High Energy Activation Data and Processes

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Outline

- Introduction
- EAF-2005, first high energy file
- New tools for library analysis
- EAF-2007,EAF-2005.1
- Deuteron-induced activation
- Proton-induced activation
- Summary
- EASY-2009
- Conclusions

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Introduction

- Understanding and predicting effect of neutrons on materials is fundamental to fusion, but also particle source devices and still fission technologies
- European Activation System (EASY) is the European tool
- Previous versions such as EASY-2003 have an energy range < 20 MeV
- Materials test facilities (IFMIF) use accelerators, high energy neutron tail ⇒ upper energy limit is ~55 MeV
- Need to extend EASY, carried out over 4 years, EASY-2007 is current version

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Theory

Set of differential equation to be solved

S_i term only for actinides or (z,anything) mt=5 yields

$$\frac{dN_i}{dt} = -N_i(\lambda_i + \sigma_i\phi) + \sum_{j\neq i} N_j(\lambda_{ij} + \sigma_{ij}\phi) + S_i$$

$$S_i = \sum_k N_k \sigma_k^f \phi Y_{ik}$$

Depletion

Source

H. Bateman, Proc. Camb. Phil. Soc. 16, (1910) 423, 28 years old

New SAFEPAQ-II features

- Able to read, high energy IEAF and TALYS libraries
- New Modification type - enables a merge of the existing data above an energy with data from a different type of reaction
  - e.g. (n,α) reaction can have low energy region replaced with data from an (n,γ) reaction
- New group structures with 211 and 351 energy groups
- New uncertainty group between 20 and 60 MeV
- MT numbers for summed reactions (MT >200)
  - e.g. (n,α+) = (n,α) + (n,n′h) + (n,pt) + (n,n′pd) + (n,2n2p)
- Validation histograms showing (C/E) for the various reaction classes produced for any source library
- C/E plots against *A* and |*Q*| possible

New SAFEPAQ-II features

- Plotting compatibility of single reaction channel (**relevant** < 20 MeV , weak > 20 MeV) and lumped reaction channels:

(n,d)+ = **(n,d)** + **(n,n'p)**

(n,t)+ = **(n,t)** + (n,n'd) + (n,2np) +

(n,h)+ = **(n,h)** + (n,n't) + (n,pd) + (n,n'2p) +

(n,a)+ = **(n,a)** + (n,n'h) + (n,pt) + (n,2d) +

(n,n'a)+= **(n,n'a)** + (n,2nh) + (n,n'pt) + (n,n'2d) +

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EAF-2005 cross sections

- EAF-2005 requires data from 20 – 60 MeV
- Calculated data produced by TALYS for data > 20 MeV
- SAFEPAQ-II automatically smoothly joins TALYS-5 data at 20 MeV to existing data in EAF-2003
- For new reactions (generally with high thresholds) TALYS-5 data are used
- A set of new MT numbers agreed allowing up to 8 particles to be emitted
- 62,637 reactions (12,617 in EAF-2003)
- 50 data sources
- 86 different reaction types (23 in EAF-2003)

New reaction types (but standard ENDF)

Reaction	MT value
(n,2nd)	11
(n,n´3a)	23
(n,2n2a)	30
(n,n'd2a)	35
(n,n´t2a)	36
(n,3np)	42
(n,n´2p)	44
(n,n´pa)	45
(n,3a)	109
(n,t2a)	113
(n,d2a)	114
(n,pd)	115
(n,pt)	116
(n,da)	117

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New reaction types (non-standard)

Reaction	MT value
(n,5n)	152
(n,6n)	153
(n,2nt)	154
(n,ta)	155
(n,4np)	156
(n,3nd)	157
(n,n´da)	158
(n,2npa)	159
(n,7n)	160
(n,8n)	161
(n,5np)	162
(n,6np)	163

- Plus 37 further reactions

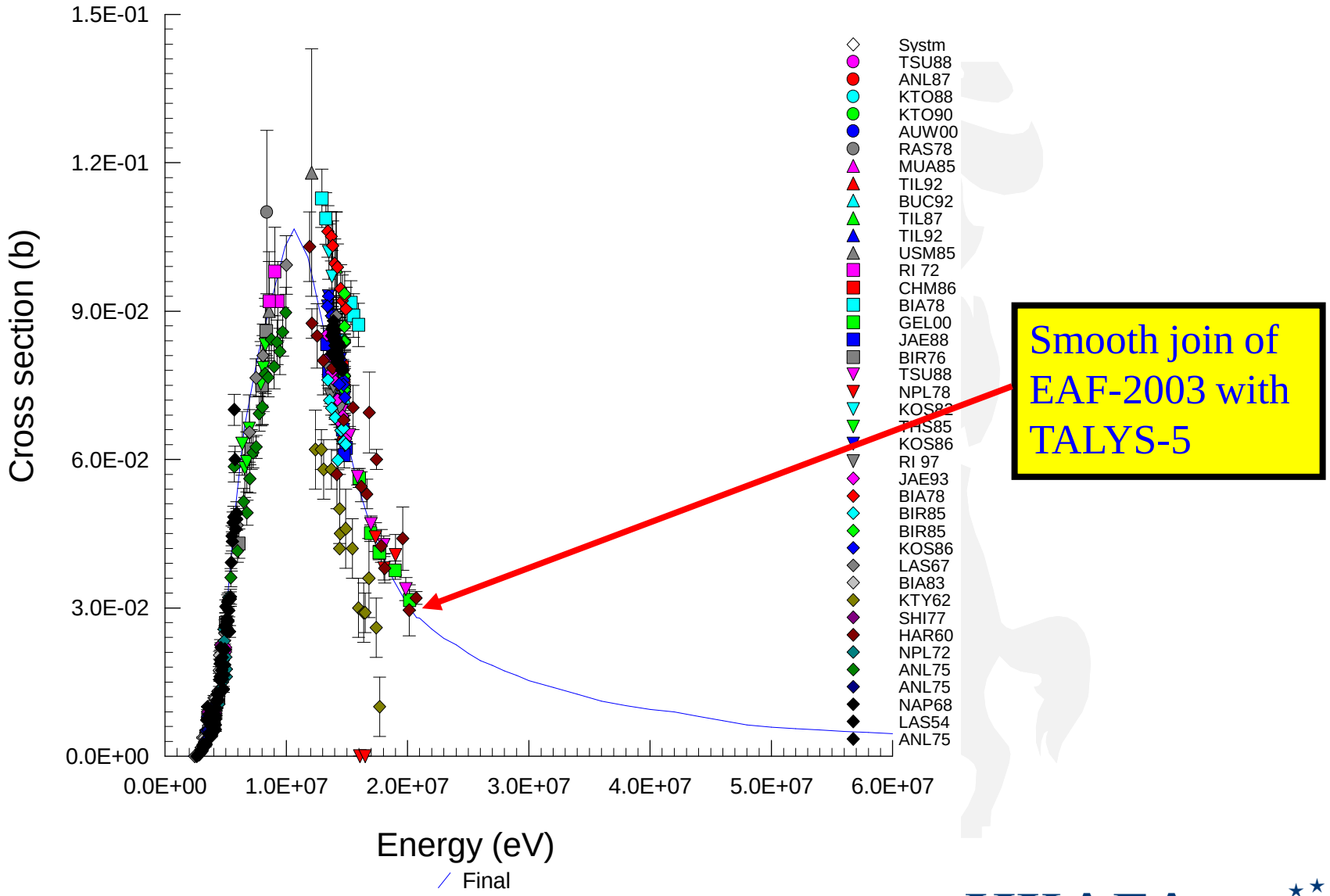
Reaction types , MT Values

- Grid of reactions including all **36 MT numbers** defined in ENDF and some of the 86 now defined in EAF-2007

	N-7	N-6	N-5	N-4	N-3	N-2	N-1	N	N+1
Z	(n,8n) 161	(n,7n) 160	(n,6n) 153	(n,5n) 152	(n,4n) 37	(n,3n) 17	(n,2n) 16	(n,n') 4	(n,γ) 102
Z-1					(n,2nt) 154	(n,nt), (n,2np) 33,42	(n,t), (n,nd) 105,32,41	(n,d), (n,np) 104, 28	(n,p) 103
Z-2	(n,6na) 167		(n,4na) 165	(n,3na) 25, **200**	(n,2na) 24	(n,n'a) 22	(n,a), (n,nh) 107,34,116	(n,h), (n,pd) 106,44,115	(n,2p) 111
Z-3					(n,2npa) 159	(n,da),(n,npa) 117,45	(n,pa) 112		(n,3p) 197
Z-4			(n,2n2a) 30	(n,n2a) 29	(n,2a) 108				
Z-5		(n,nt2a) 36	(n,t2a) 113,35	(n,d2a) 114					
Z-6		(n,n3a) 23	(n,3a) 109						

Classical MT's
New MT's

Data for $^{27}Al(n,p)^{27}Mg$



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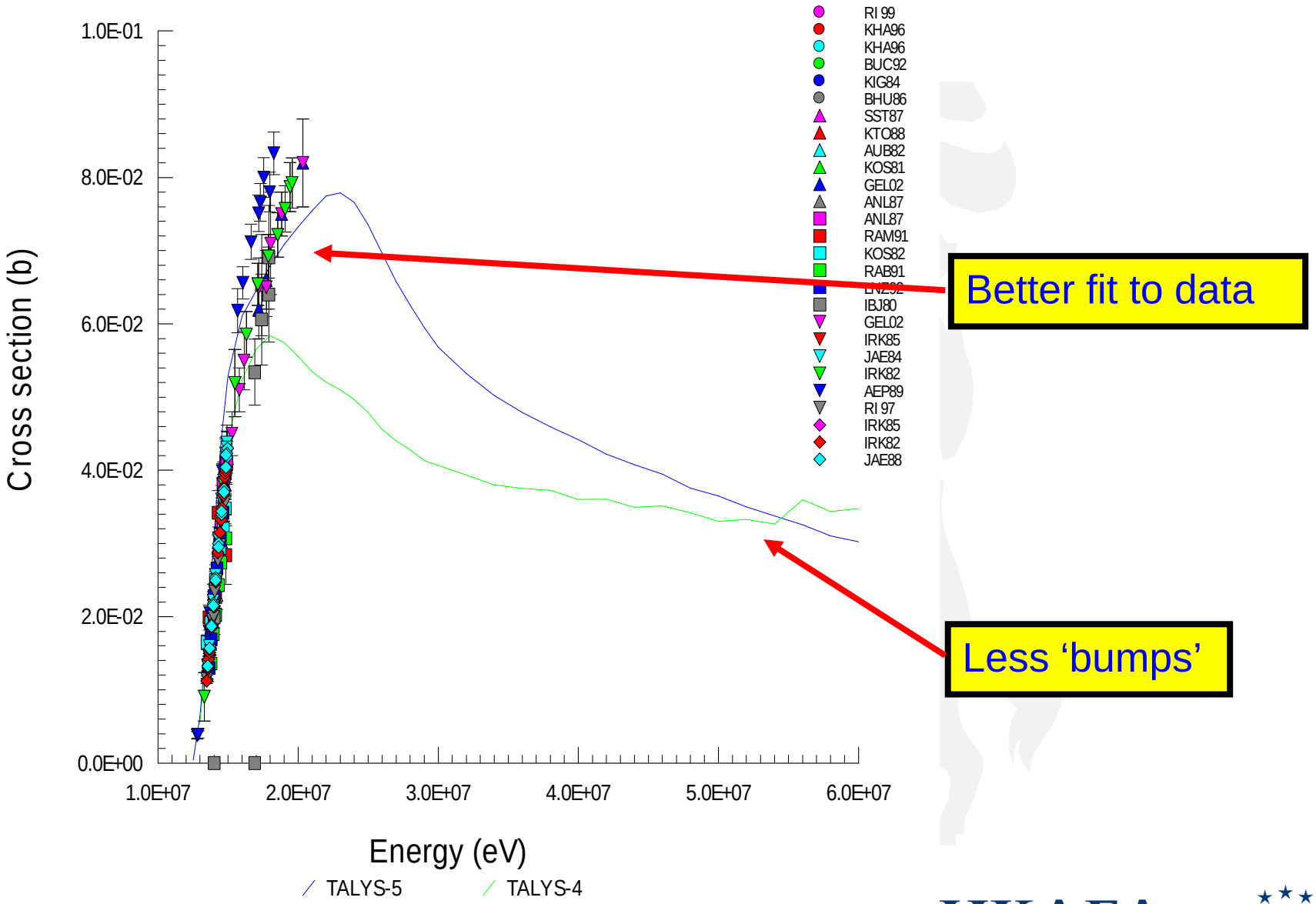
New differential and integral data

- Filatenkov has measured 14 reactions that were discrepant
- Kopecky has searched EXFOR to find all data > 20 MeV
- New source of integral data identified:
  - S. Qaim et al., KfK Jülich in late seventies, 53 MeV deuterons on a Be target. The resulting neutron spectrum extends from 4 to 50 MeV, with its maximum around 22.5 MeV and FWHM = 15.8 MeV.
- New integral data for Y, Pb, Ta and Mo
- Use of FZK and Řež integral data > 20 MeV
- Pseudo “Differential” data
  - Full 20 – 60 MeV scale measurements, coming from two laboratories: Louvain-La-Neuve and Tohoku University activation measurements with the Li-7(p,n) neutron source.
  - “Just above 20 MeV” measurements (activation measurements), data mostly between 20-25 MeV

TALYS-6, -5 and -5a data

- A calculation for all targets using global parameters output in EAF format
- Corrects many problems identified in TALYS-4, -5
  - Better physics
  - 'Smoother' high energy data
  - Charged particle emission improved (still not perfect)
- Is default choice for > 20 MeV data

TALYS-6,-5 improvement – $^{58}Ni(n,2n)^{57}Ni$



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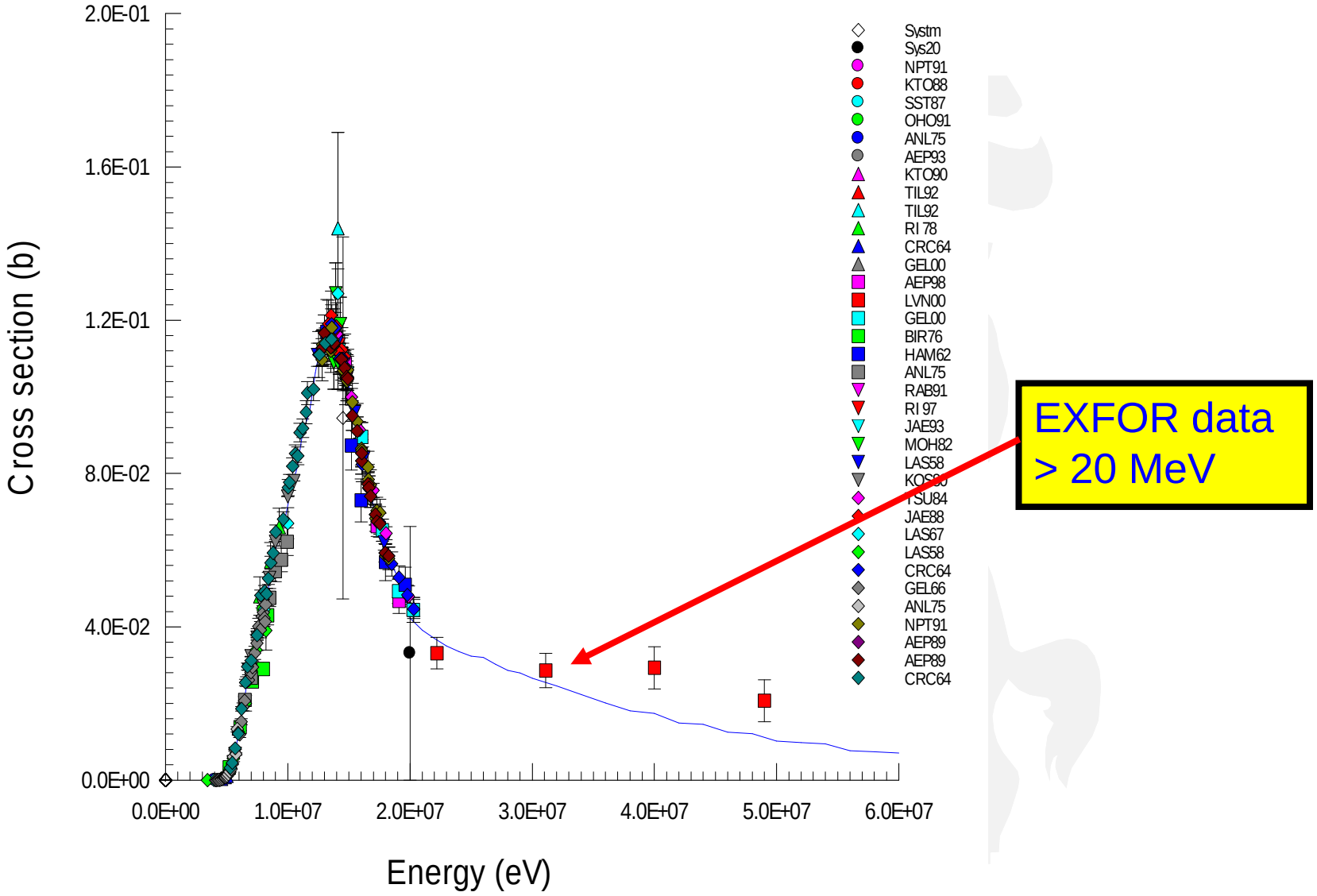
New EXFOR data – $^{56}Fe(n,p)^{56}Mn$



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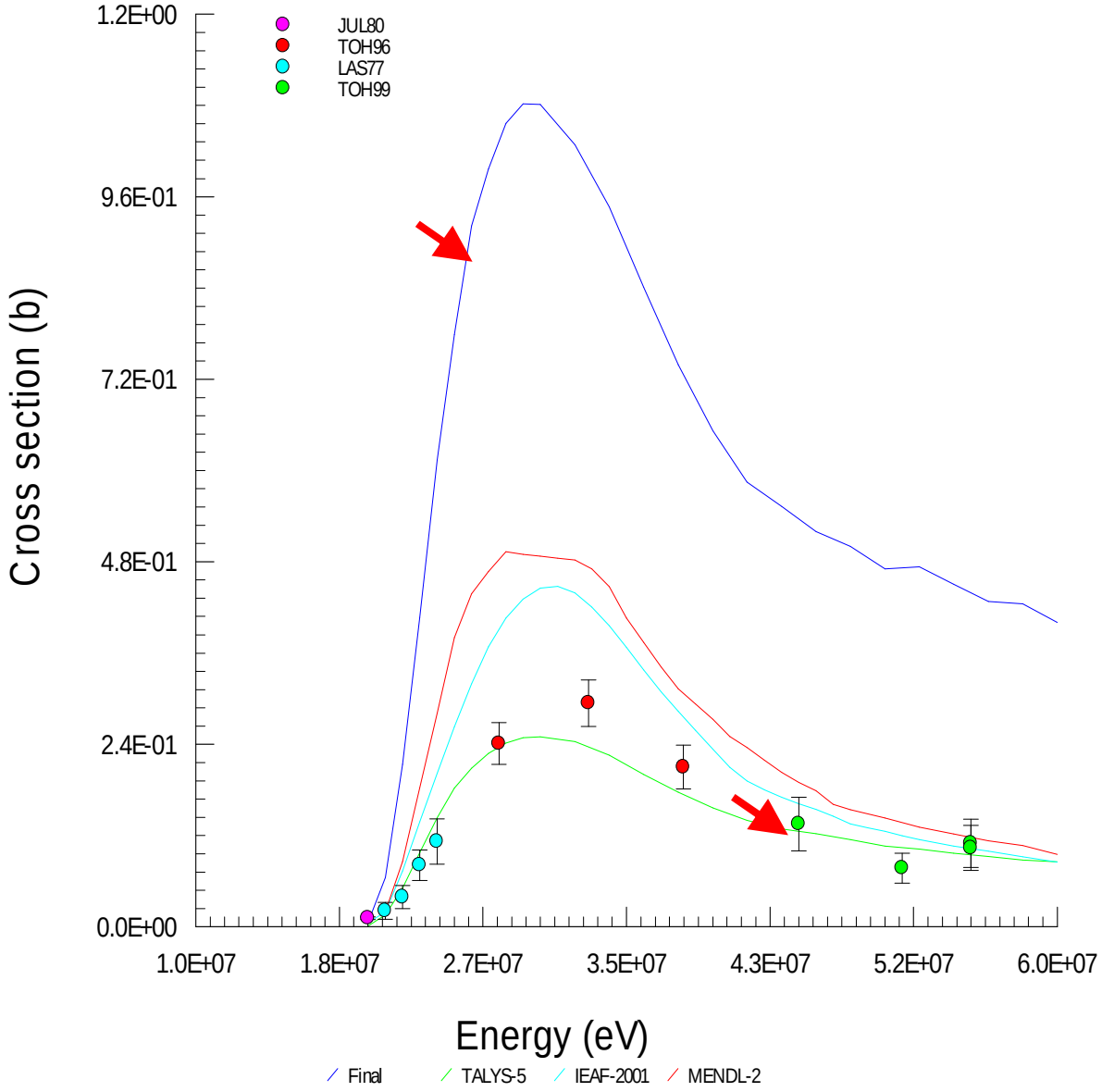
New EXFOR data - $^{59}Co(n,3n)^{57}Co$



TALYS-5 in very good agreement with new high energy data

Significant improvement over EAF-2004

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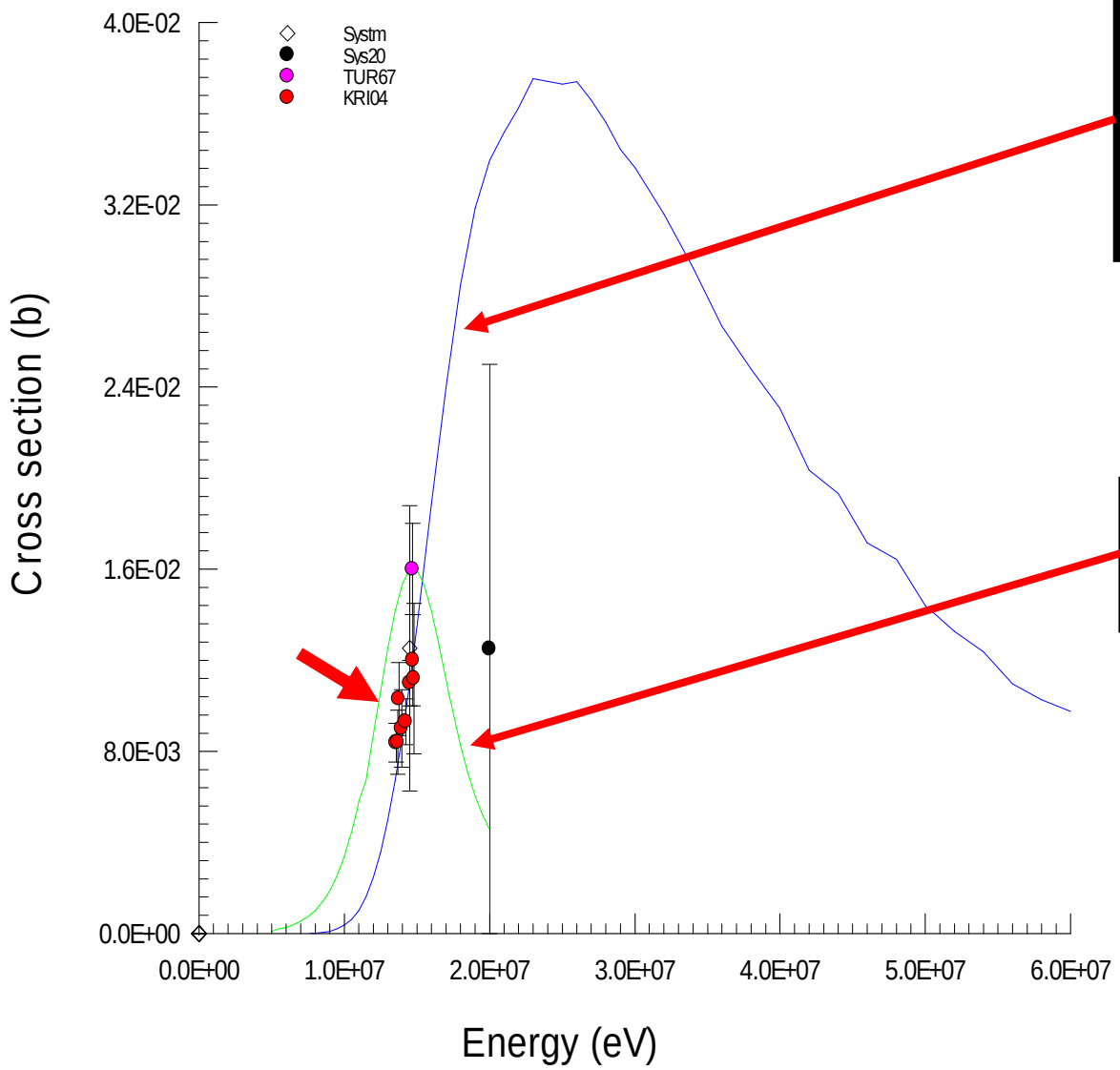
New differential data – $^{80}Se(n,p)^{80}As$



EAF-2005 based on TALYS-5 renormalised to Filatenkov data

EAF-2003 based on JEF-2.2

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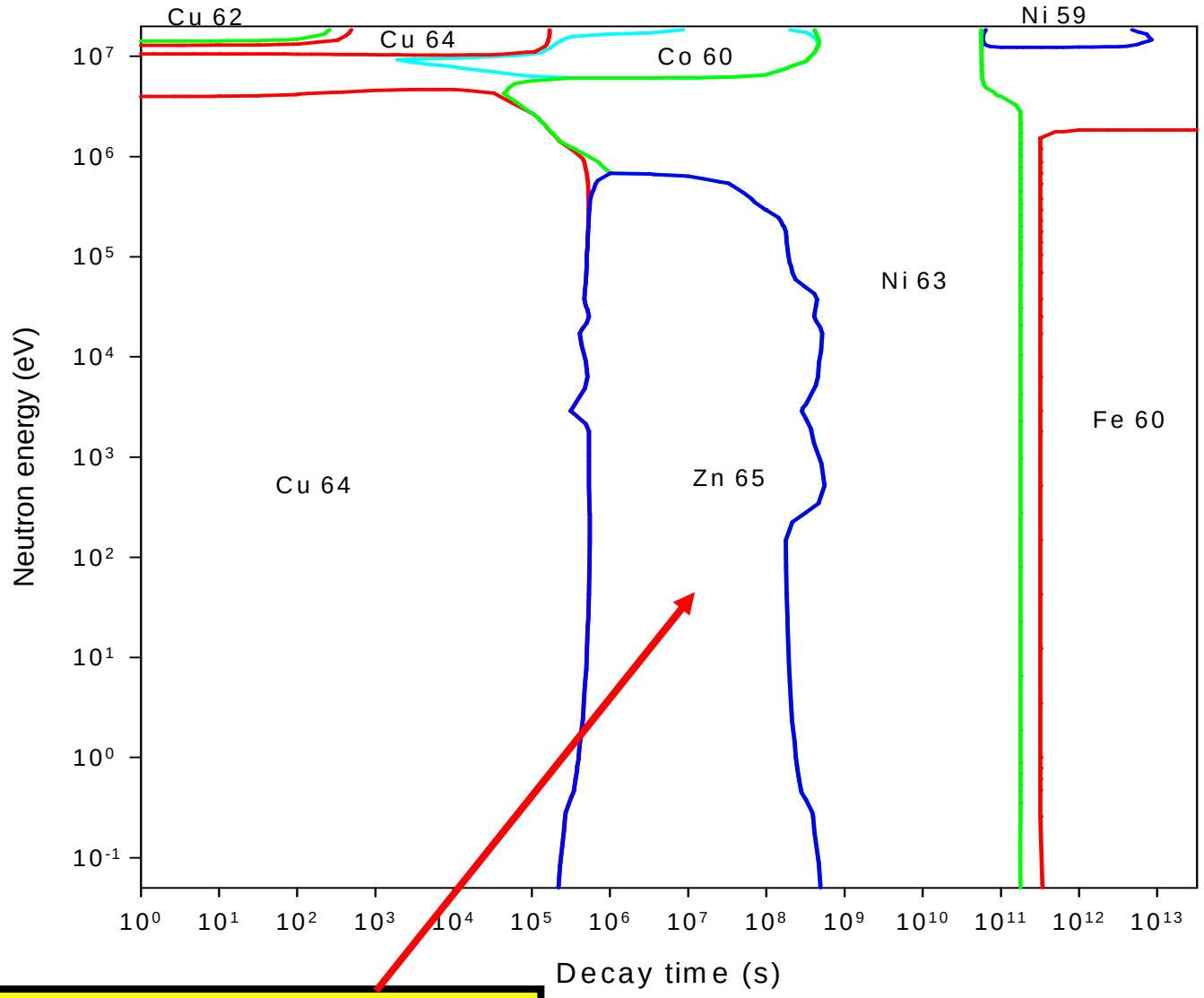
Importance diagrams

- A neutron spectrum needed for activation calculations
- FISPACT output files contain a large amount of data
- How to summarize – ideally as a picture?
- Importance diagrams give a picture of the dominant nuclides for all neutron energies and all decay times
- They are largely independent of the neutron flux
- Set of activation calculations for mono-energetic neutrons
- Identify dominant nuclides for a quantity e.g. activity
- Find regions in (decay time, energy) space where a nuclide contributes more than 50%

Activity importance diagram for Cu



Zn-65 contributes > 50%

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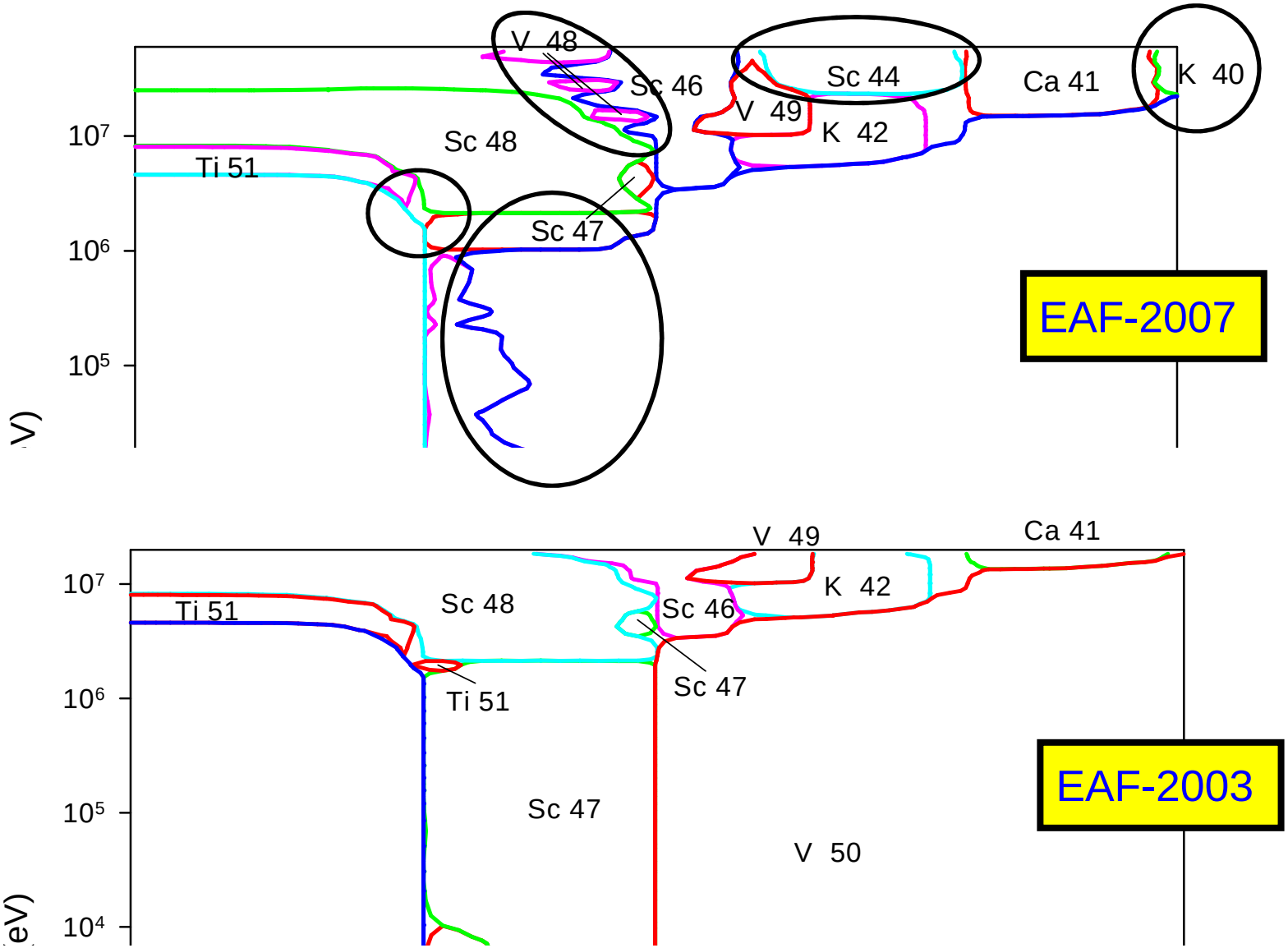
Information from importance diagrams

- Nuclides shown are primary nuclides (> 50%)
- Secondary nuclides (1-50%) also identified
- Further FISPACT runs at a set of particular energies gives the pathways and hence reactions that produce the primary nuclides
- Use of EAF-2007 allows study to cover energies < 60 MeV
- By considering all elements get:
  - List of the dominant nuclides (primary and secondary)
  - List of important reactions
- Lists allow focus on which nuclides and reactions to improve
- What is new for E > 20 MeV?

Dose rate importance diagram for V



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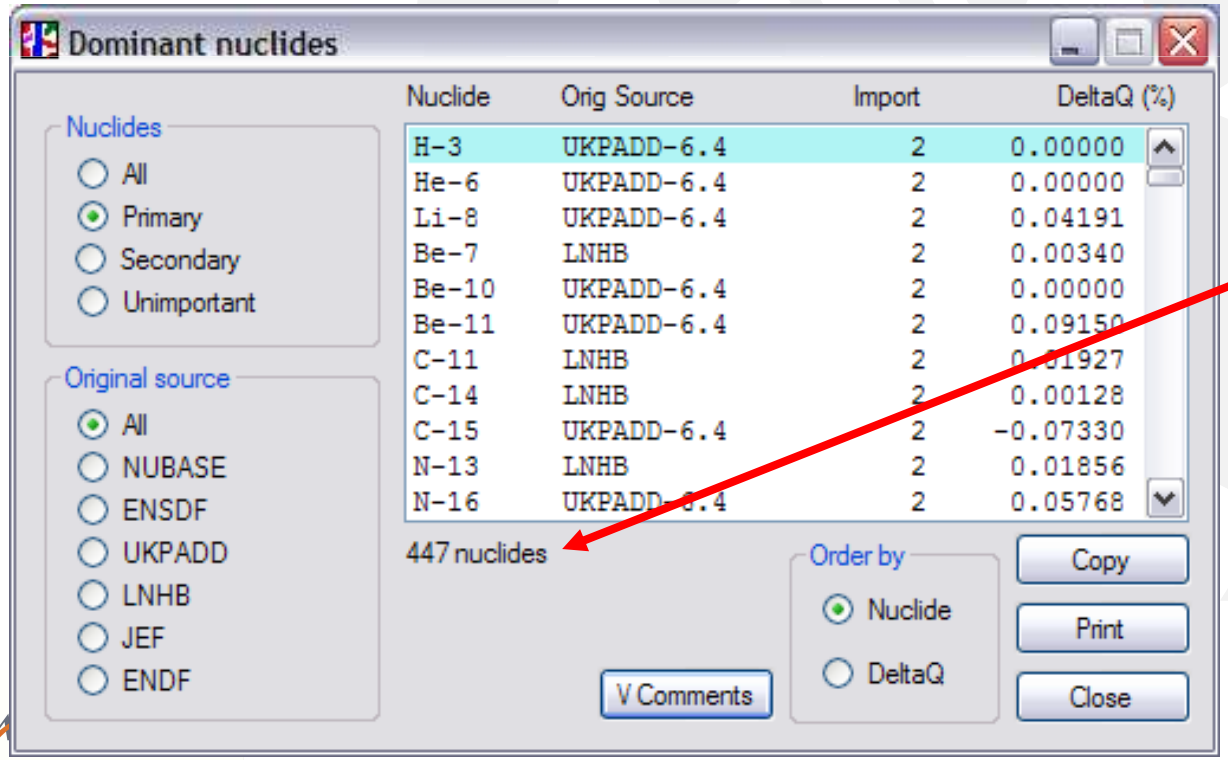
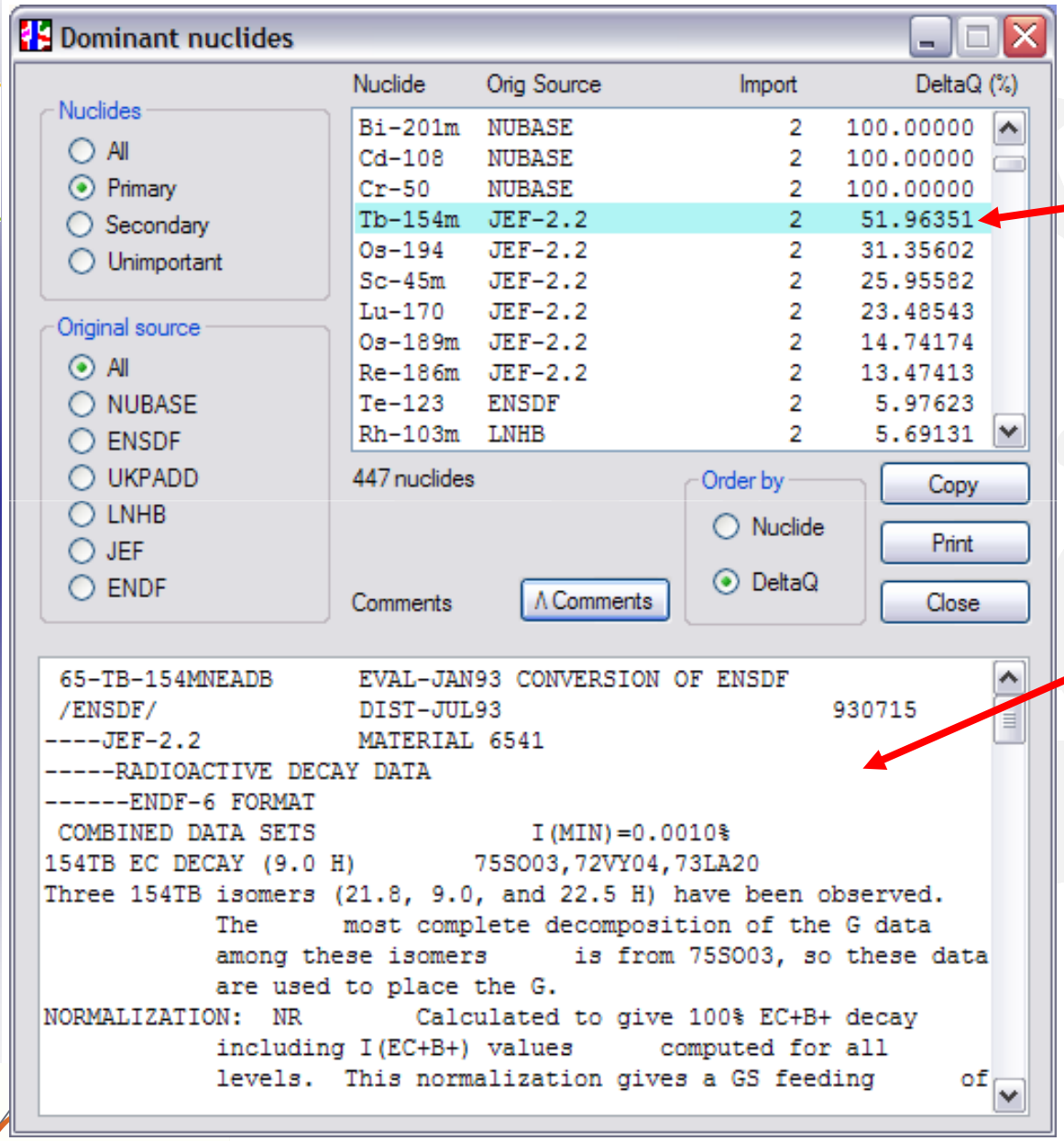
Dominant nuclides

- Primary nuclides seen on importance diagrams (> 50%)
- Secondary nuclides (1-50 %)
- SAFEPAQ-II can now show:
  - Original source for each nuclide
  - ΔQ, indicates consistency of evaluation
  - File comments



447 primary nuclides

Dominant nuclides



Ordered by ΔQ

Comments shown

Importance diagrams for EAF-2007

- New primary nuclides are seen for E > 20 MeV
  - For V: ^{48}V, ^{44}Sc and ^{40}K
- Diagrams for H – Bi analysed
- 36 new primary nuclides
  - ^{7}Be, ^{11}C, ^{19}Ne, ^{48}Ca, ^{50}Cr, ^{64}Zn, ^{66}Ga, ^{72}As, ^{76}Br, ^{82m}Rb, ^{86}Y, ^{108}Cd, ^{114}Cd, ^{109}Sn, ^{124}Sn, ^{124}I, ^{124}Xe, ^{130}Cs, ^{136}Ce, ^{138m}Pr, ^{139m}Nd, ^{160}Gd, ^{154m}Tb, ^{156}Dy, ^{158}Ho, ^{162}Er, ^{168}Yb, ^{170}Lu, ^{171}Hf, ^{172}Hf, ^{176}Ta, ^{183}W, ^{184}Os, ^{192}Au, ^{196}Hg, ^{201m}Bi
- 'Exotic' reactions seen for E > 20 MeV
  - ^{54}Fe(n,dα)^{49}V in pathways → ^{39}Ar, ^{42}Ar and ^{44}Sc
  - 18% of ^{39}Ar formed has ^{54}Fe(n,dα)^{49}V as first step

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Importance diagrams for EAF-2007

- Define an importance value to each reactions
- If the reaction is in a pathway that contributes:
  - ≥ 50% then importance = 5
  - ≥ 20% then importance = 4
  - ≥ 10% then importance = 3
  - ≥ 5% then importance = 2
  - ≥ 1% then importance = 1
- Previously ‘major’ reaction ≡ importance 5 and 4
- 2,272 major reactions

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Activation handbook

- Current Handbook produced with EAF-2003, needed to be updated for EAF-2007
- Production of Importance diagrams using EAF-2007 and extending to 60 MeV completed
- Work on ‘cooling curves’ for 5 neutron spectra completed, production of new handbook by March 2009 (658 pages!)
- Primary and secondary nuclides identified
- Important reactions (using scale 1 to 5) identified
- Results can be seen in the User Interface ‘Importance viewer’
- New features in SAFEPAQ-II:
  - Important and measured reaction statistics
  - Analysis plots can use new importance results

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Importance diagrams for EAF-2007

- Compared to total of 65,565 only 3.5% are major
- 2,272 major reactions are:
  - mostly of 'traditional' types e.g. (n,γ) 432, (n,2n) 365, (n,α) 236
  - Some 'exotic' types e.g. (n,5n) 69, (n,6n) 41, (n,2nt) 25, (n,dα) 25, (n,tα) 14
- Analysis shows:
  - 923 of the 2,231 nuclides describe activation properties of all elements < 60 MeV
  - 5,105 of the 65,565 reactions needed for all dominant nuclides
  - Allows focus of future work
- Will be able to give a list of reactions that need new measurements
- Reactions that cannot be measured will need improved model calculations

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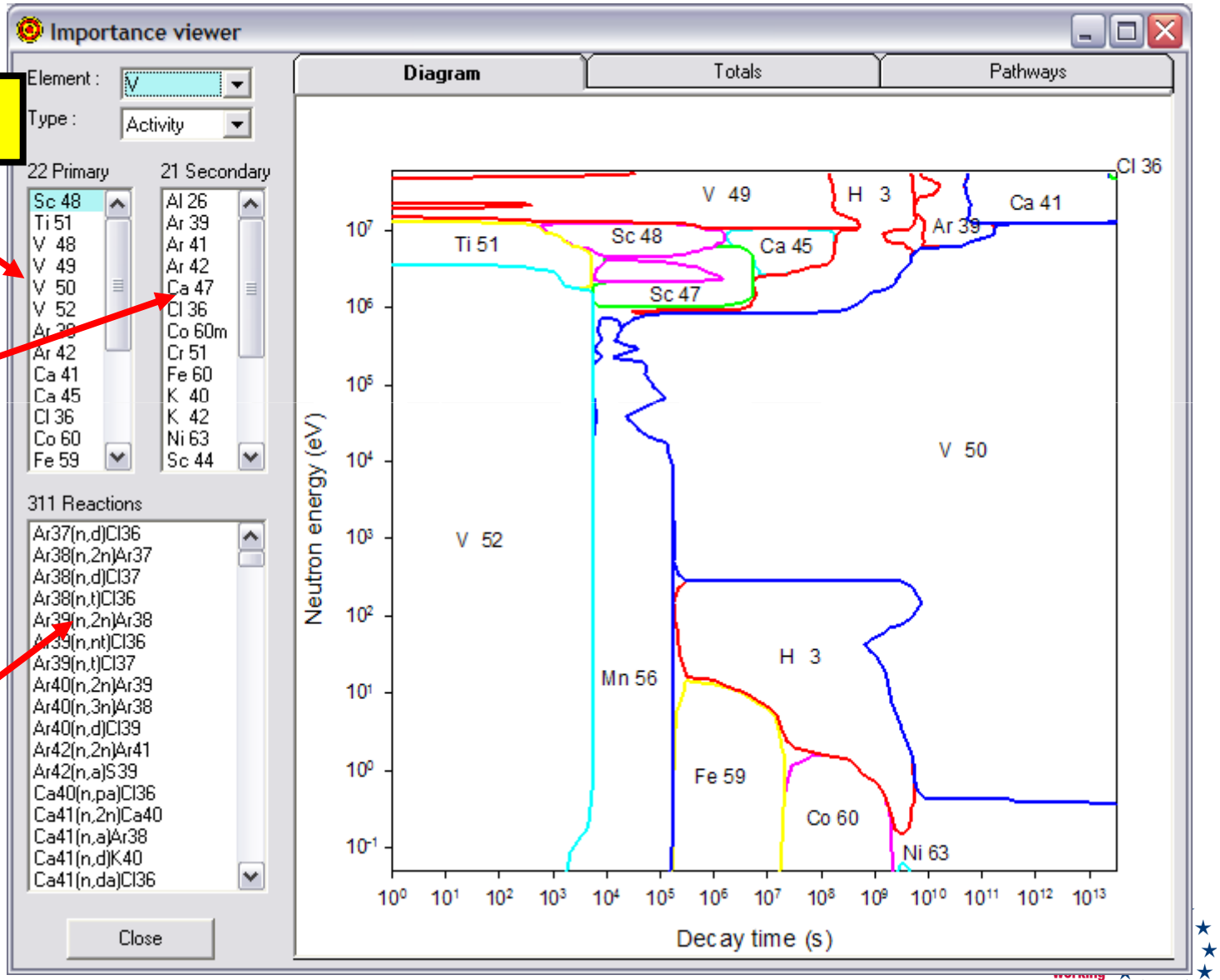
Importance viewer (1)



Primary nuclides

Secondary nuclides

Reactions

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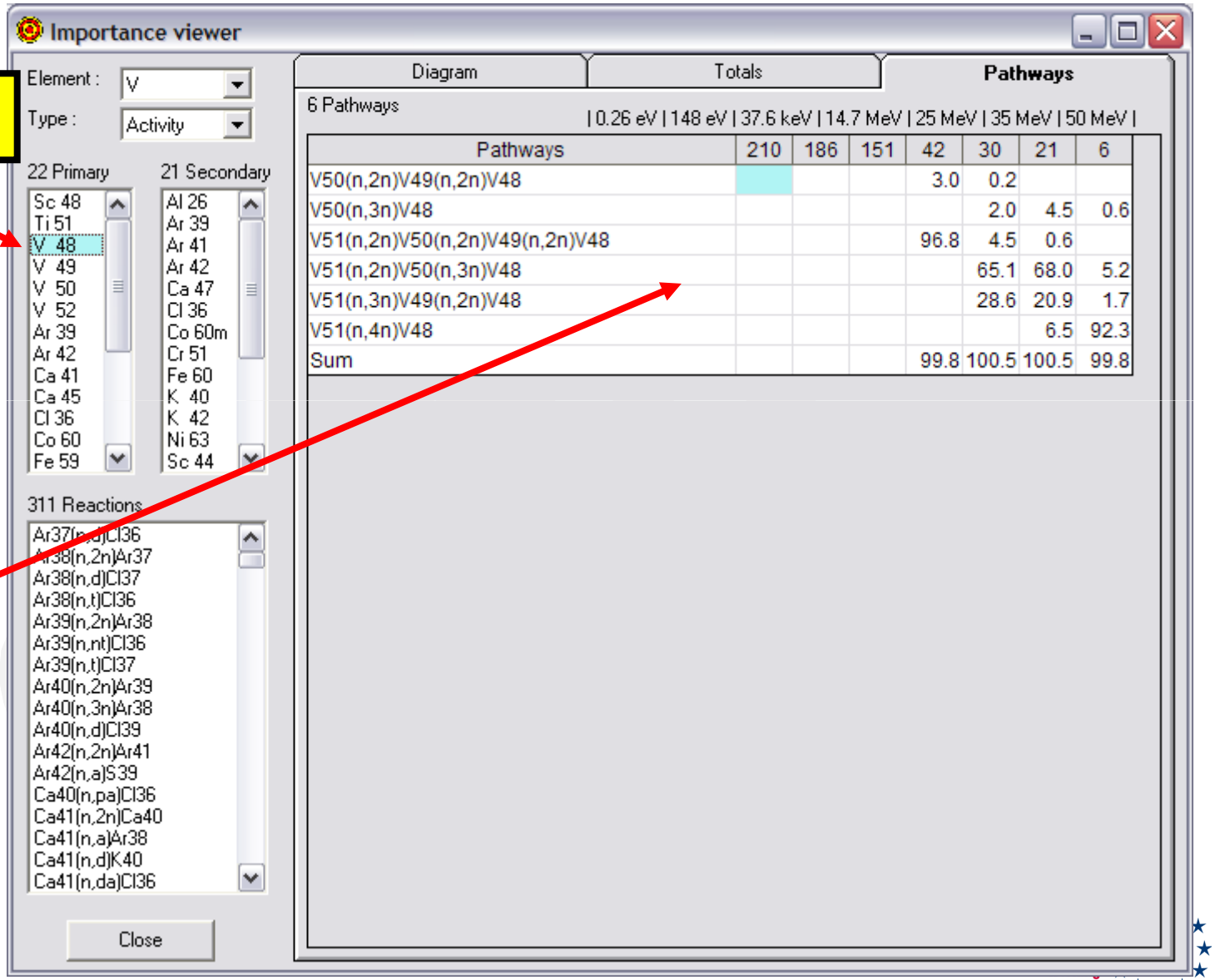
Importance viewer (2)

Primary nuclide

Pathway contributions at various energies



Validating and testing EAF libraries

- Consider only the n-induced data in EAF-2007
- Huge number (65,565) of reactions
- All methods of testing are built into SAFEPAQ-II
- Compare with EXFOR (~1,800 reactions)
- Compare to integral data (470 reactions)
  - "Decay Power: A Comprehensive Experimental Validation" 184p, CEA-R-6213, 2009
  - "Validation of EASY-2007 using integral measurements" 564p, UKAEA Fus 547, 2008
  - Validation of EASY-2005, -2003, -2001, FENDL/A-2.0 reports, numerous EFF docs
- Only a small fraction of library can be compared to exp.
- Statistical Analysis of Cross Sections (SACS) method

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New SAFEPAQ-II tools

- Verification and validation of very large EAF library is difficult – need for additional tools
- Systematics show that cross sections at particular energies have a good correlation with parameters such as *A* or $s = (N - Z) / A$
- Work on maximum cross sections by Manokhin for (n,2n) shows similar trend
- SAFEPAQ-II can extract such data from EAF or one of the data sources (such as TALYS) and display a scatter plot against *A*, *Z* or *s*
- Line of best fit can be added and reactions discrepant from the trend identified

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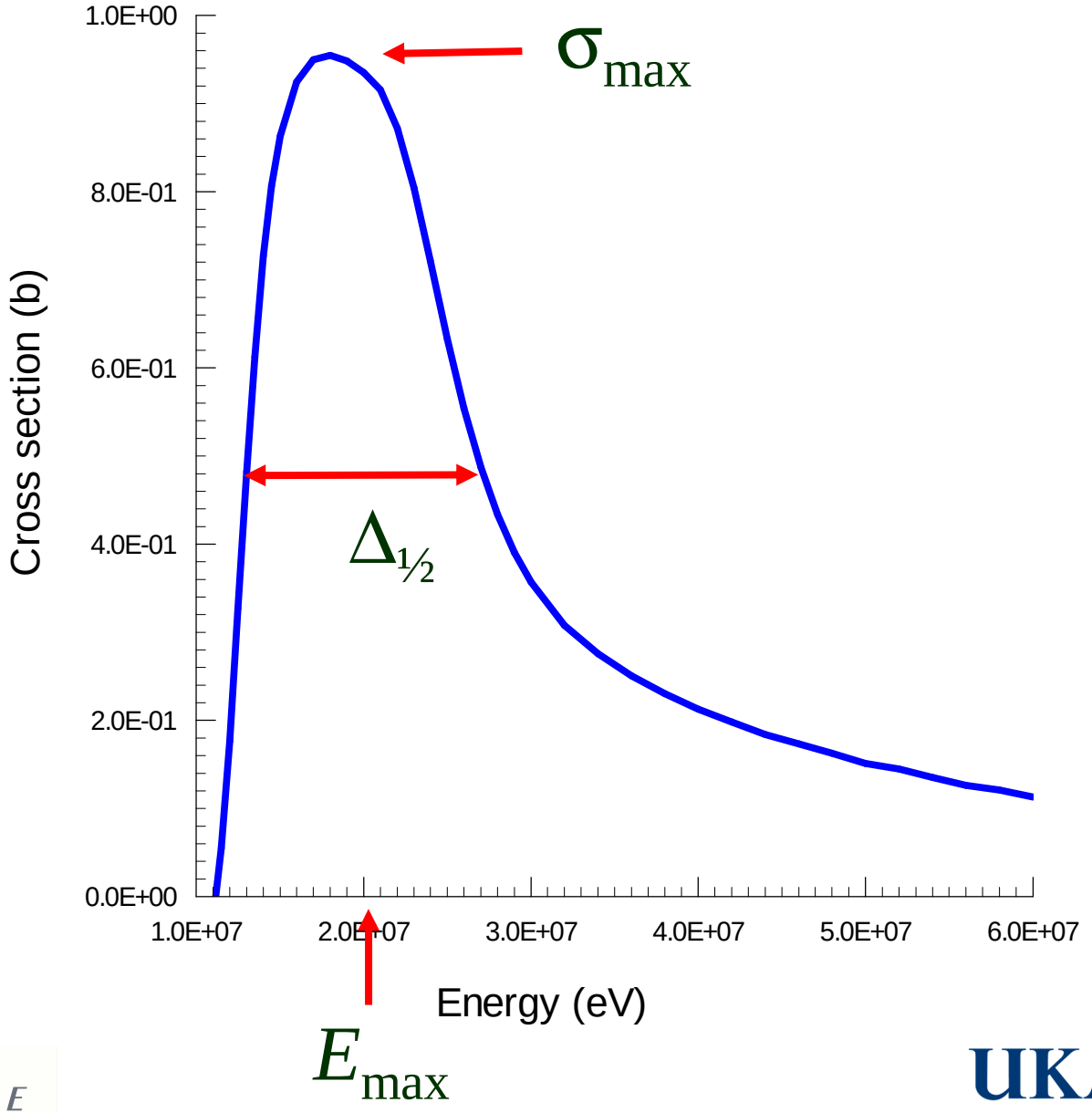
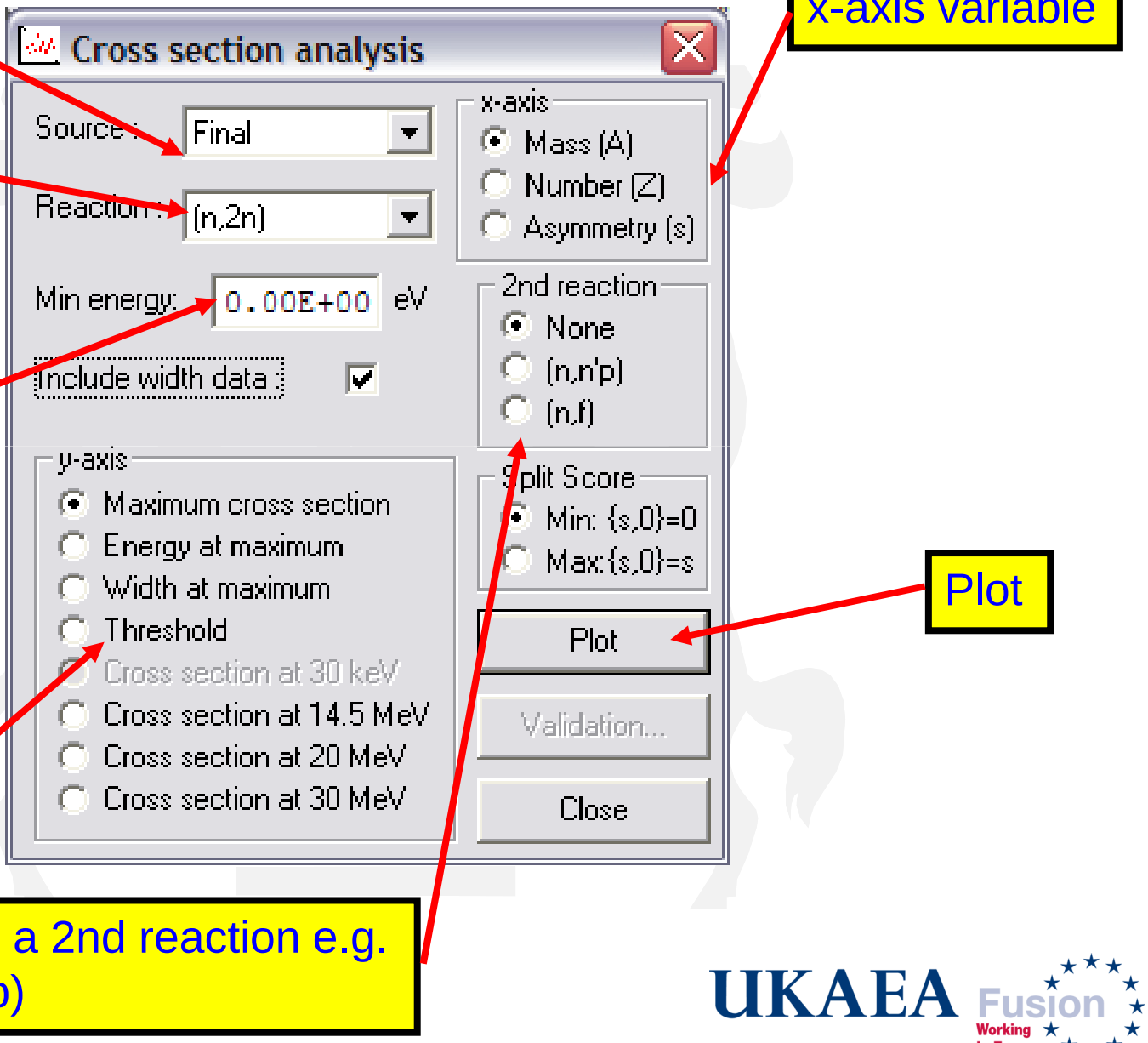
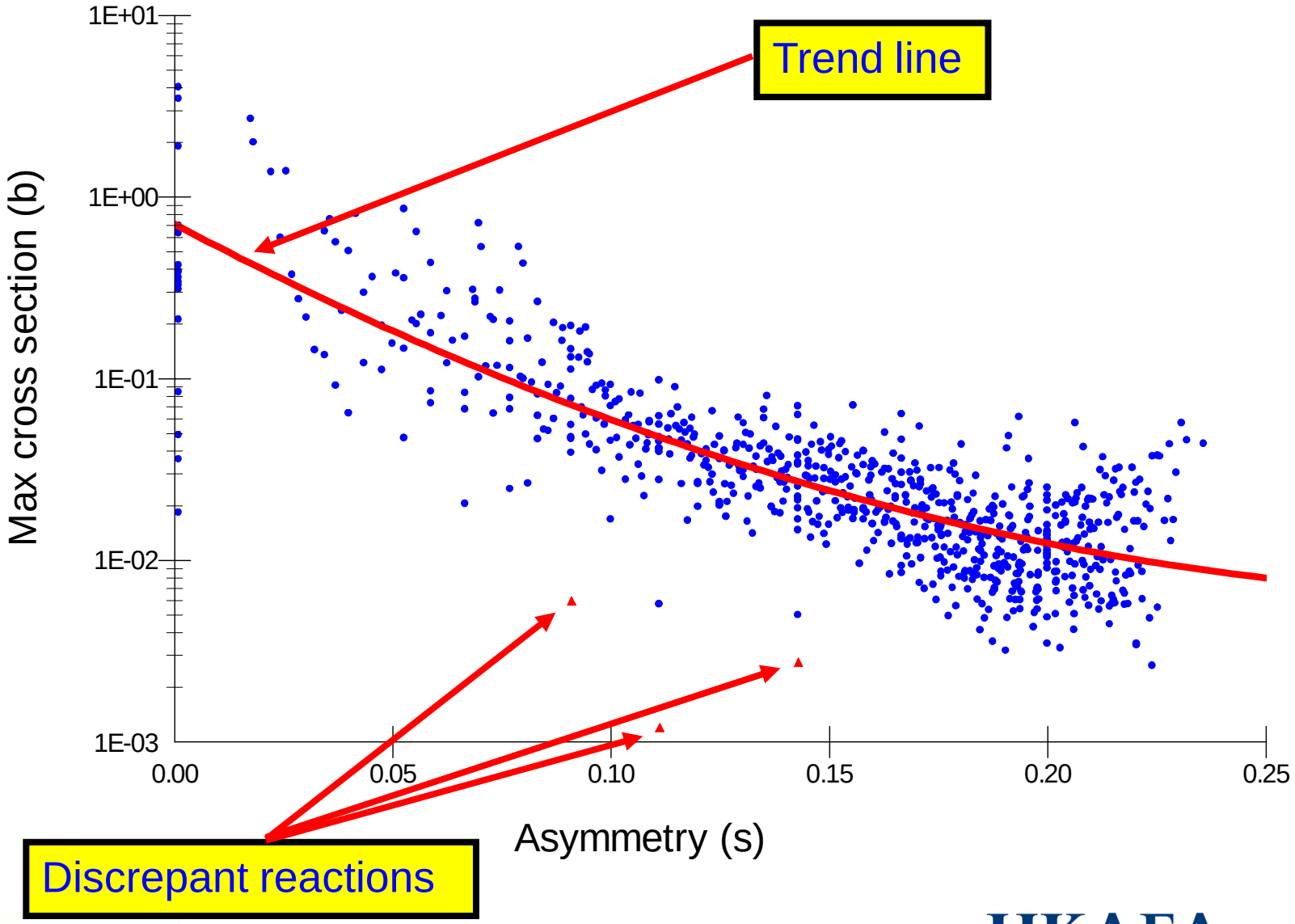
Definition of statistics



Cross section analysis



EAF-2005 – $\sigma_{max}(s)$ for (n,p)



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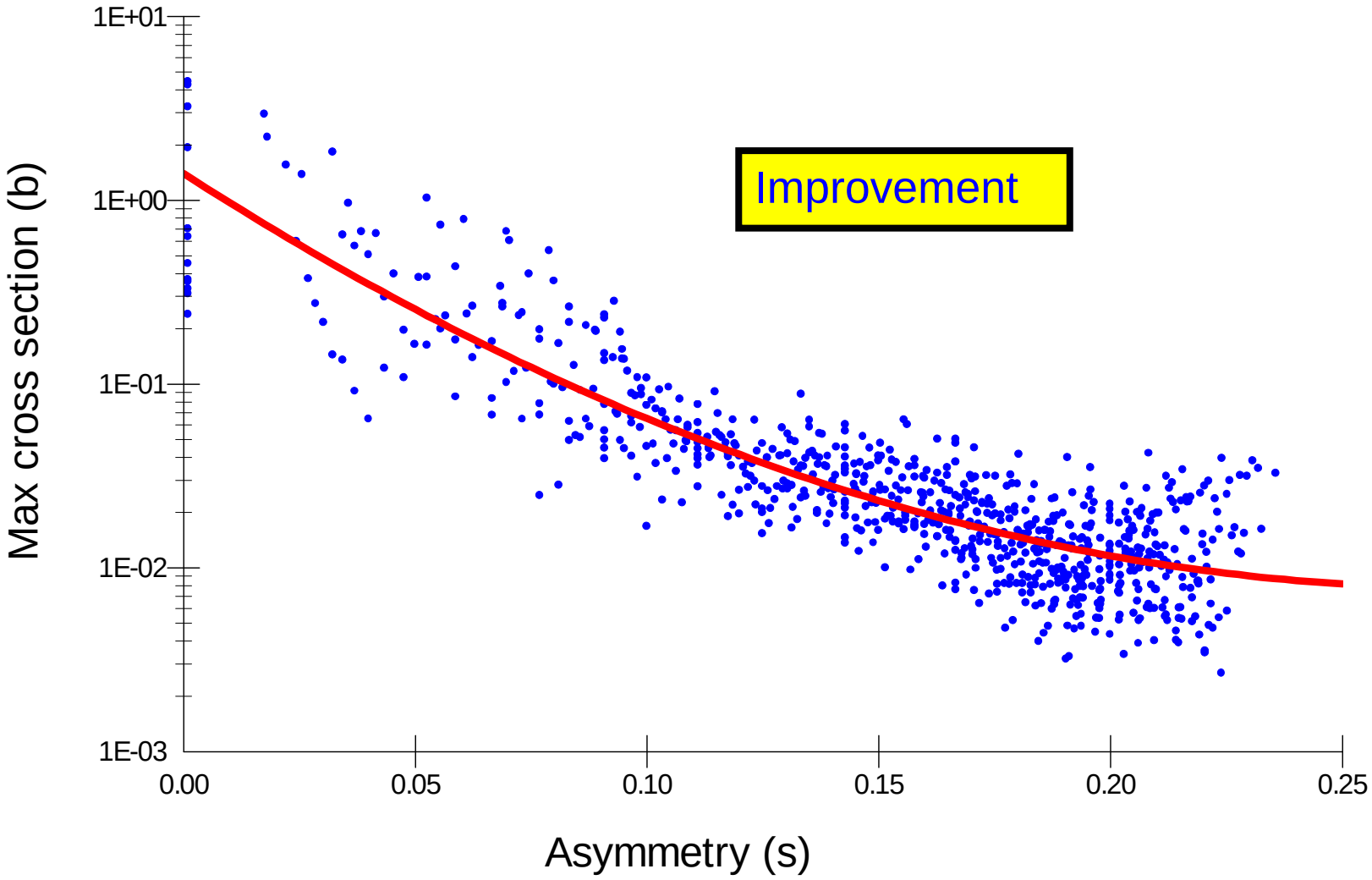
EAF-2007 – $\sigma_{max}(s)$ for (n,p)



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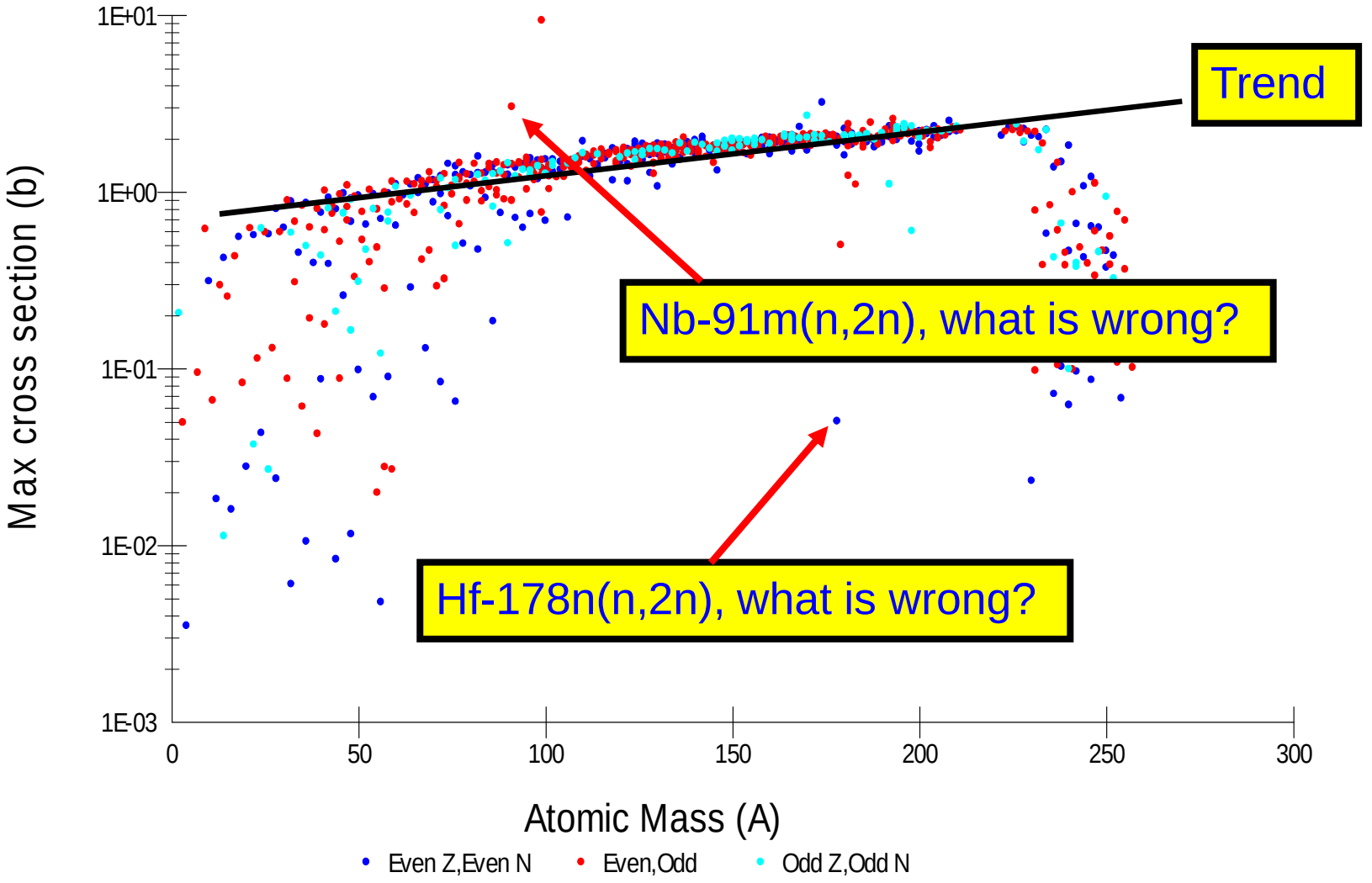
Maximum cross section - (n,2n) for EAF-2005



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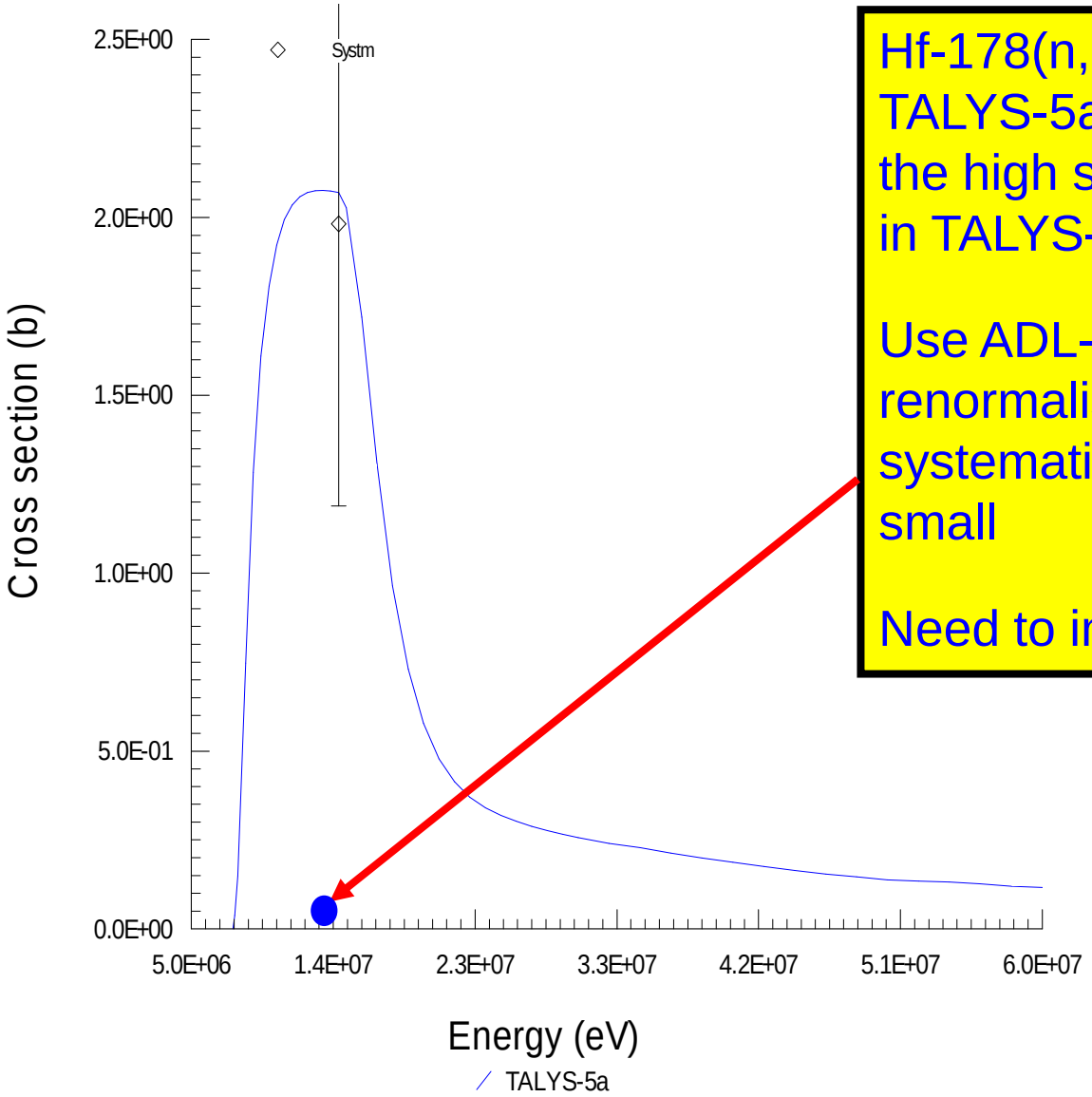
^{178}Hf(n,2n) and ^{178m}Hf(n,2n)



Hf-178(n,2n) data from TALYS-5a, but no data for the high spin Hf-178n isomer in TALYS-5a

Use ADL-3, no renormalisation to systematics and data very small

Need to improve

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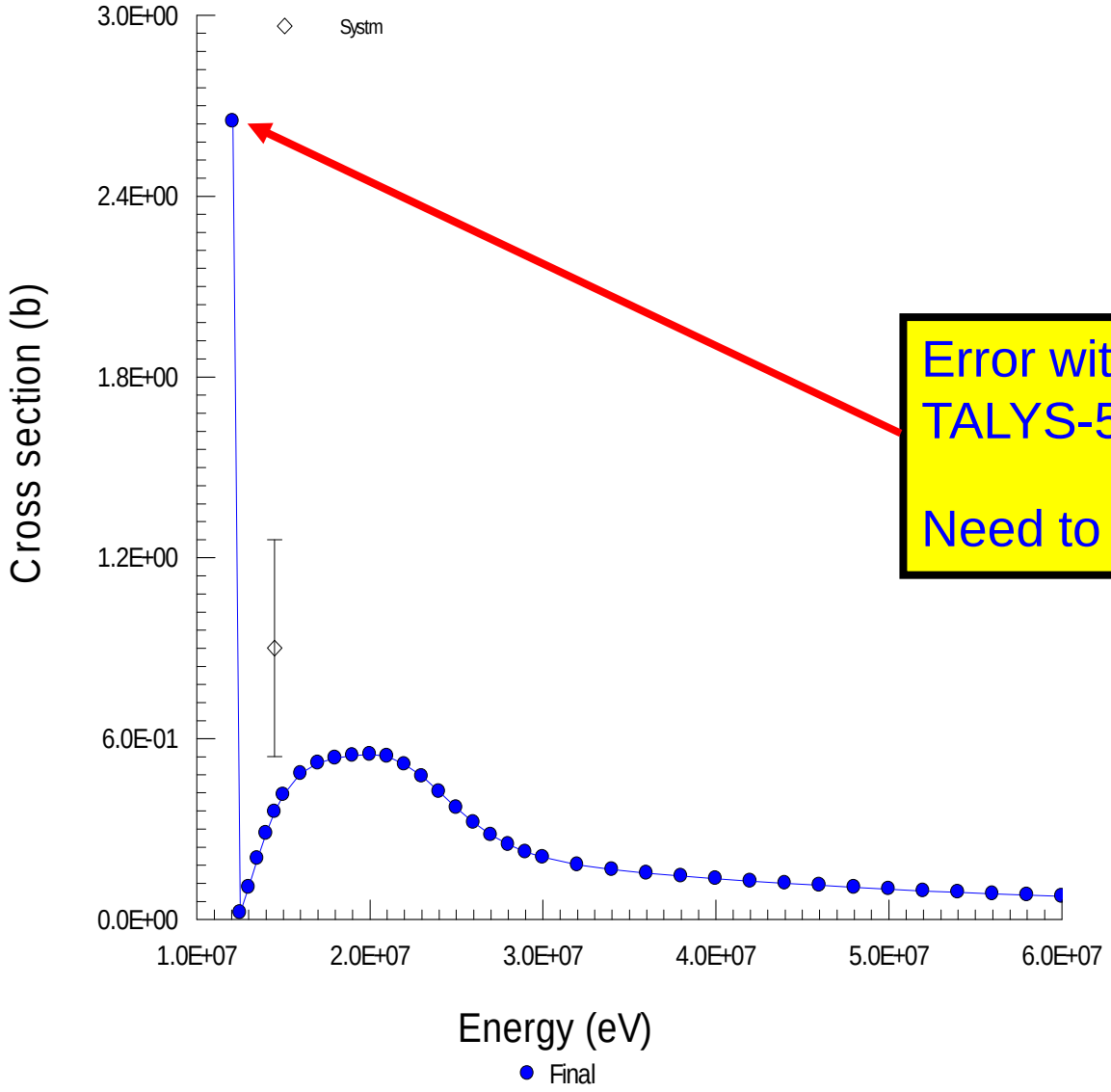
$^{91m}Nb(n,2n)^{90g}Nb$



Error with first point in TALYS-5, should be 0

Need to improve

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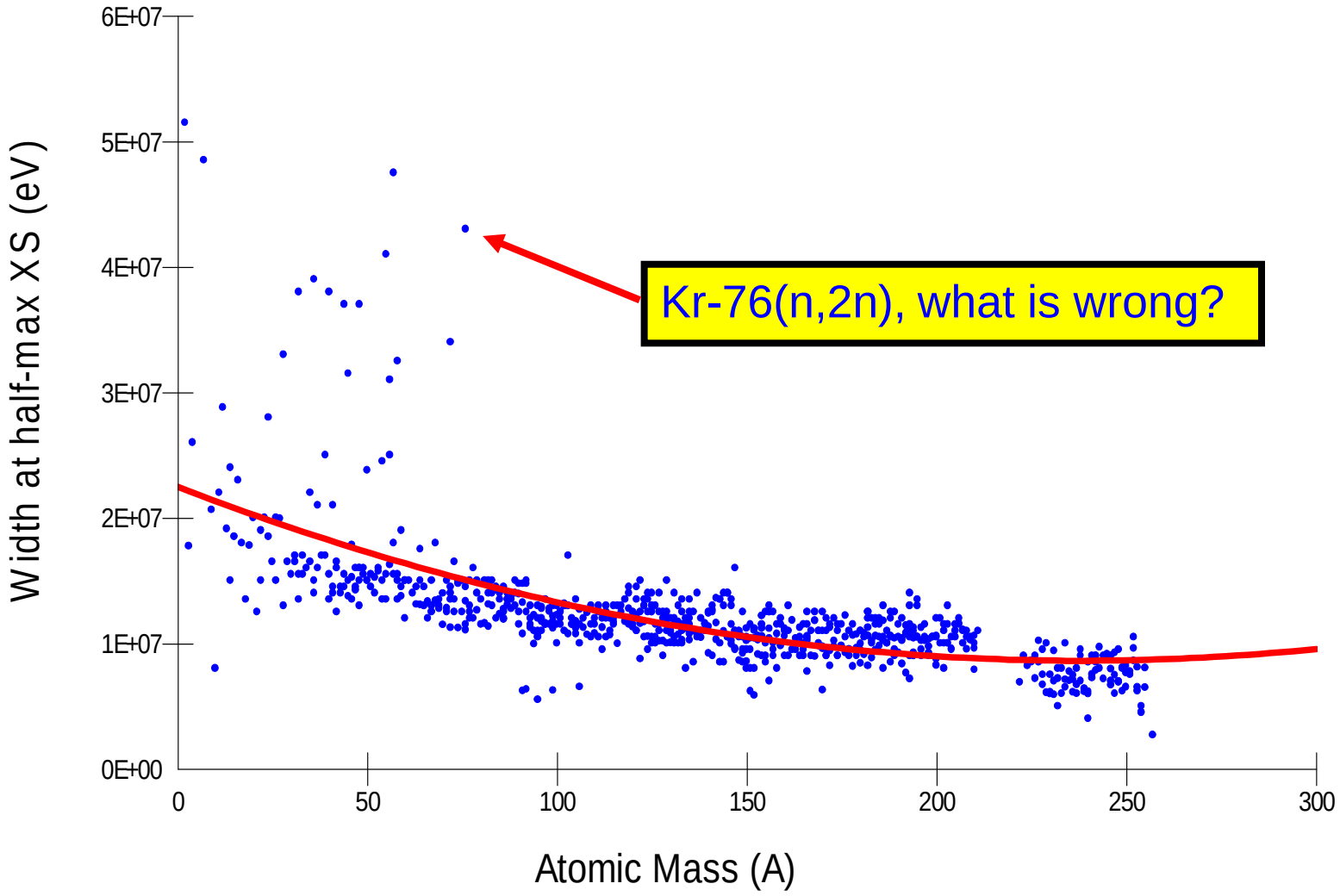
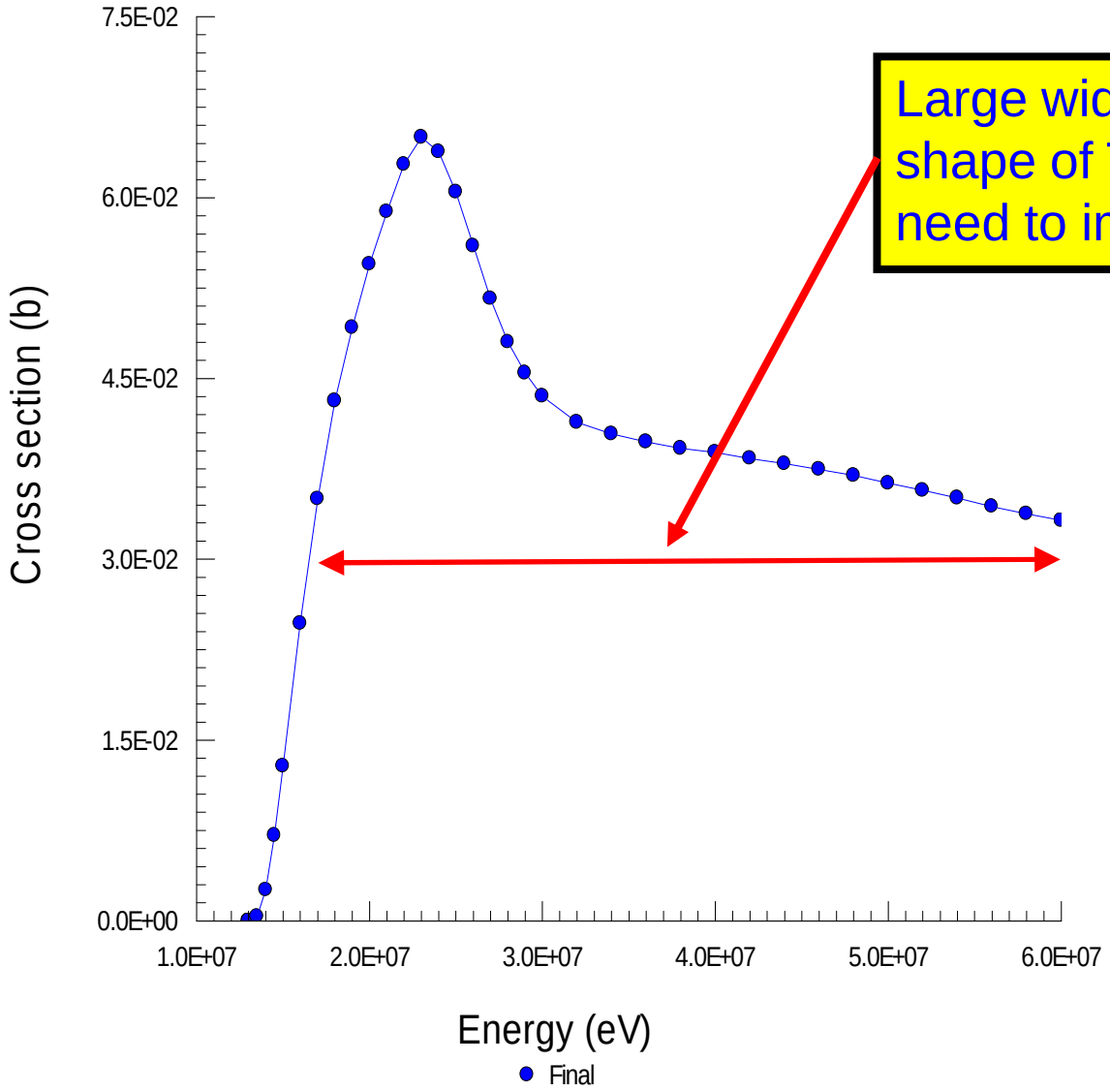
Width at half-maximum - (n,2n) for EAF-2005



$^{76}Kr(n,2n)^{75}Kr$



Large width is due to shape of TALYS-5 data, need to improve?

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From EAF-2005 to EAF-2007

- Improvements over EAF-2005(.1) due to
  - Integral data validation
  - SACS
  - New data sources
  - New measurements

- Improvements over EAF-2005 due to
  - Obvious errors such as these were corrected
  - Maintenance release at beginning of 2006
  - Corrected 250 reactions
  - Includes d-induced data

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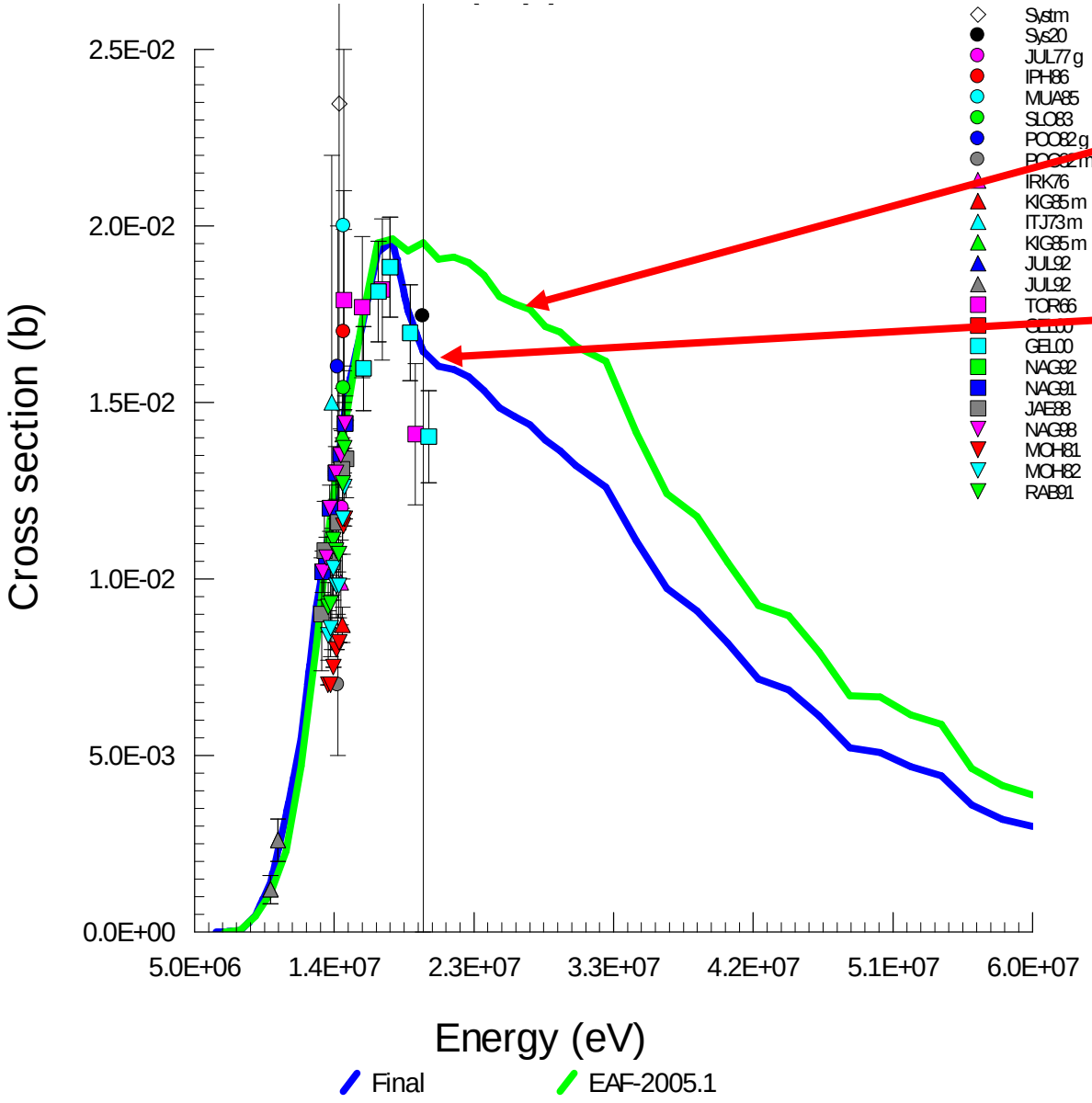
Use of new source – JEFF-3.1 for $^{50}Ti(n,p)^{50}Sc$



EAF-2005.1

EAF-2007

EAF-2007 use JEFF-3.1 + TALYS-6 renormalised

Agrees with recent Geel data

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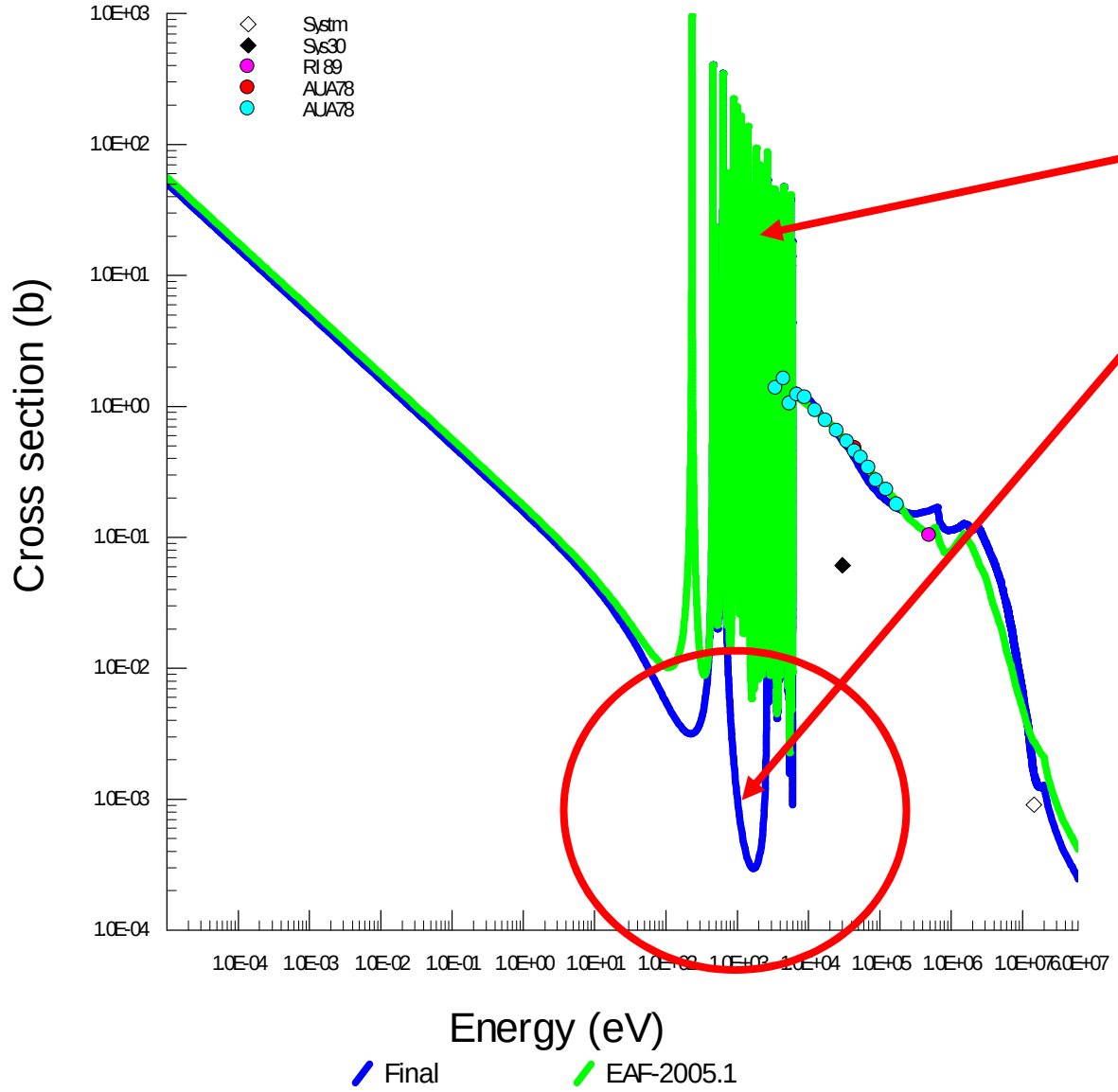
Use of new source – ENDF/B-VII for $^{106}Cd(n,\gamma)^{107}Cd$



EAF-2005.1

EAF-2007

EAF-2007 use ENDF/B-VII + TALYS-6 renormalised

Better resonance data

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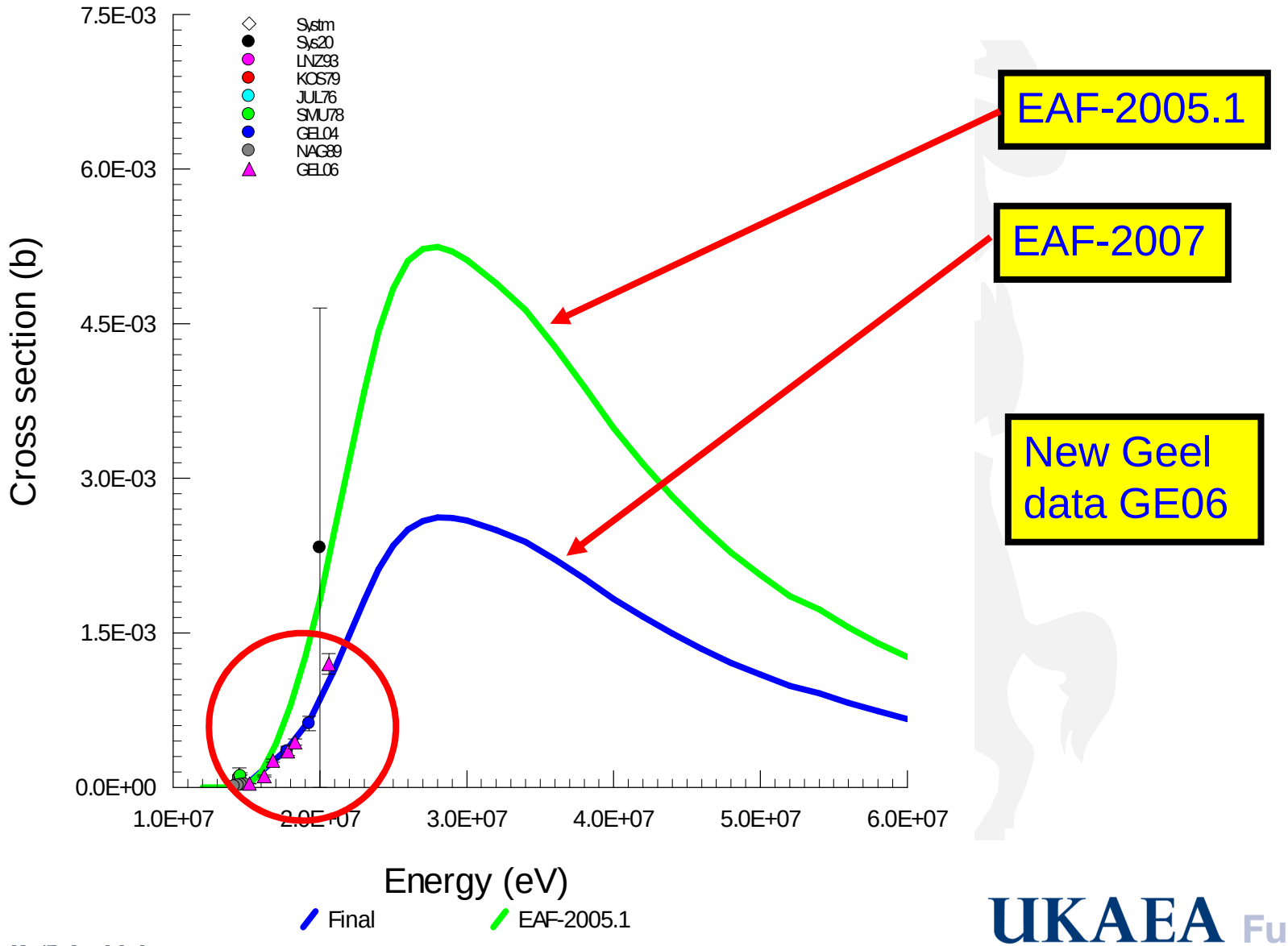
$^{58}Ni(n,t)^{56}Co$



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EAF-2007 deuteron-induced cross sections

- IFMIF uses high energy d beams on a flowing lithium target
- Corrosion products in the lithium means that reactions of d with a wide range of elements possible
- Need to be able to calculate the d-induced activation
- Calculated data from model code TALYS used for most data
- Improvements over EAF-2005.1 due to
  - New data sources
    - 66,274 from TALYS-6d (global)
    - 219 from NIPNE-d (local)
    - 346 from TALYS-d (global)
    - 21 from ACSELAM-d (ALICE)
    - 4 from FENDL/C-2
  - Additional targets (H, He)
  - Renormalisation to EXFOR for 33 reactions

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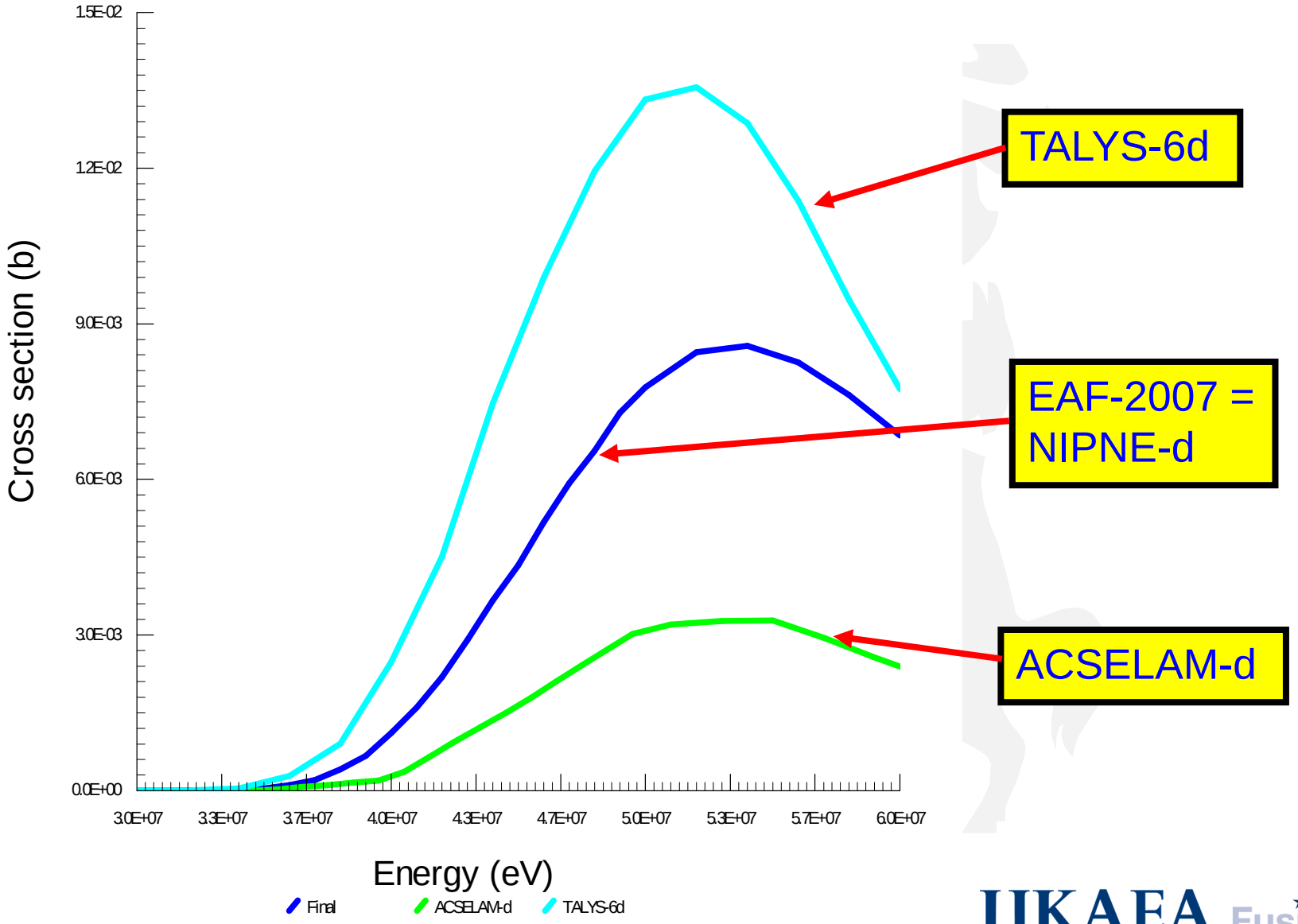
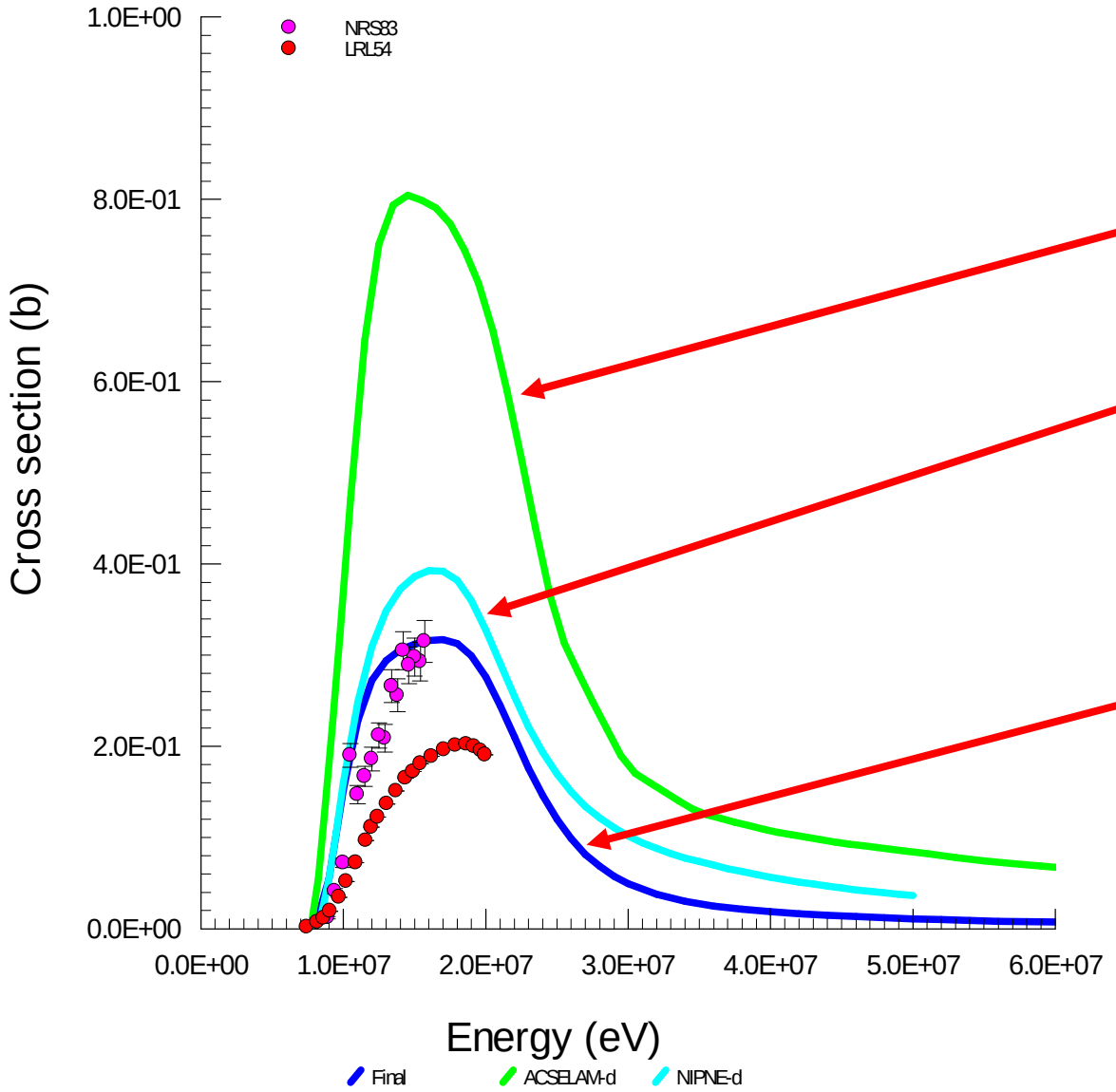
Large variation between sources – $^{63}Cu(d,2n2\alpha)^{55}Fe$



EXFOR discrepant – $^{56}Fe(d,2n)^{56}Co$



ACSELAM-d

NIPNE-d

EAF-2007
=TALYS-6d

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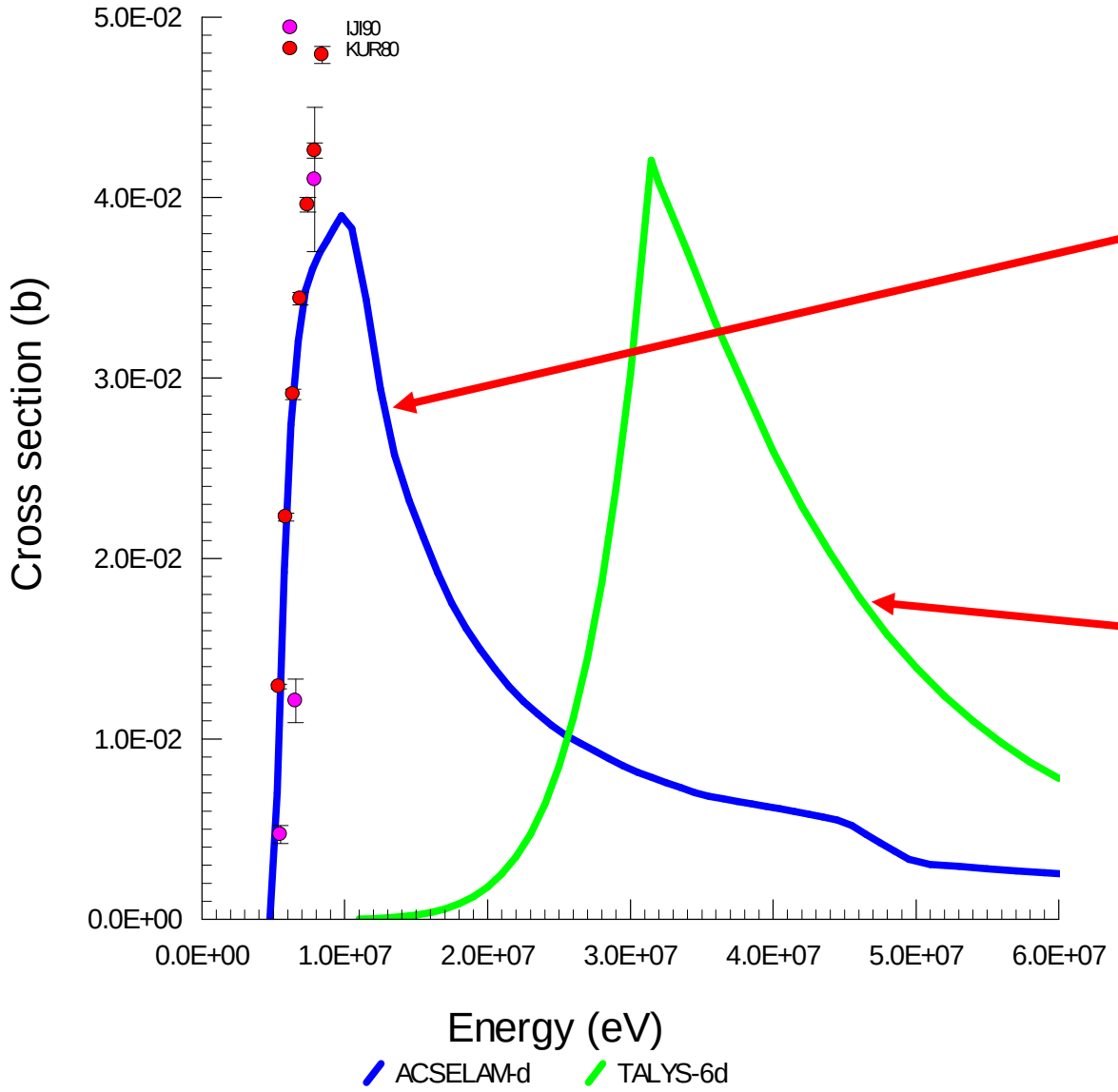
Missing from EAF-2005.1 - $^{7}Li(d,2n)^{7}Be$



EAF-2007 = ACSELAM-d

TALYS-6d

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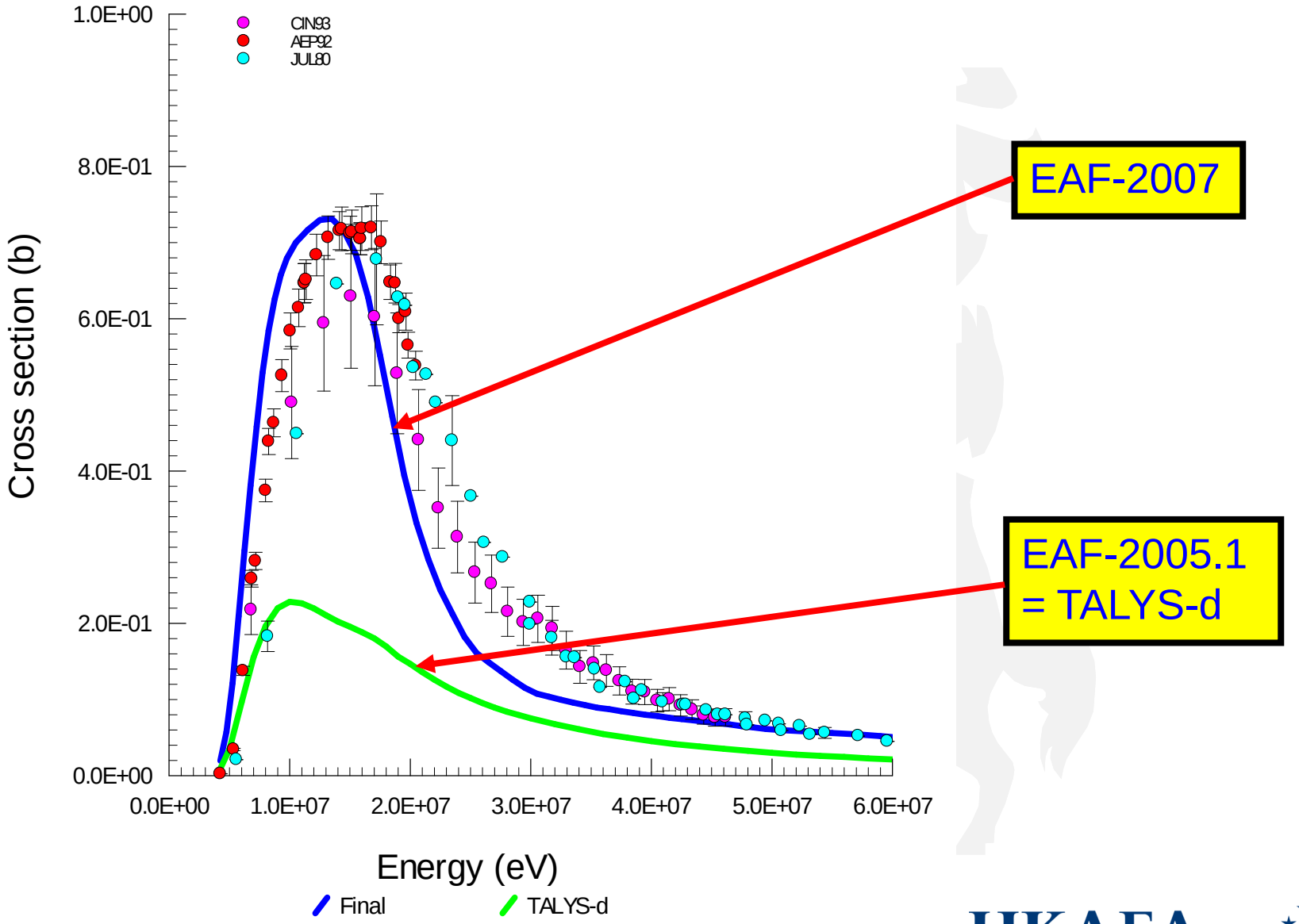
Improvement over EAF-2005.1 – $^{51}V(d,2n)^{51}Cr$



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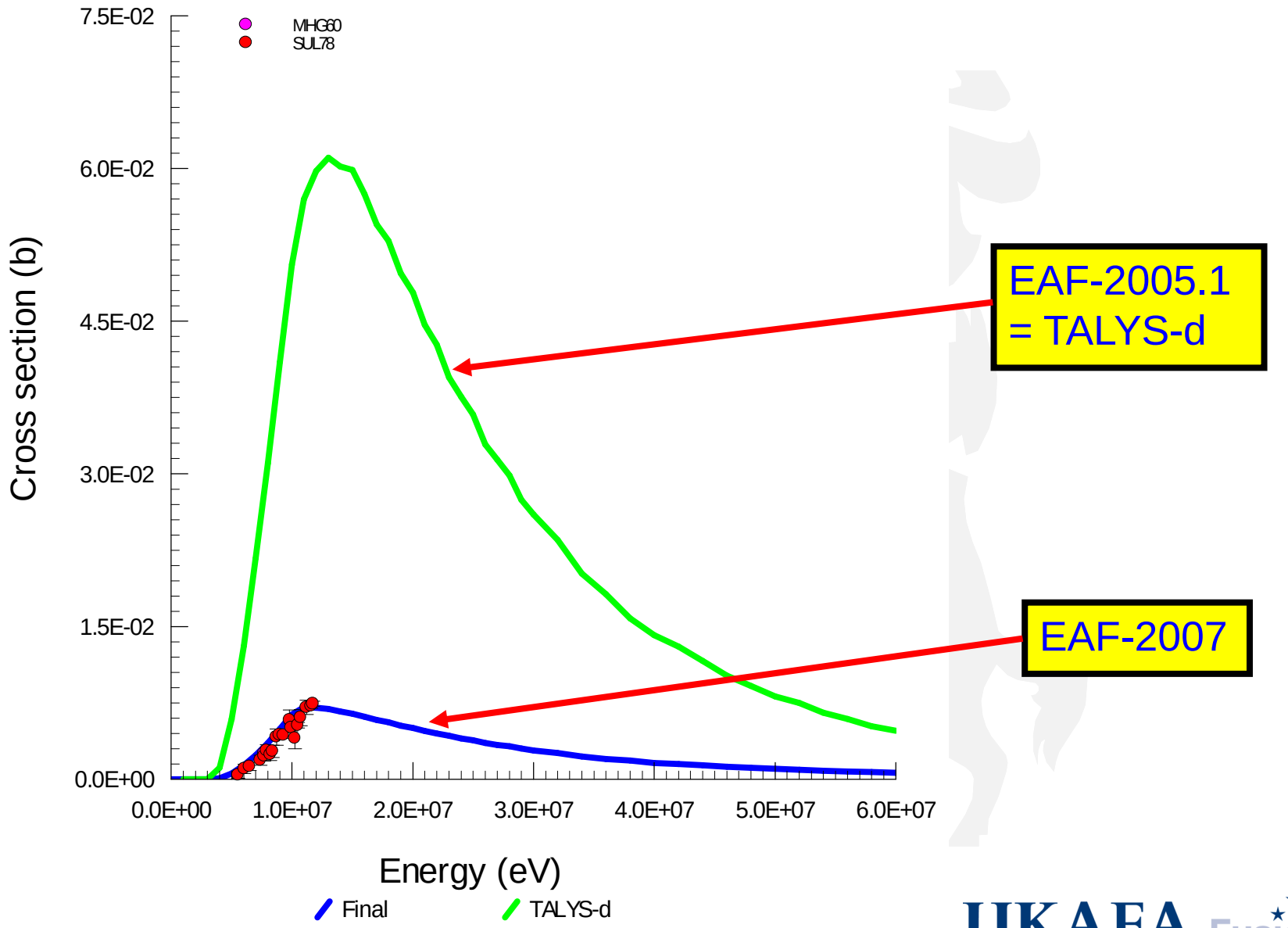
Improvement over EAF-2005.1 – $^{98}Mo(d,\alpha)^{96}Nb$



EAF-2007 proton-induced cross sections

- First time in EAF
- Included because in testing phase of IFMIF H^+ or H_2^+ rather than D^+ beams will be used
- Calculated data from model code TALYS used for all data
- Comparison with EXFOR, but no renormalisation

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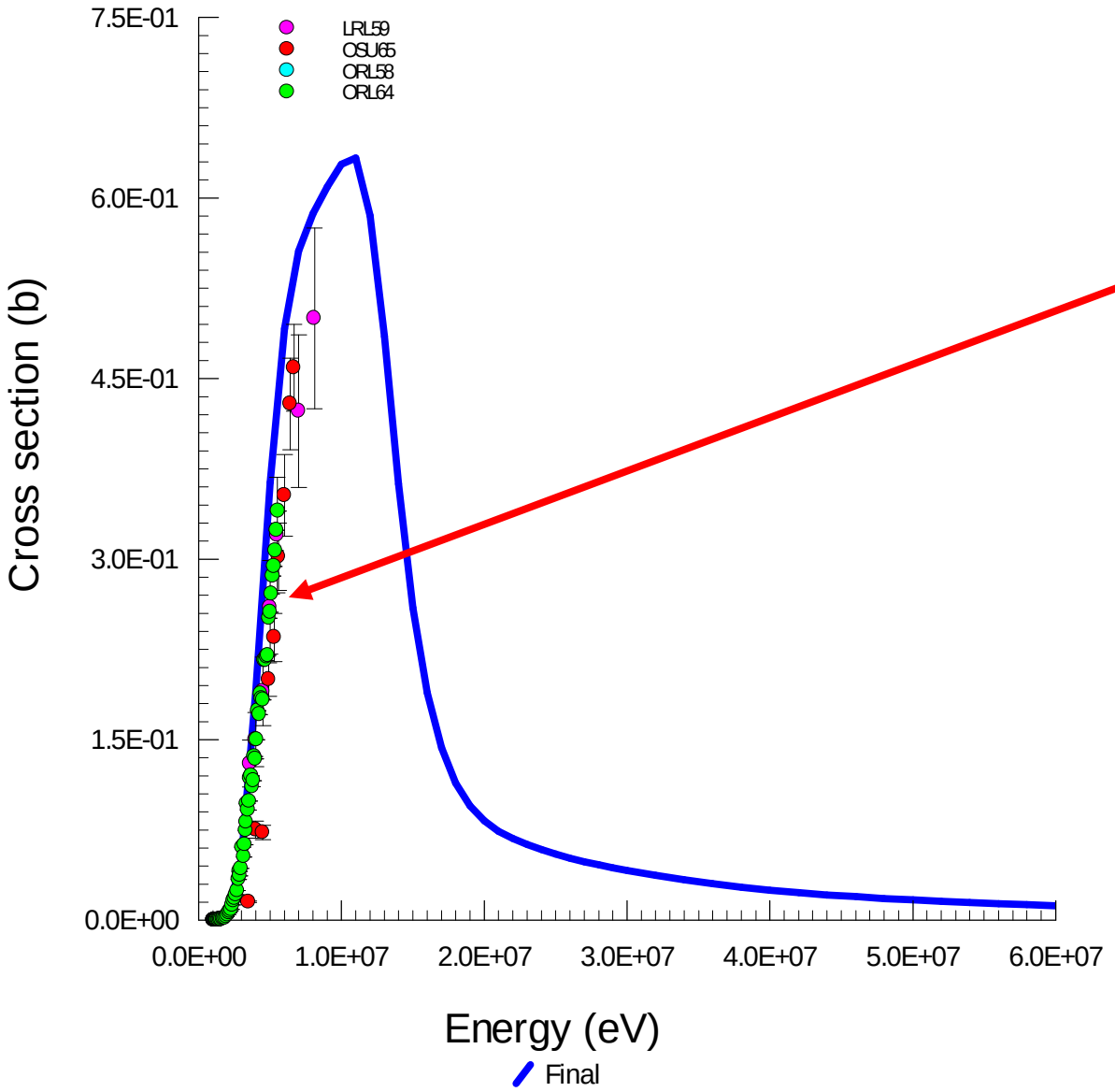
$^{55}Mn(p,n)^{55}Fe$



Good agreement with EXFOR

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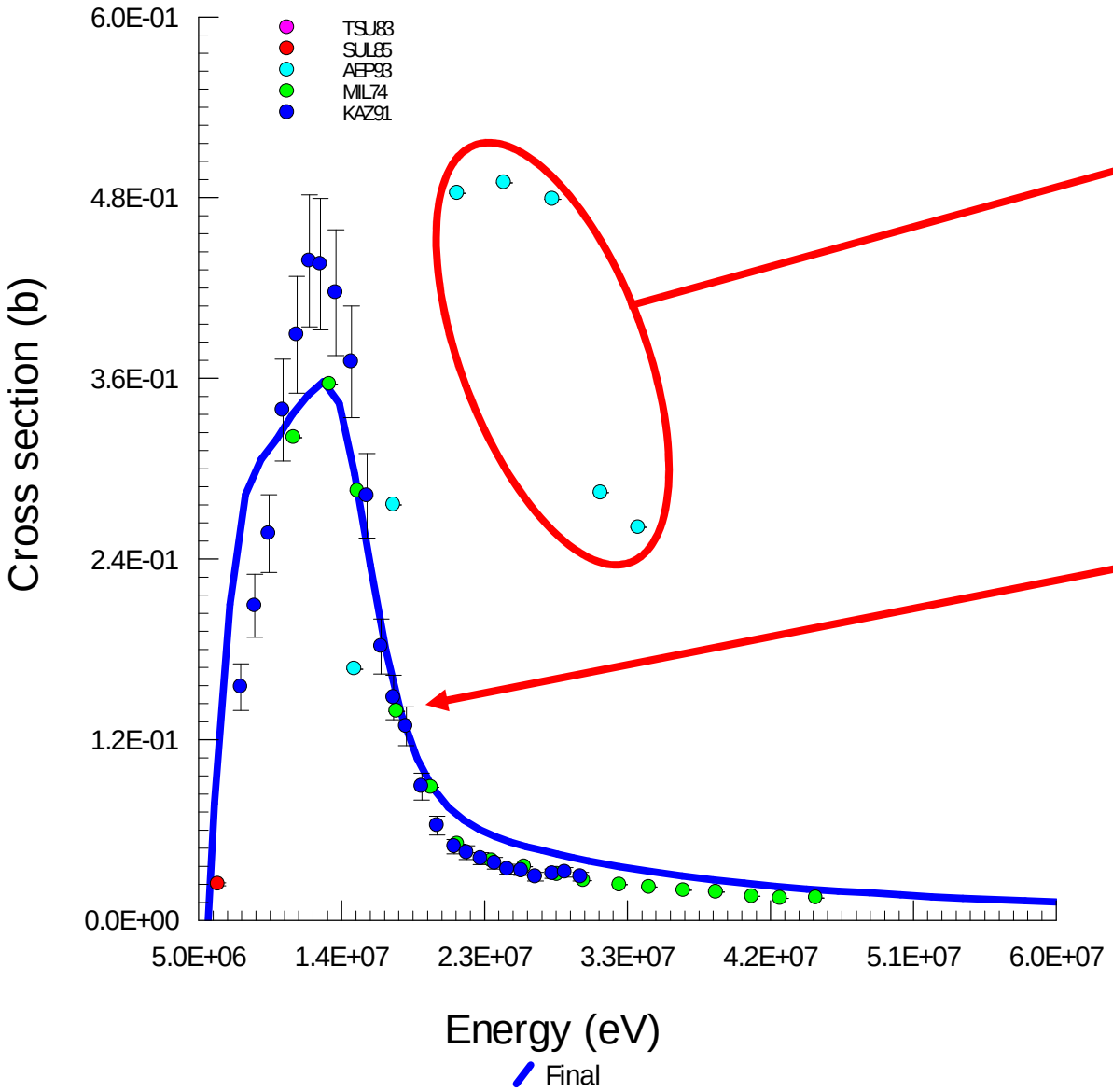
$^{56}Fe(p,n)^{56}Co$



AEP93 data discrepant

Agreement with EXFOR

CADARACHE

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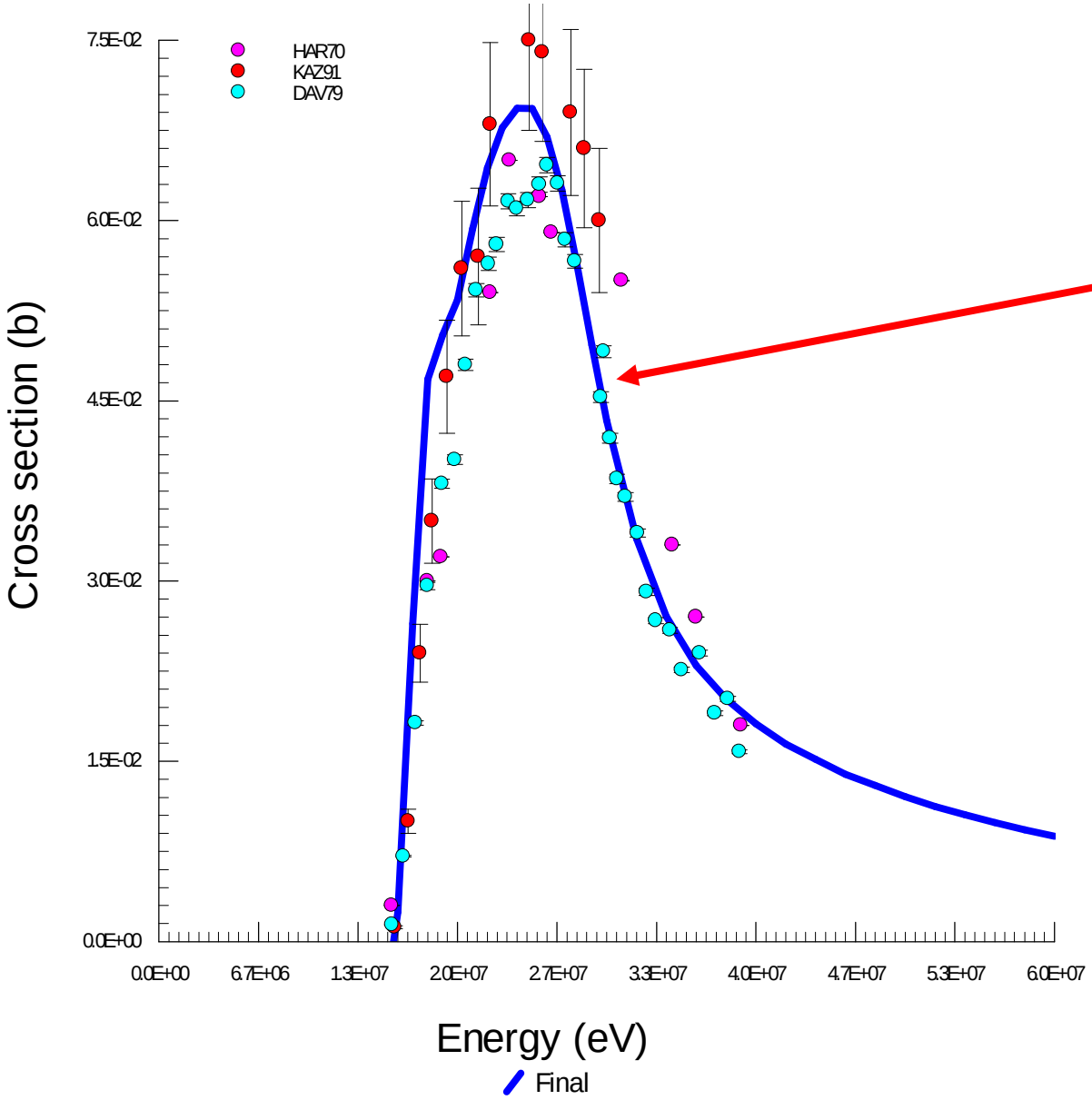
$^{56}Fe(p,2n)^{55}Co$



Excellent agreement with EXFOR

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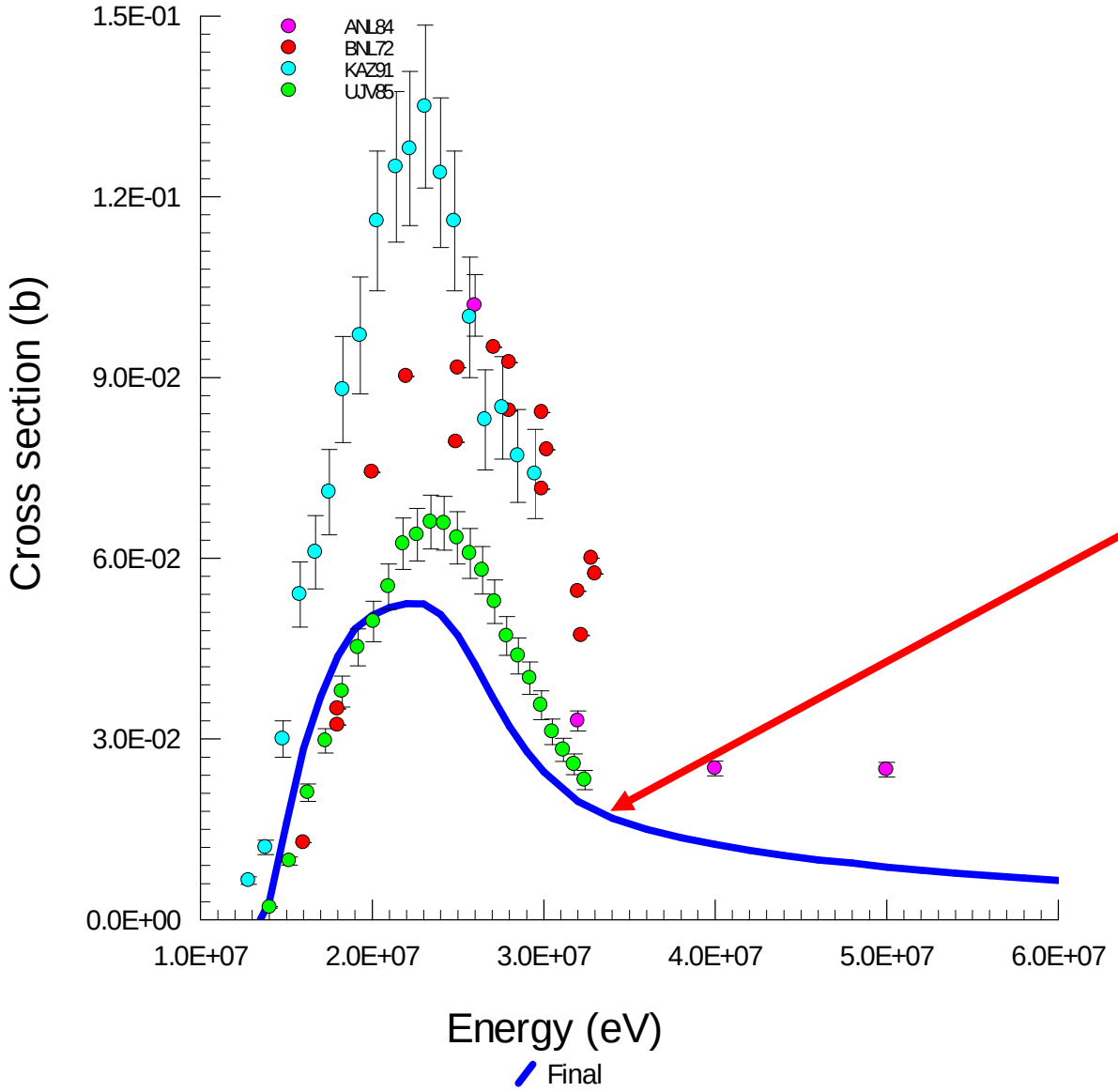
$^{63}Cu(p,2n)^{62}Zn$



EXFOR data discrepant

EAF-2007 low?

Summary

- EAF-2007 contains data up to 60 MeV
- Data for n-, d- and p-induced reactions
  - n- since 1987, with uncertainty
  - d-, p- since 2005, second generation only
- ~ 200,000 reactions
- Validation with integral data important, but only available for few reactions, mainly n- induced
- SACS important for testing large libraries

EAF-2009

- Improvements to n-induced cross section data based on:
  - New data sources
  - New experimental data
  - Feedback from EAF-2007 validation exercise
  - Feedback from SACS analysis
- Decay data improved by 20 new evaluations and use of JEFF-3.1.1
- n-induced data will be improved by use of TALYS code to give uncertainties in ~40 groups for set of important targets
- The complete n-induced uncertainty data will be improved
- FISPACT will also be updated to use the new data
- New d calculations will be used to improve d-induced data
- No plans to improve p-induced data

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EASY-2009

- EAF-2009
- FISPACT is being rewritten in FORTRAN 95 using new algorithm and few approximations, note that the changes will be transparent to the user
- Available March 2010, but is not expected to be distributed until extensive testing and validation have been done
- FISPACT-2009 will (probably) use modified version of current code
- Conversion of User Interface from VB5 to VB.NET (planned, but also may not be available for distribution)
- Documentation
- Distribution as EASY-2009 beginning 2010
- May be called EASY-2010

Conclusions

- SAFEPAQ-II updated, new features
- Activation handbook (EAF-2007) – available from April 2009
- Based on importance diagrams (H-Bi)
- Identifies all dominant nuclides and important reactions
- Importance diagram part in the 2009 User Interface
- SACS analysis tool updated
- 2007 Validation report – feedback
- EASY-2009 planned for beginning 2010

Vision is the art of seeing what is invisible to others- Jonathan Swift (1667-1745)