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Angular distribution: LRF7 processing trails with NJOY2016

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RML-LRF-7 angular distribution processing trails

- Calculation of Legendre polynomials from resonance parameters in RML-LRF7 forms (CSEWG, November 4-7, 2003)
- Implemented in NJOY2010 reconr, based on Nancy Larson's SAMRML code converted to f90/95 style and integrated into NJOY2010 by R. MacFarlane (in 2010)
- The reconstruction generates 0K pointwise cross sections **and** Legendre coefficients up to P8 now
  - MF4-mtx sections are simply added to the NJOY pendf tape
  - At the time Bob made a few patches to Acer to accept the MF4 data and merge it with the ENDF angular data above the RRR
  - Today the new MF4 data is extracted from the reconr pendf tape to be merged with the original ENDF tape above the RRR and create a new ENDF tape
- PREPRO2021 does not handle this type of angular distribution calculation, only the LRF7's MF3

LRF-7 angular distribution processing trails

- In reconr.f90
  - Set the logical, public variable Want_Angular_Dist=.true. then recompile
- Run a “normal” reconr
- Look into the “normally” pure MF3 pendf, MF4 blocks have appear there

- Caveats in reconr Card 4
  - *err* fractional reconstruction tolerance .001\
  - *tempr* as we do not have a method to Doppler broaden Legendre coefficients
  - given on the OK resonance energy grid

19 evaluations using LRF7

- Parity problem *

```
ier    energy-range    lru lrf  method
 1  1.000E-05 1.900E+05   1   7   sammy
 *** Parity problem ***
    Group and channel #    3    1
    Spin, L, Chspin =   -1.0   0    0.0
 *** Parity problem ***
    Group and channel #    3    2
    Spin, L, Chspin =   -1.0   2    1.0
```

- Fe057 samm max legendre order: 0 for mt 51
- Ca40: (n,p0) thresh. glitch
- Pu239 samm max legendre order: 0 for mt 2 102 18

- Fe054 wrong MF1 451 !!

JEFF-4.0T2	ENDF/B-8.1b1	JENDL-5
O016		
Si028	Si028	
Si029	Si029	
Si030	Si030	
Cl035	Cl035	Cl035
	Ca040 **	
Cu063 *	Cu063 *	
Cu065 *	Cu065 *	
Fe054	Fe054	Fe054
Fe057 **	Fe057 **	Fe057 **
	Mo095	
Rh103 *	Rh103	
	W182	
	W183 *	
	W184	
	W186	
Gd155		
Gd157		
	Pu239 *	

JEFF-4.0T2.2 LRF7's MF4

- NJOY2016 pendf's MF4 addition
- lines /2 ~= number of points !! 90986 for Rh103 MF4-mt2
- Fe057 MT51 isotrope below 190 KeV – Thres. 14.6 KeV for mt 51

	MF	MT	Lines
rendf0k/Cl035p.asc	4	2	51579
rendf0k/Cl035p.asc	4	600	51579
rendf0k/Cu063p.asc	4	2	92759
rendf0k/Cu065p.asc	4	2	74207
rendf0k/Fe054p.asc	**4**	**2**	**95377**
rendf0k/Fe057p.asc	4	2	34089
rendf0k/Fe057p.asc	**4**	**51**	**0**
rendf0k/O016p.asc	**4**	**2**	**7929**
rendf0k/O016p.asc	**4**	**800**	**4153**
rendf0k/Rh103p.asc	4	2	181975
rendf0k/Si028p.asc	4	2	13833
rendf0k/Si029p.asc	4	2	7857
rendf0k/Si030p.asc	4	2	10065

Fe054 example (no URR)

```
ier    energy-range       lru  lrf   method
1   1.000E-05  1.036E+06    1    7    sammy
```

samm resonance reactions: **2** 102

samm max legendre order: 0 !! but in fact 4

resolved resonance range upper limit = 1.036E+06 eV.

final maximum energy for broadening/thinning = 1.036E+06 eV

broadened mat2625 from 0.0000E+00 to 2.9360E+02 k

points in= 48582 points out= 32153

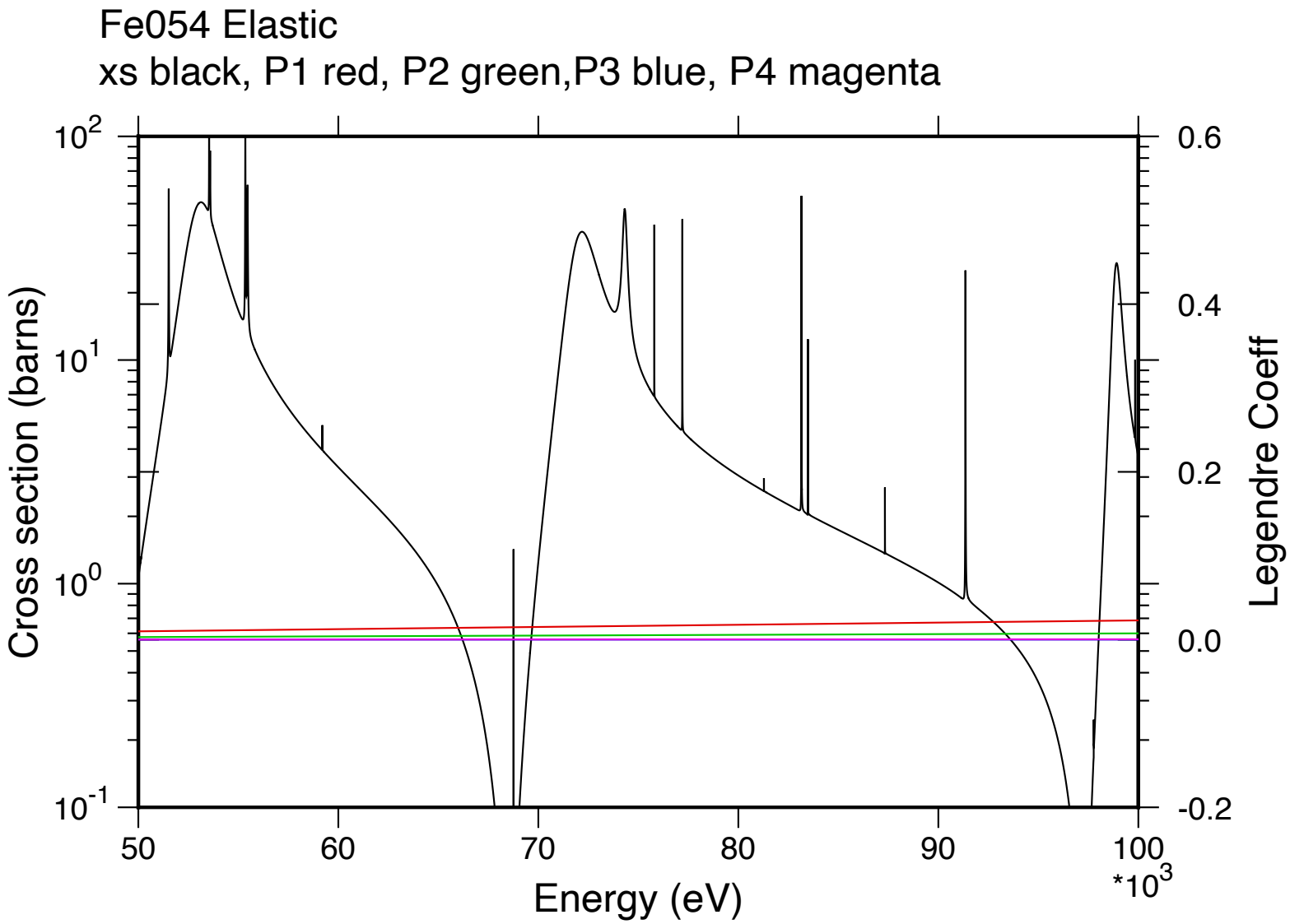
mt **2** 5 102 103 107 600 601 602 603 604 605 606 607 800 801 802 803 804 805 806

Fe054 example (no URR)

- even with err .01 (not the default .001)
- energy grid 18447 points from 1.000000-5 to 1.035999+6 eV
- up to P4 but a_1 = 6.9-12 @ 1.0E-5 !!

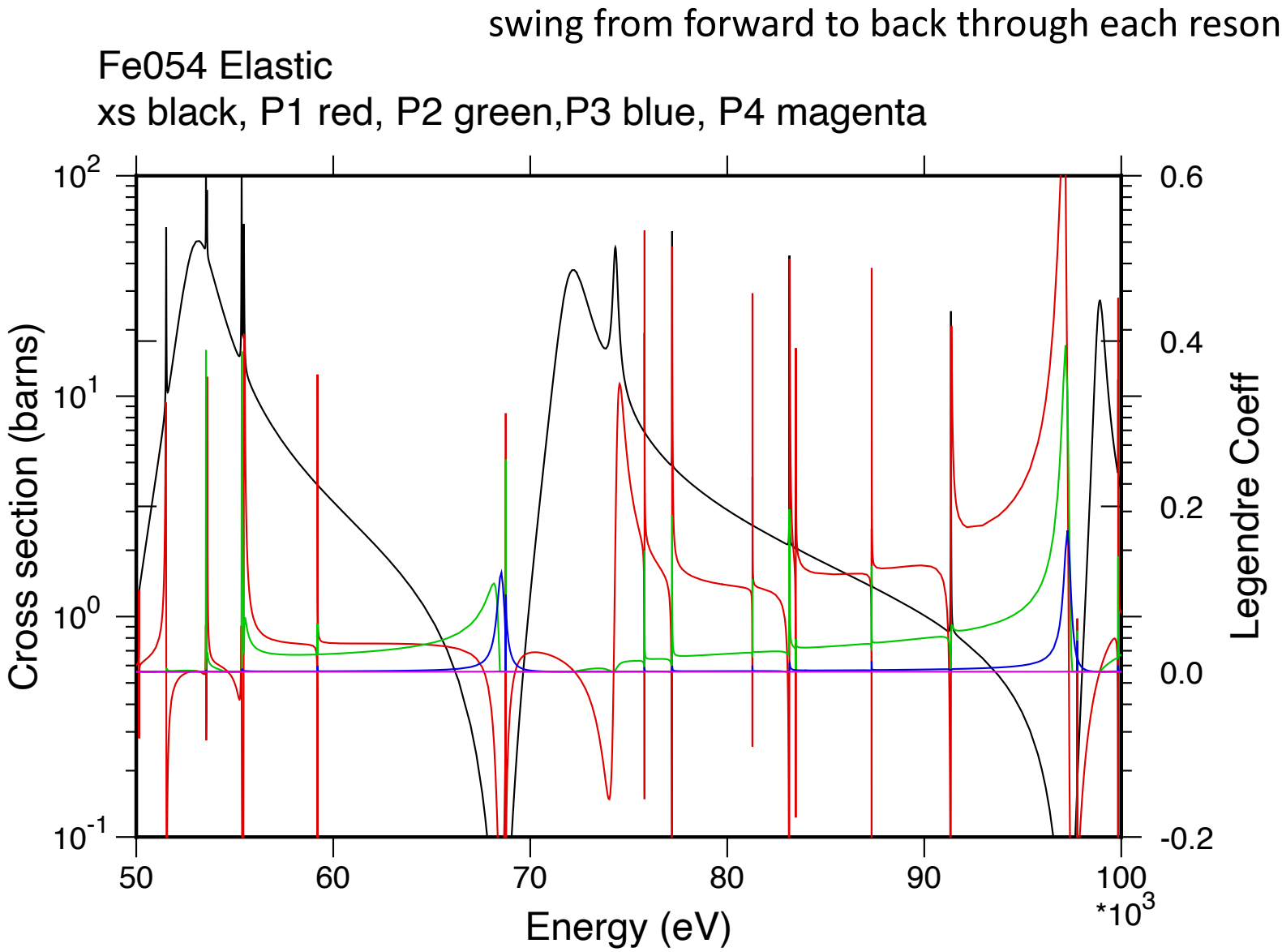
```
 2.605400+4 5.347624+1          0          1          0          02625 4   2
 0.000000+0 5.347624+1          0          2          0          02625 4   2
 0.000000+0 0.000000+0          0          0          1      18447625 4   2
      18447          2                                           2625 4   2
 0.000000+0 1.000000-5          0          0          1          02625 4   2
 6.96064-12                                                       2625 4   2
 0.000000+0 1.125000-5          0          0          1          02625 4   2
 7.83115-12                                                       2625 4   2
 0.000000+0 1.250000-5          0          0          1          02625 4   2
******
******
 0.000000+0 1.035092+6          0          0          4          02625 4   2
 2.612169-2 0.10574953 5.367891-2 8.247226-3                      2625 4   2
 0.000000+0 1.035152+6          0          0          4          02625 4   2
 2.395527-2 0.10620593 5.269484-2 8.011644-3                      2625 4   2
 0.000000+0 1.035273+6          0          0          4          02625 4   2
 2.017353-2 0.10605018 5.057259-2 7.553813-3                      2625 4   2
 0.000000+0 1.035515+6          0          0          4          02625 4   2
 1.278824-2 0.10559563 4.614209-2 6.588903-3                      2625 4   2
 0.000000+0 1.035999+6          0          0          4          02625 4   2
-6.612680-3 0.10839903 3.353650-2 3.630147-3                      2625 4   2
```

Fe054 example original (no URR) 50-100 KeV



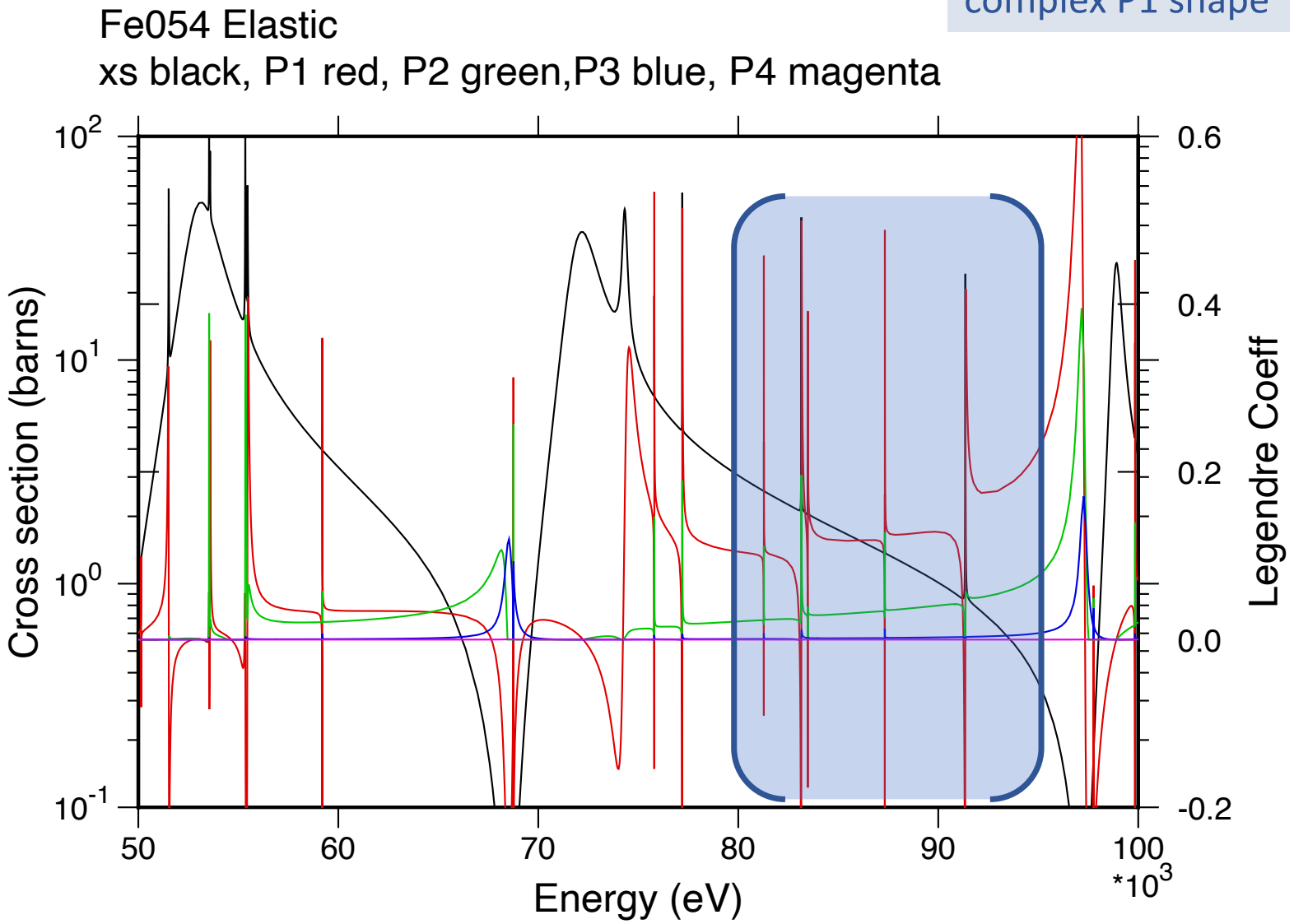
Fe054 example LRF7's MF4 (no URR) 50-100 KeV

swing from forward to back through each resonance



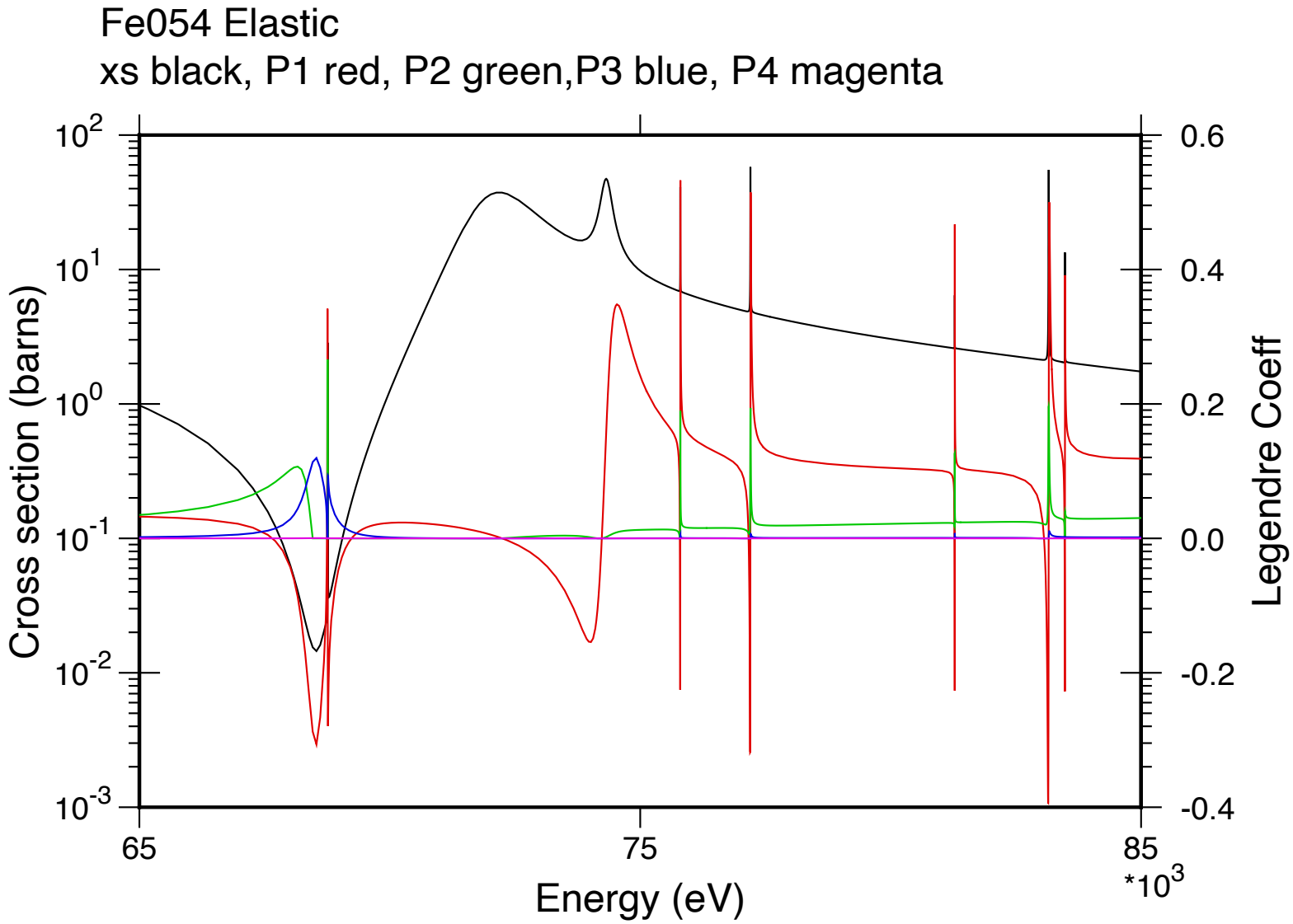
Fe054 example (no URR) LRF7's MF4 50-100 KeV

complex P1 shape

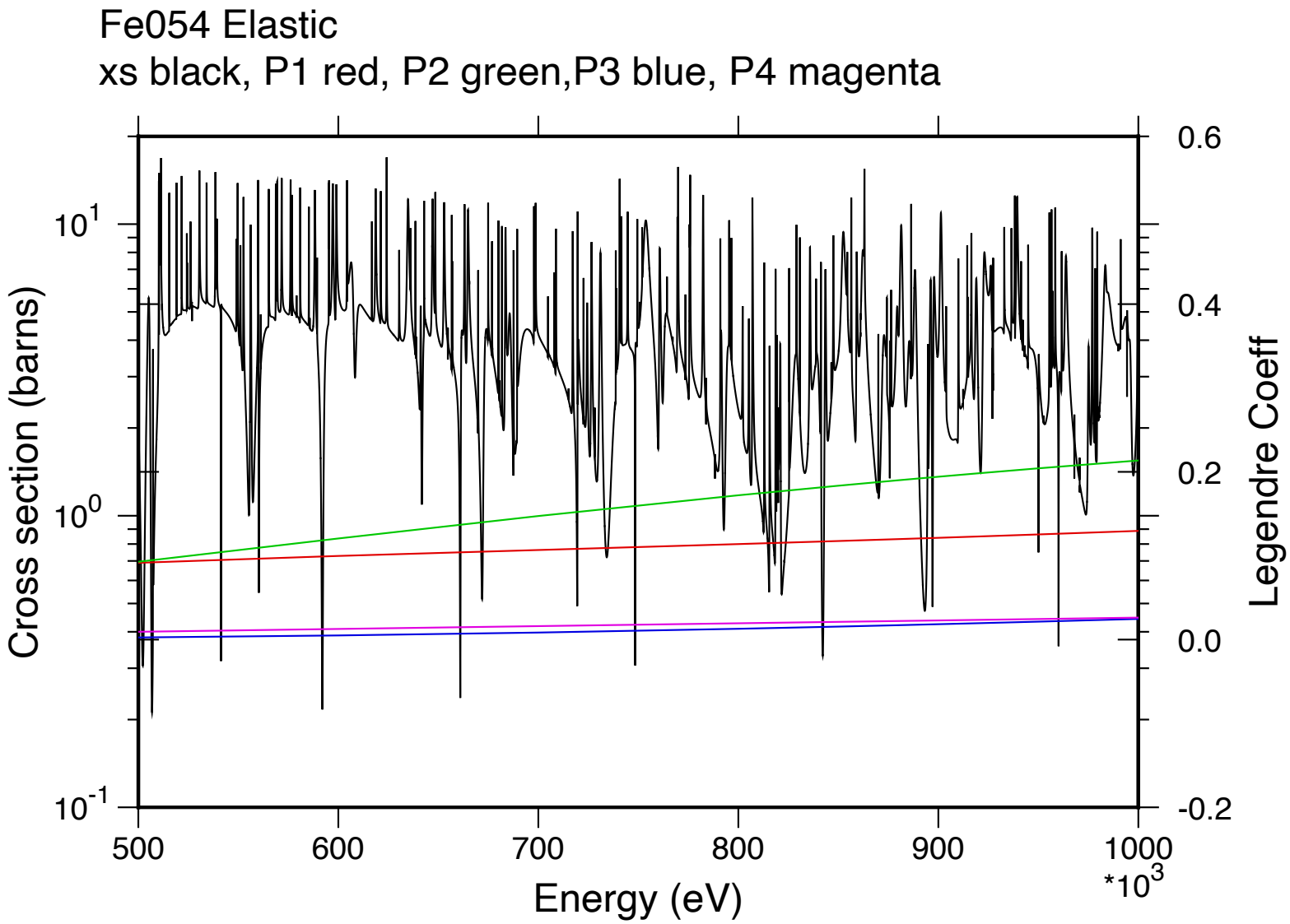


Fe054 example (no URR) LRF7's MF4zoom

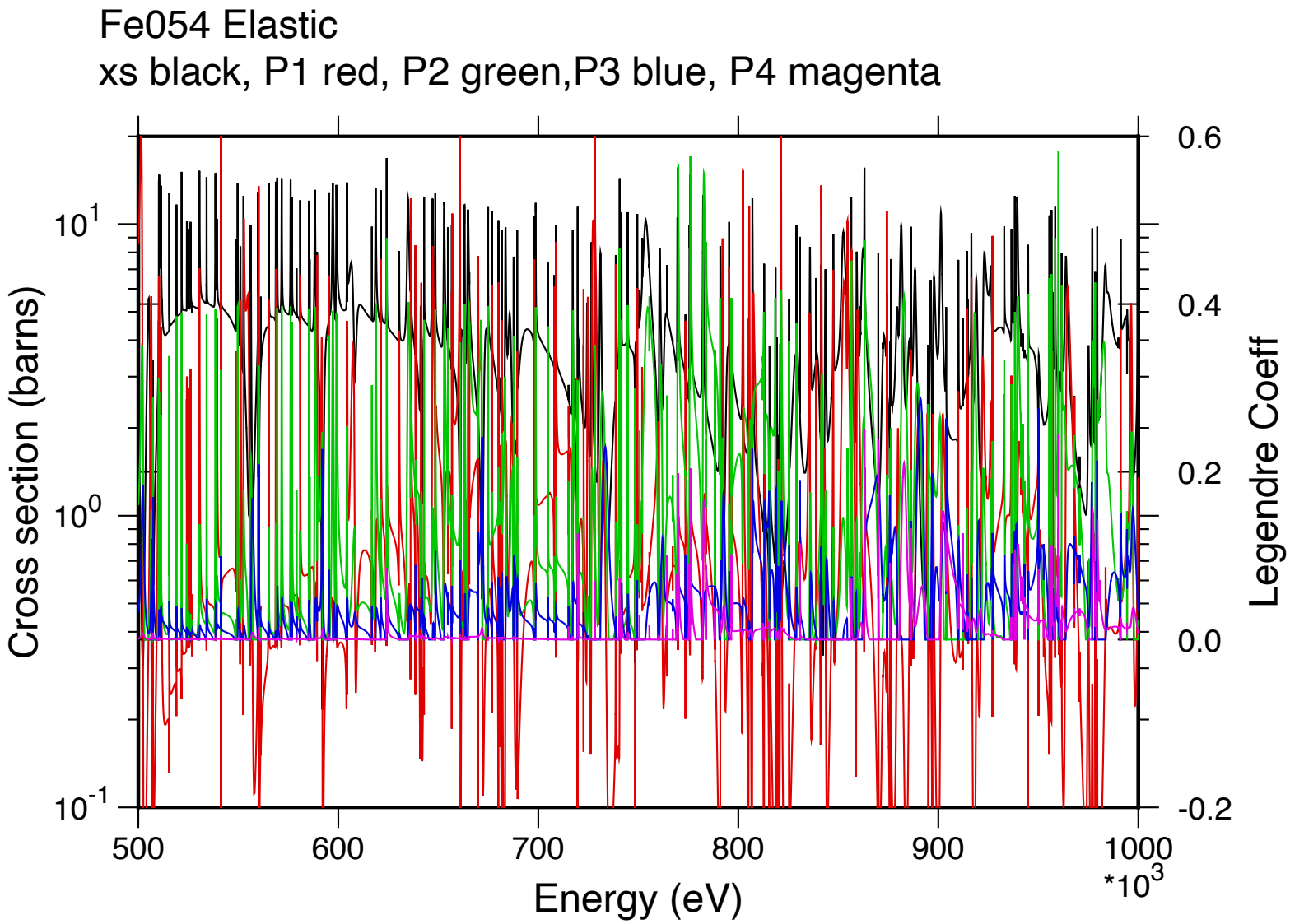
- P's coefficient sharp swings



Fe054 example (no URR) original 0.5 –1 MeV



Fe054 example (no URR) LRF7's MF4 0.5 –1 MeV



O016 example (no URR)

```
ier    energy-range       lru lrf   method
1   1.000E-05 6.000E+06    1    7    sammy
```

samm resonance reactions: **2** 102 **800**

samm max legendre order: 0 !! but in fact P8

resolved resonance range upper limit = 6.000E+06 eV.

final maximum energy for broadening/thinning = 6.000E+06 eV

broadened mat 825 from 0.0000E+00 to 2.9360E+02 k

points in= 5129 points out= 3740

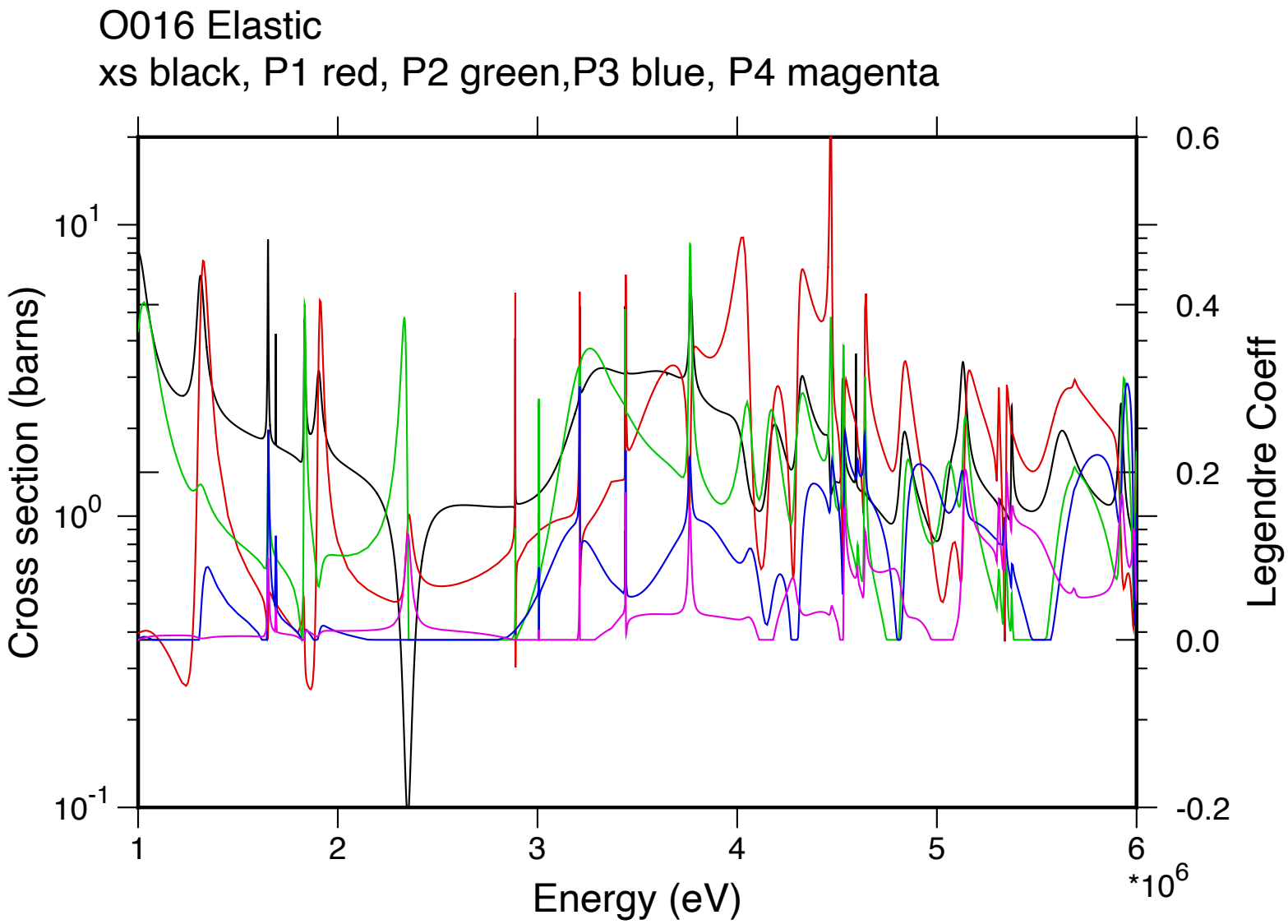
mt **2** 102 107 **800** 801

O016 example

- even with err .01 (not the default .001)
- energy grid 1490 points from 1.000000-5 to 5.99999+6 eV
- up to P8 but a_1= -3.4E-12 @ 1.0E-5 !!

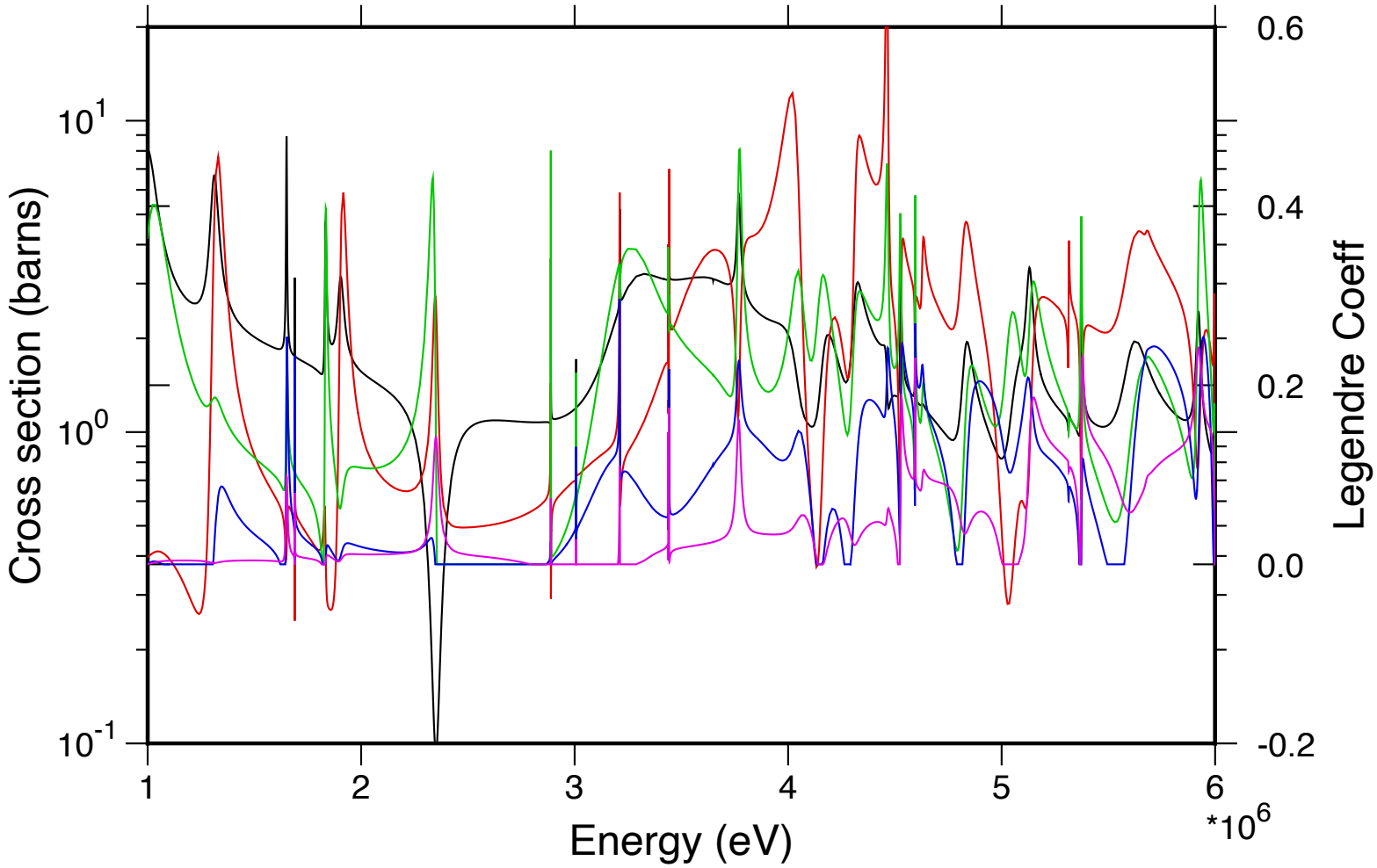
```
 8.016000+3 1.585751+1          0          1          0          0 825 4   2
 0.000000+0 1.585751+1          0          2          0          0 825 4   2
 0.000000+0 0.000000+0          0          0          1       1490 825 4   2
       1490          2                                             825 4   2
 0.000000+0 1.000000-5          0          0          1          0 825 4   2
-3.40677-12                                                        825 4   2
 0.000000+0 1.125000-5          0          0          1          0 825 4   2
-3.83277-12                                                        825 4   2
 0.000000+0 1.250000-5          0          0          1          0 825 4   2
-4.25868-12                                                        825 4   2
******
******
 0.000000+0 5.997000+6          0          0          8          0 825 4   2
 0.27787261 0.16187109 2.328558-2 7.568938-2-1.801033-2 1.810356-2 825 4   2
-2.860278-3-1.276187-3                                             825 4   2
 0.000000+0 5.998000+6          0          0          8          0 825 4   2
 0.29040075 0.17026649 4.044223-2 7.081754-2-1.496721-2 1.639703-2 825 4   2
-2.655751-3-1.188121-3                                             825 4   2
 0.000000+0 5.999000+6          0          0          8          0 825 4   2
 0.30261113 0.17978684 6.128253-2 6.732909-2-1.106630-2 1.491657-2 825 4   2
-2.477444-3-1.111461-3                                             825 4   2
 0.000000+0 5.999999+6          0          0          8          0 825 4   2
 0.31384543 0.18975903 8.439431-2 6.531068-2-6.603552-3 1.370011-2 825 4   2
-2.334023-3-1.050175-3                                             825 4   2
```

O016 example original 1-6 MeV



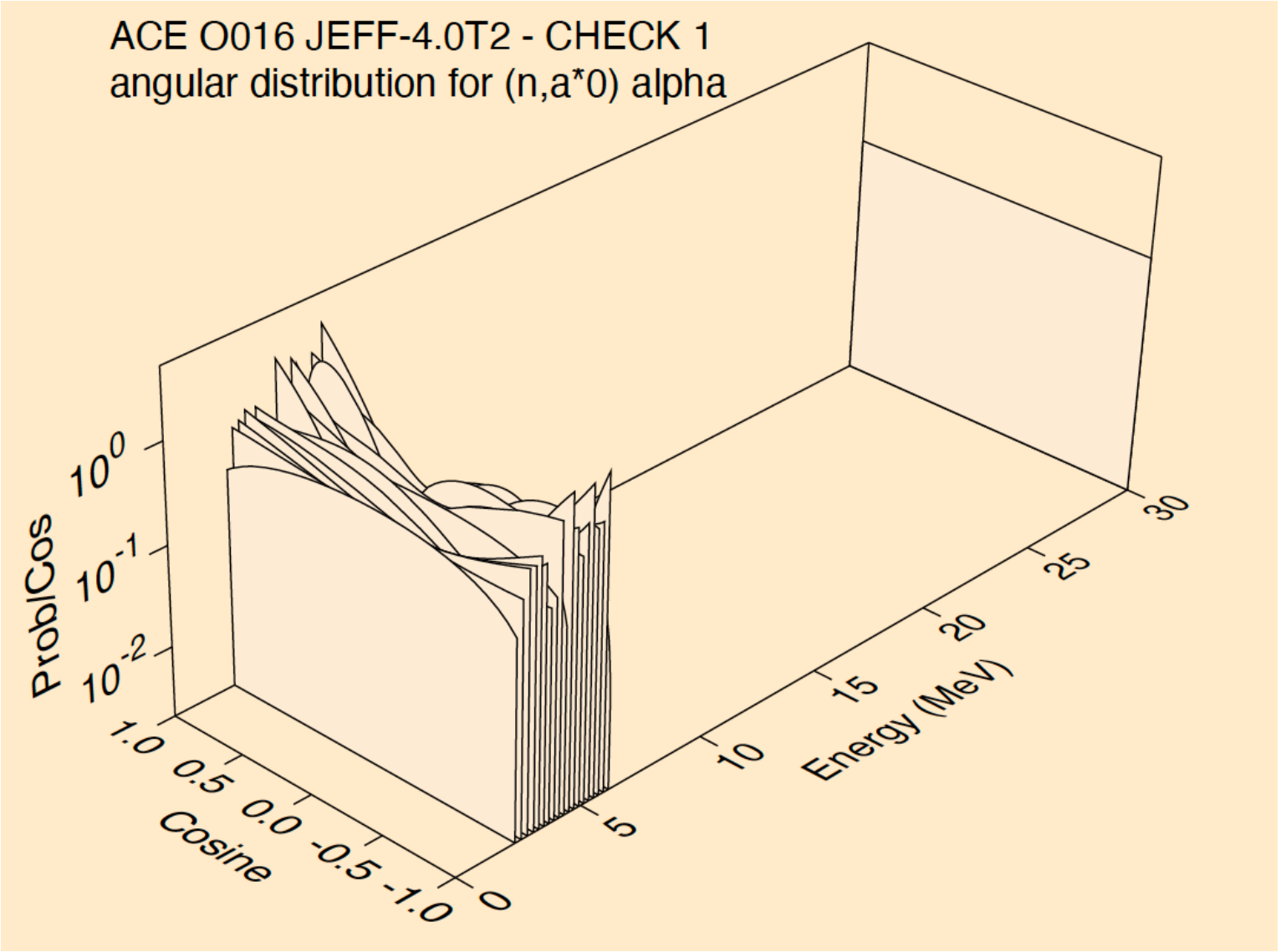
O016 example LRF7's MF4 1-6 MeV

subtle differences, higher P1, P2, more leaks ?



O016 example LRF7's mt800

- New Acer forms, emitted alpha angular distribution in the RRR else isotropic



Conclusions

- Evaluations
  - Why only MF4 mt2 when so many representable in LRF7 but not represented channels are open?
  - Why for mt600, mt800 MF4? or who needs those (in that energy range)
  - A lot of structure, Legendre coefficients is some range: numerical instability, interpretation or reality?
  - Very theoretical (Nancy's admission), complicated structure, mature enough for all JEFF's applications?
- Processing
  - Currently there is no method to Doppler broaden the Legendre coefficients
  - Legendre coefficients calculation on the same unionised grid as the cross-sections !!
    - @ OK or 293.6K ? .01 or .001? as they need to be unique
  - Elastic angular distribution given in the TSL range !!
  - Big application file: 125M Fe045 Acer forms
- Applications
  - Correlated sampling may be needed, with many, many, many more histories to converge properly

Conclusions

- The burden of proof is the responsibility of the evaluator(s) and/or their institution(s)
- At the moment the 12 JEFF-4.0T2 LRF-7 evaluations can be interpreted with a twist: some MF4 from the RRR MF2
- Around 2012 it was work in progress in NJOY2012, still has preliminary, unfinished tag attached to it in NJOY2016
  - Scattering MF-4 in the TSL energy range !!
  - Given on the same energy grid as the cross-sections !!
  - Swing from forward to back through each resonance, tends to cancel out when integrated over energy !!
- Sammy has been updated (had to be) to reproduce the MF4 from the parameters. As it produces the MF2 why not the MF4 for the MF2 channels in the MF2 range? How does it compare with NJOY2016 calculation?
- Frame CM-LAB translation issues (0.96 cosine cut-off)
- A unique recommendation is needed

Thank you for your attention!

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