **radD** code to calculate R_o for odd-odd and odd-mass nuclei
- Language: FORTRAN77, updated to FORTRAN90
- Documentation: readme-alphad.pdf
- Input ENSDF file: alphad.inp
- Calculation report: alphad.rpt
- Output ENSDF file: alphad.new
- alphad_new: combines alphad and radD; need to be tested

Electromagnetic Decay Processes



EM decay: energy and momentum carried away

Energetics

Gamma $E_\gamma = E_i - E_f + T_r$

CE $E_{CE,i} = E_i - E_f - E_{BE,i} + T_r$

PF $E^+ + E^- = E_i - E_f - 2m_oc^2 + T_r$

Selection *rules* (πL)

$|L-j_i| \leq j_f \leq L+j_i$

$\pi = (-1)^L$ for EL

$\pi = (-1)^{L+1}$ for ML

Transition probability

$\lambda_T = \lambda_\gamma + \lambda_K + \lambda_L + \lambda_M \ldots\ldots + \lambda_{PF}$

Conversion coefficient

$\alpha_{CE,PF} = \lambda_{CE,PF} / \lambda_\gamma$

$\lambda_{CE,PF} = \lambda_\gamma \times \alpha_{CE,PF}$

E0 transitions:

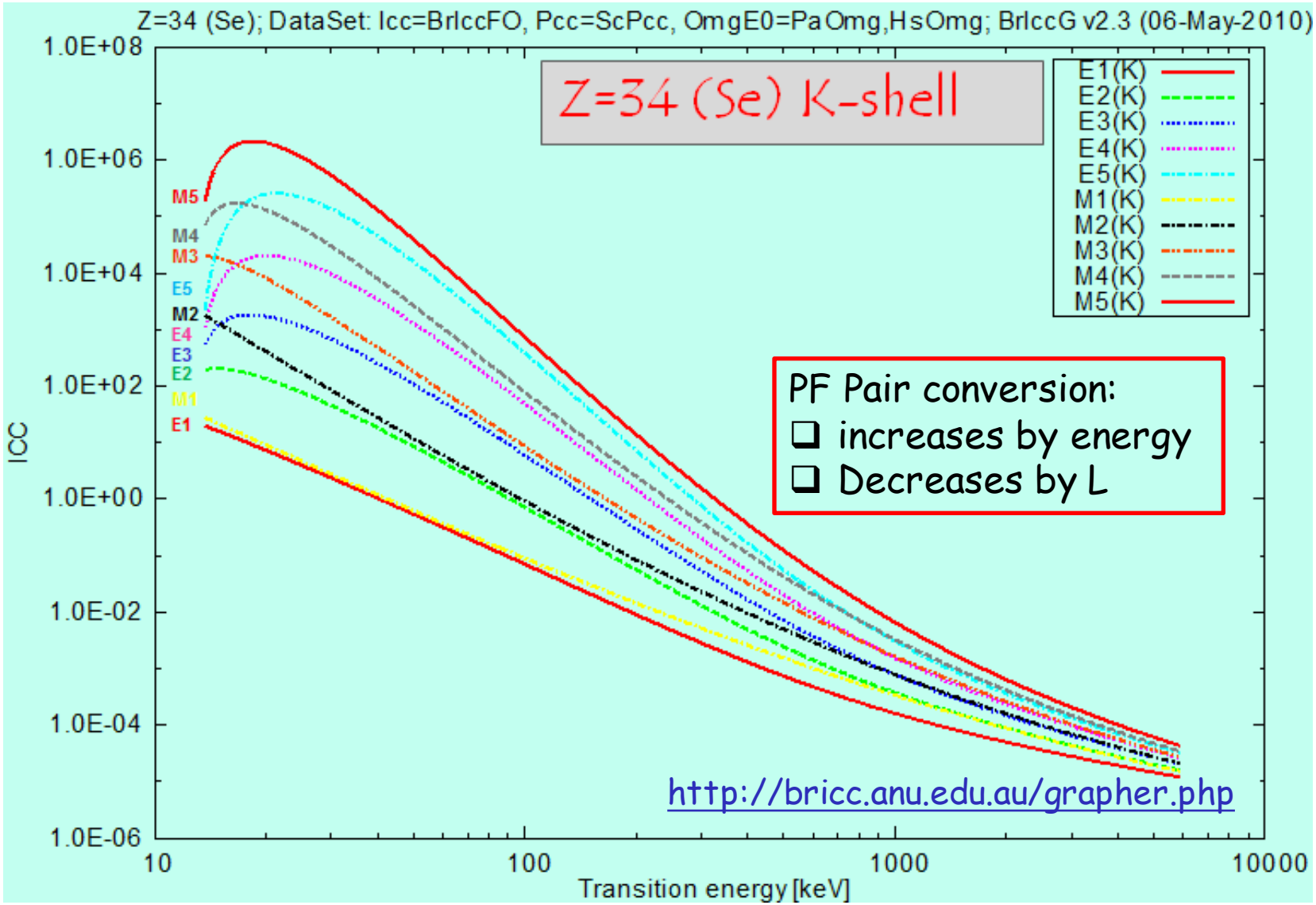
$j_i = j_f$

No single photon emission is allowed!

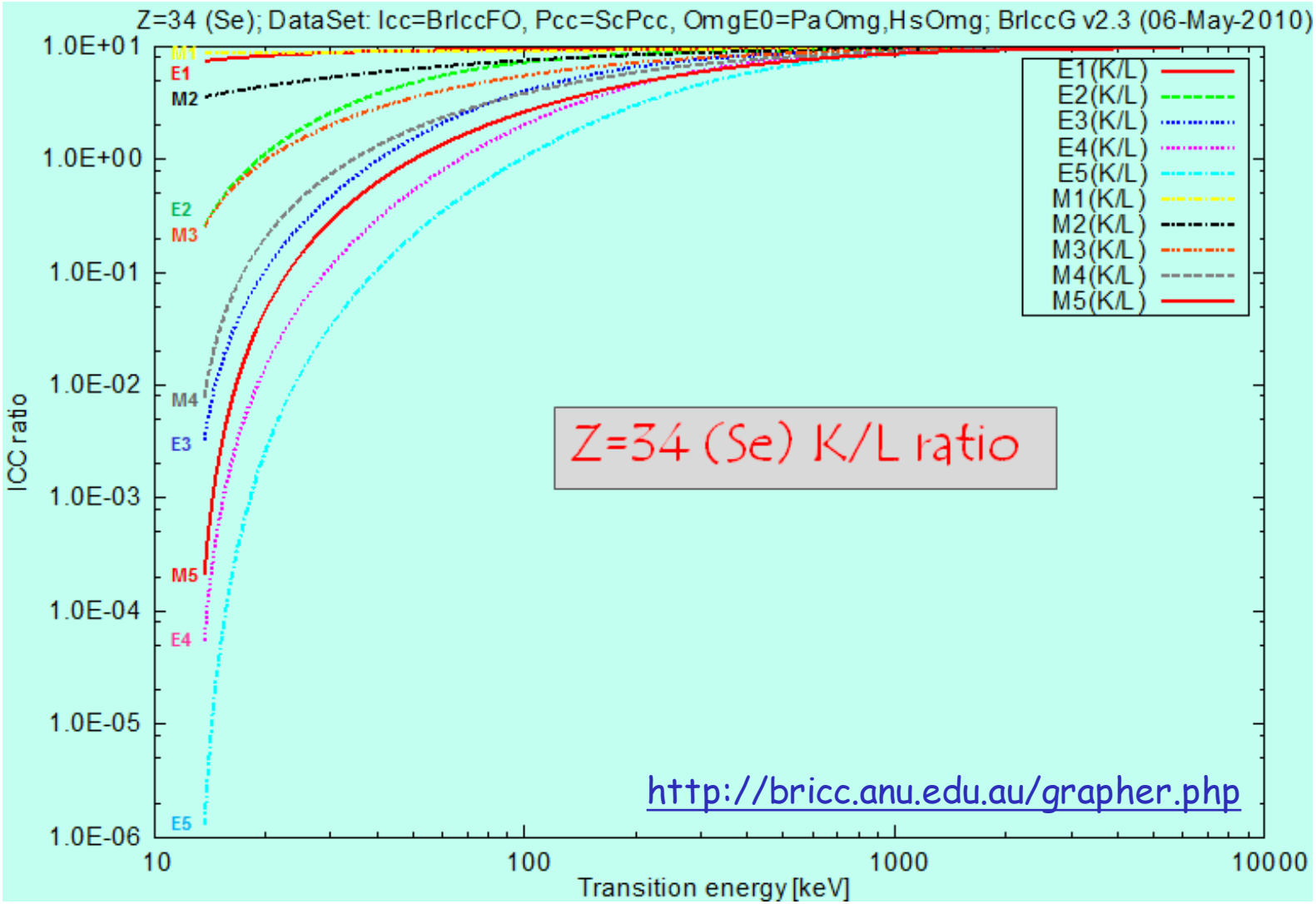
Conversion coefficient is not defined

$\lambda_{CE,PF} = \rho^2(E0) \times \Omega_{CE,PF}$

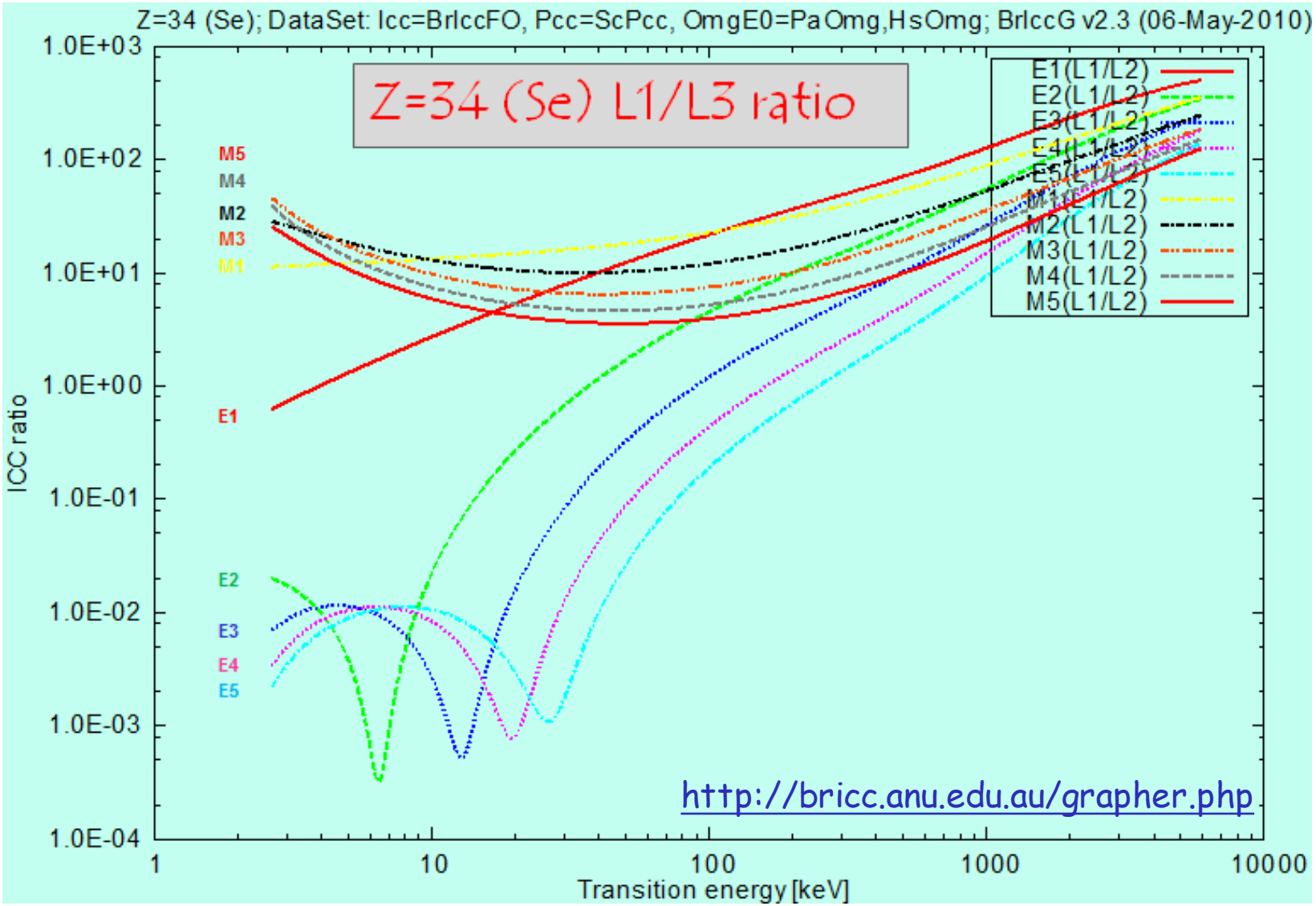
ICC - energy & multipol dependence



ICC - shell dependence



ICC - shell dependence



Mixed Transitions

	Δπ=+1		Δπ=-1	
πL	M1	M3	E1	E3
π'L'	E2	E4	M2	M4

Mixing ratio (MR)

$$\delta^2(\pi' L'/\pi L) = \frac{\lambda_\gamma(\pi' L')}{\lambda_\gamma(\pi L)}$$

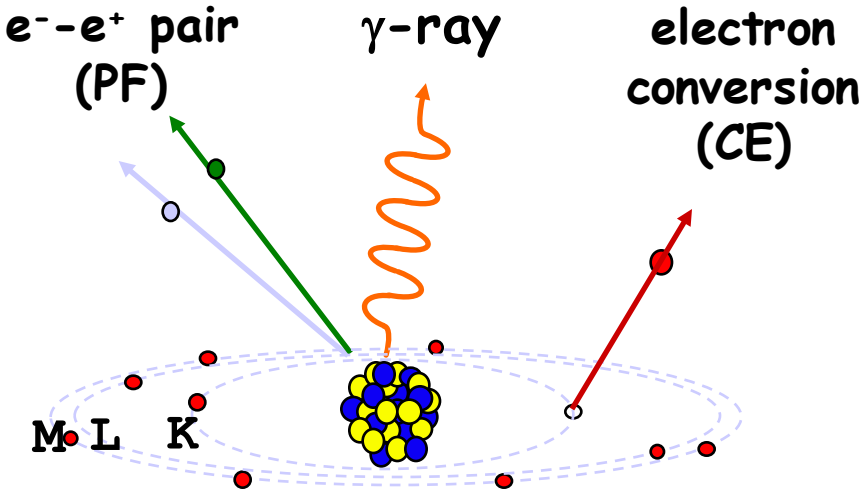
Conversion coefficient for CE and PF

$$\alpha(\pi' L'/\pi L) = \frac{\alpha(\pi L) + \delta^2 \alpha(\pi' L')}{1 + \delta^2}$$

Special cases of mixed transitions with 3 multipolarities

- 184W 536.674(15) keV E1+M2+E3, ME(M2/E1)=+0.070(6), MR(E3/M2)=-0.025(4), λ=-2.1(2); very few known cases; none of the codes can handle two MR
- M1+E2+E0: more common, not discussed here

Theoretical conversion coefficients



Energetics of CE-decay

$E_i - E_f = E_{CE,i} + E_{BE,i} + T_r$

Transition probability

$\lambda_T = \lambda_\gamma + \lambda_K + \lambda_L + \lambda_M \ldots\ldots + \lambda_{PF}$

Conversion coefficient

$\alpha_{CE,PF} = \lambda_{CE,PF} / \lambda_\gamma$

$\lambda_{CE,PF} = \lambda_\gamma \times \alpha_{CE,PF}$

α_{CE}: 2002Ba85 Band et al.
2008Ki07 Kibedi et al.
2012Ki04 Kibedi et al.

α_{PF}: 1979Sc31 Schluter et al.
1996Ho21 Hofman et al.

Ω_{CE}: 1969Ha61 Hager-Seltzer
1970Be87 Bell et al.
1986PaZM Passoja et al.

Use BrIcc to obtain values by interpolation

E0 transitions:

$j_i = j_f$

No single photon emission is allowed!

Conversion coefficient is not defined

$\lambda_{CE,PF} = \rho(E0) \times \Omega_{CE,PF}$

ENSDF Analysis - BrIcc

Calculates Band-Raman Internal Coefficients for gamma-rays based on atomic number, gamma-ray energy, multipolarity, mixing ratio and atomic shell

- Language: FORTRAN90
- Documentation: BrIcc.pdf
- Data files: BrIccFO.idx, BrIccFO.icc, BrIccNH.idx, BrIccNH.icc
- Installation: Compressed archive (Linux&MacOS); installer package (Windows)
- "BrIccHome" environment variable to find data files
- HsIcc (Hager and Seltzer Internal ICC) used for older (pre ~2009) datasets
- Step_1: generates new cards
- Input ENSDF file: myFile.ens
- Calculation report: BrIcc.lst
- New ENSDF records: Card.new
- Old/new card comparison report: Compar.lst
- Step_2: merge (delete/replace/insert) new cards to ENSDF file
- Output ENSDF file: cards.new

More on today afternoon practice session

ENSDF Analysis - BrIccMixing

BrIccMixing – Calculates multipole mixing ratios from internal conversion coefficients, ratios of internal conversion coefficients and multipol mixing ratios

- Language: FORTRAN90; uses GnuPlot for plotting
- Documentation: BrIccMixing.pdf; sign convention: 1970Kr14
- Data files: BrIcc & Gnuplot (http://www.gnuplot.info) need to be installed
- Installation: Compressed archive (Linux&MacOS); installer package (Windows)
- Input ASCII file: myFile.in
- Calculation report: BrIccMixing.lst
- GnuPlot script and data file for each data set

More on today afternoon practice session

Conversion coefficient for CE and PF

$$\alpha(\pi' L'/\pi L) = \frac{\alpha(\pi L) + \delta^2 \alpha(\pi' L')}{1 + \delta^2}$$

ENSDF Analysis - DELTA

Analyses angular correlation and conversion coefficient data, and calculates the best values of mixing ratios

Language: FORTRAN77

- Documentation: readdelt.me
- Installation: executable
- Input ASCII file: delta.dat
- Calculation report: delta.rpt

Replaced by BrIccMixing

ENSDF Analysis - GABS

Calculates absolute gamma-transition intensities and decay scheme normalization factors NR for converting relative decay intensities to absolute intensities per 100 decays

Language: FORTRAN77 updated using FORTRAN90

- Documentation: Gabs-Manual.pdf;

  1986Br21 E. Browne, Calculated Uncertainties of Absolute gamma-ray Intensities and Decay Branching Ratios Derived from Decay Schemes,

  Nucl. Instr. Meth. A249 (1986) 462

- Installation: executable
- Input ENSDF file: myEnsdf.in (a minimum of one transition going to g.s. need to be marked)
- Calculation report: myEnsdf.rpt
- Output ENSDF file: myENSDF.new

More on today afternoon practice session

ENSDF Analysis - JGAMUT

Tool to create ADOPTED dataset by combining gamma-ray energies and intensities from different input data sets. Two ways of taking input gamma-ray energy and intensity measurements and producing adopted values.

Language: java

- Documentation: jgamutManual.pdf
- Installation: executable
- Input ENSDF file: myEnsdf.in (a minimum of one transition going to g.s. need to be marked)
- Calculation report: myEnsdf.rpt
- Output ENSDF file: myENSDF.new

More on today afternoon practice session (ask Balraj)

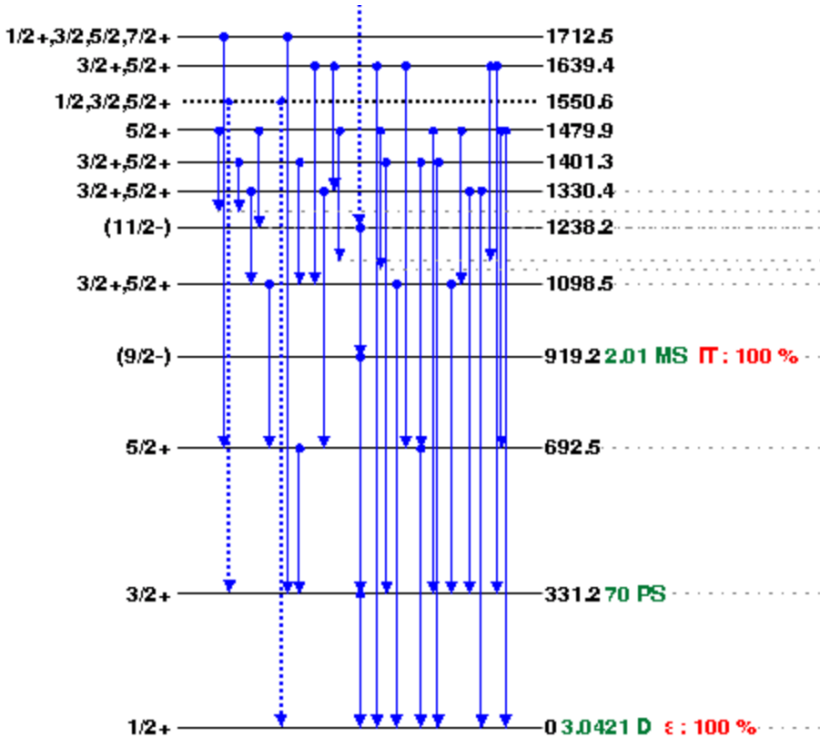
ENSDF Analysis - GTOL

Tool to perform a least-squares fit to the gamma-energies to obtain level energies and to calculate the net feedings to levels.

Language: FORTRAN77 converted to FORTRAN90

- Documentation: readme-gtol-2.pdf
- Installation: executable
- Input ENSDF file: gtol.inp (special commands to control execution)
- Calculation report: gtol.rpt
- Output ENSDF file: gtol.out

More on today afternoon practice session



ENSDF Analysis - LOGFT

Tool to calculate

- logft for beta decay
- partial capture fractions for electron capture decay
- electron capture to positron ratio for positron decay
- Average β-ray energies

Language: FORTRAN77 converted to FORTRAN90

- Documentation: readmelogft.me
- Installation: executable; radial wave function data: LOGFT.DAT
- Input ENSDF file: data.tst
- Calculation report: logft.rpt
- Output ENSDF file: logft.new

More on today afternoon practice session

ENSDF Analysis - PANDORA

Tool to carry out physics checking on ENSDF datasets

- Decay data sets, other than IT and SF decays have a P-card and vice versa
- An L-record with $T_{1/2}$ > 0.1 sec should have MS FLAG
- Consistency of spin/parity of levels with multipolarity connecting transitions
- For a transfer reaction with even-even target J=L±1/2
- β-decay: log ft, J_i, J_f, parity change
- α-decay: HF, J_i, J_f parity change
- Levels out of order

Language: FORTRAN77 converted to FORTRAN90

- Documentation: readmepandora.pdf
- Installation: executable
- Input ENSDF file: pandora.inp
- Several output files: pandora.err, pandora.gam, pandora.gle, pandora.lev, pandora.rad, pandora.rep, pandora.xrf
- Output ENSDF file: pandora.out

More on today afternoon practice session

ENSDF Analysis - RADLIST

Calculates the nuclear and atomic radiations associated with the radioactive decay of nuclei:

- β^+, β^-, ε decay
- α decay
- γ-rays, conversion electrons, electron-positron pairs
- X-rays and Auger electrons

Language: FORTRAN77

- Documentation: readme-pandora.pdf; radlistdoc.pdf (description of physics)
- Installation: executable; atomic mass data RADMAS.DAT; atomic data MEDNEW.DAT
- Input ENSDF file: radlist.inp
- Several output files: radlist1.out, radlist2.out, radlist3.out, radlist4.out, radlist5.out

Code is not maintained, replacement (BrIccEmis) under development (Friday)

Use myEnsdf at https://www-nds.iaea.org/exfor/myensdf.htm

ENSDF Analysis - RULER

Calculates

a) reduced electromagnetic transition strengths and compares these to the Recommended Upper Limits (RUL)

b) BEλ and BMλ

- Language: FORTRAN77
- Documentation: ruler.pdf, readme-ruler.pdf; Ruler-NewFeatures.pdf
- Installation: executable
- Input ENSDF file: ruler.inp
- Output files: (a) ruler1.rpt, (b) ruler2.rpt

More on today afternoon practice session

Code is not maintained, replacement under development

Recommeded Upper Limits RUL

	Γ_γ/Γ_W (Upper Limit)		
Character*	A=6–44[a§]	A=45–150[b,c]	A>150[d]
E1 (IV)	0.3[#]	0.01	0.01
E2 (IS)[e]	100	300	1000
E3	100	100	100
E4	100	100[†]	
M1 (IV)	10	3	2
M2 (IV)	3	1	1
M3 (IV)	10	10	10
M4		30	10

ENSDF Utility codes - ADDGAM

Adds gamma transitions to the adopted dataset when all gamma's come from one data set

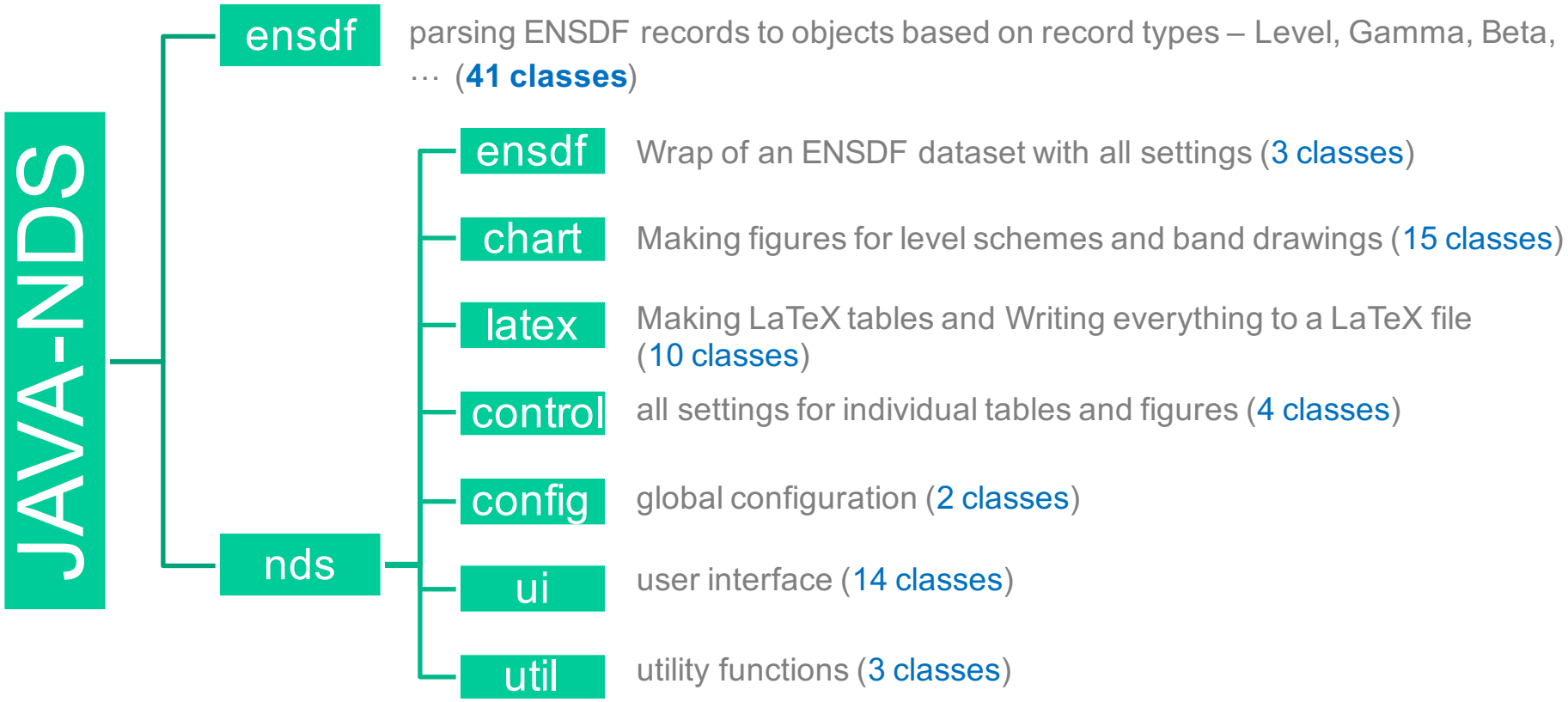
- Language: FORTRAN 77
- Documentation: readaddg.me
- Installation: executable
- Input1: ADOPTED data set; sample: ADDGAML.DAT
- Input2: A decay/reaction data set with gammas to be added;
  Sample: ADDGAMG.DAT
- Output: Merged dataset; sample: ADDGAM.NEW
- The relative intensities (RI) will be scaled, so the strongest gamma will be 100
- If only one gamma coming from the level, no uncertainty in RI given; DRI=0
- If gammas come from more than one data set but are non-overlapping, the program may be run successively with different gamma data sets as input; care should be taken to merge intensities correctly!
- Use jGAMUT

ENSDF Utility codes - AVETOOLS

Calculates the average value and uncertainty of a set of experimental data using 5 different statistical methods

- Language: FORTRAN90
- Documentation: AveTools.pdf
- Installation: Compressed archive (Linux&MacOS); installer package (Windows)
- Input ASCII file: AveTools.in
- Output: Avetools.rpt
- V.AveLib - alternative code in java; next talk by Balraj Singh`s on Averaging methods

ENSDF Utility codes - JAVA_NDS



Courtesy of Jun Chen, NSCL/MSU

JAVA-NDS

Nuclear Data Sheets 126, 373 (2015)

JAVA-NDS
Font (10pt):
Times New Roman

Nuclear Data Sheets for A=209*

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#*Present address: Na*
East L

(Received 24 Se

Abstract: The experimental data are evaluated for
Detailed evaluated level properties and related
for level energies, half-lives, γ-ray energies and
other spectroscopic data. This work supersedes

Cutoff Date: Literature available in NSR database

General Policies and Organization of Material:
/nds/NDSPolicies.pdf.

Acknowledgements: The authors express their gra
Nuclear Data Center for their assistance during
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Nuclear Data Sheets for A = 209*

NDS-PUB

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East Lansing, Michigan 48824, USA

(Received September 24, 2013; Revised March 31, 2015)

Abstract: The experimental data are evaluated for known nuclides of mass number A=209 (Au,Hg,Tl,Pb,Bi,Po,At,Rn, Fr,Ra,Ac,Th). Detailed evaluated level properties and related nuclear structure information are presented, with the best values recommended for level energies, half–lives, γ–ray energies and intensities, decay data (energies, intensities and placement of radiations), and other spectroscopic data. This work supersedes the earlier full evaluation of A=209 by M.J. Martin (1991Ma16).

Cutoff Date: Literature available in NSR database up to September 30, 2013 has been included.

General Policies and Organization of Material: see http://www.nndc.bnl.gov/nds/NDSPolicies.pdf.

Acknowledgments: The authors express their gratitude to Dr. J.K. Tuli, Mrs. J. Totans and Mrs. M. Blennau from the National Nuclear Data Center for their assistance during the evaluation process and the preparation of the manuscript. The authors are thankf
manuscript and many useful comments
Kolkata for his help with the evaluatic

NDS-PUB
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NewCenturySchlbk

Courtesy of Jun Chen, NSCL/MSU

ENSDF Utility codes - XLS2ENS

Code to generate ENSDF file from data stored in Excel

- Language: Python 2.7.6 ONLY!
- Installation: compressed archive of Python script, documentation and sample input; requires xlrd Python module

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Summary

- Codes are for you to do your work, but you need to understand how they work and how to drive. Knowledge in programming is useful, but not essential
- ENSDF codes written by evaluators and tested by evaluators. Give feedback if you notice problems, unexpected behaviors
- Always run FMTCHK to verify that the input ENSDF file has no errors
- Observe the messages on the terminal console and in the report files
- Error messages may not be sufficient to solve problems. Look into the source code if available
- Some codes create new ENSDF files under different name. Check the new ones before overwriting the old ones
- IAEA action to replace old codes with new ones: jGamut, java_NDS, v.AveLib are already out