Why the Zr evaluation isn't getting done fast enough

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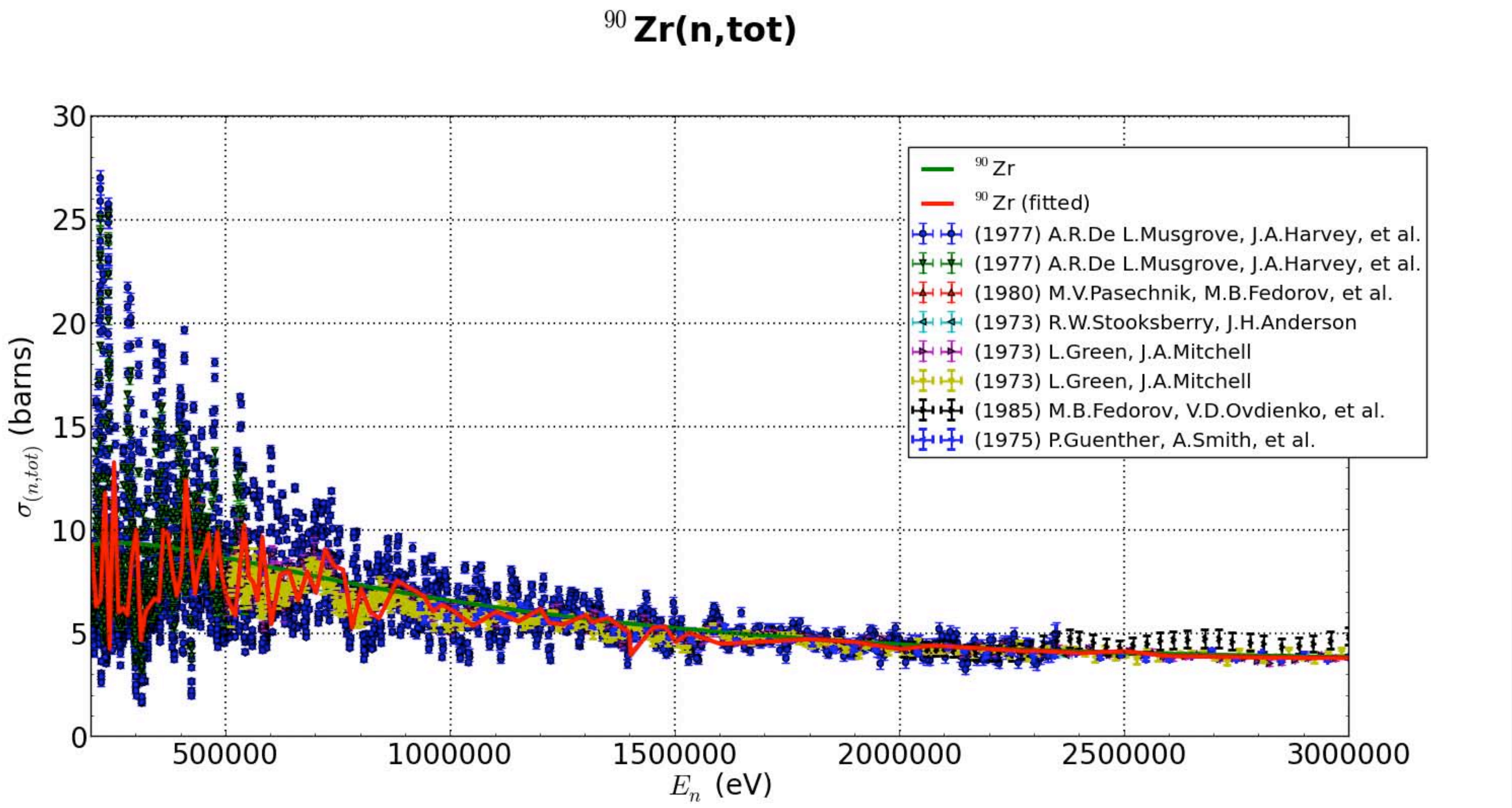
90Zr has magic neutron number, hard to evaluate (like 56Fe, 23Na...)



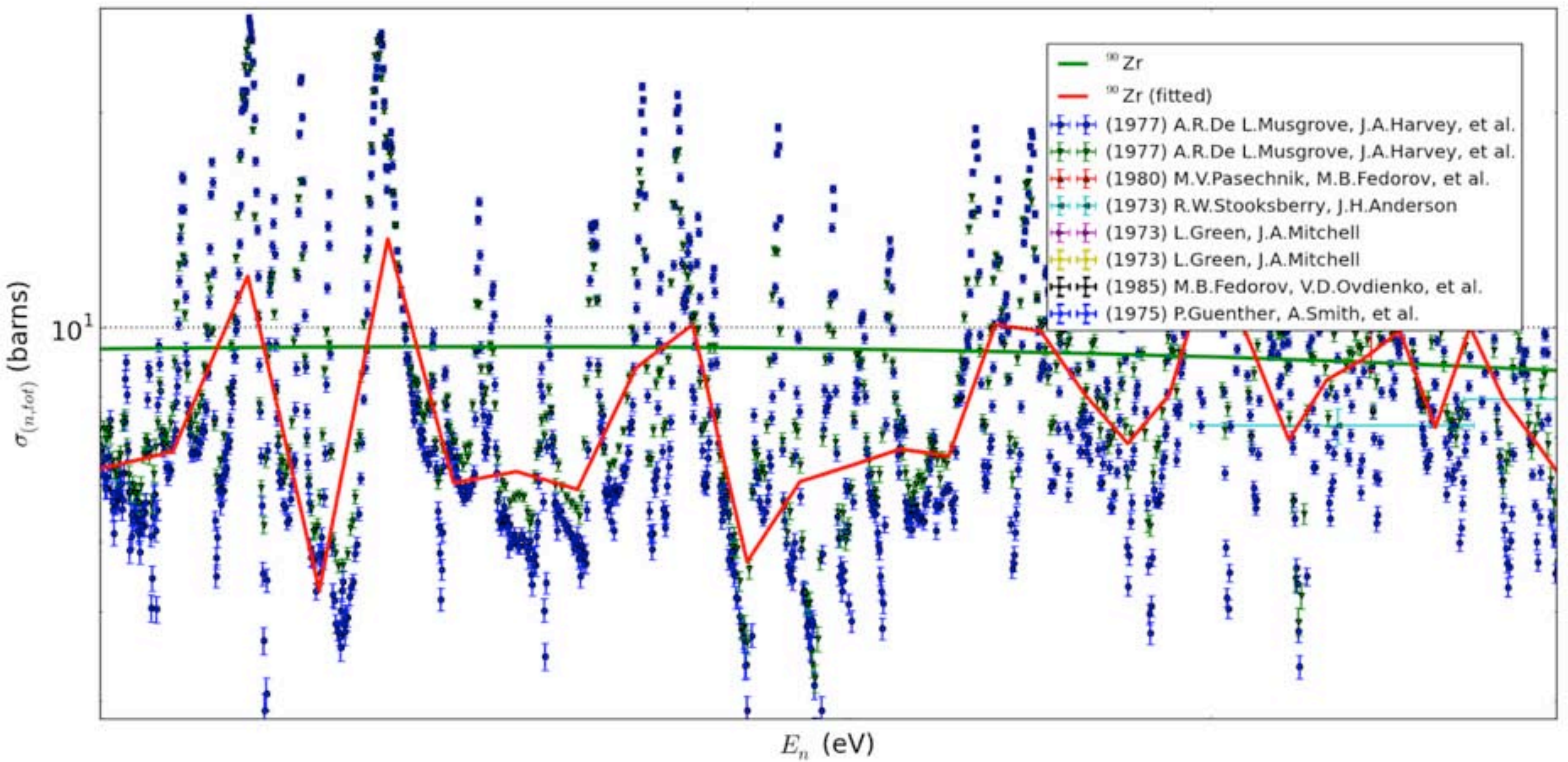
Low level density means wide resonance spacing, and resonances that go very high in energy

Testing by KAPL and others tell us that must get angular distributions correct to get leakage right

- **ENDF/B-VI.8**
  - (n,el) fluctuating cross sections fit to data
  - (n,el) angular distributions
  - No other secondary distributions
  - did well in testing
- **ENDF/B-VII.0**
  - EMPIRE based, so all secondary distributions
  - no fluctuations
  - did poorly in testing
- **ENDF/B-VII.1**
  - Fitted EMPIRE, so ..
    - All secondary distributions
    - fluctuations included
  - did well in testing
  - bug in EMPIRE meant evaluation was a “Frankenevaluation”, we glued in JENDL-4.0 angular distributions

Try one more time...

Zooming in: those fluctuations aren't overlapping resonances, they can be fully resolved



Could we extend the 90Zr RRR, then compute angular distributions from the RRR parameters?

- In ENDF/B-VII.0, JENDL-4.0, ... RRR's are given as MLBW, not unitary so angular distribution iffy

- We are likely missing many smaller resonances

- There is only one RRR set, from A.R. de L. Musgrove, J. A. Harvey, et. al., how well do we trust it?

No

Full R matrix theory isn't going to work, but what about an URR treatment?

- We don't know all the resonances, so we could treat using URR prescription

$P(\sigma_{ab}|E)$ where pdf defined by $\langle\Gamma\rangle$, D, etc.

- Will need average resonance parameters from RRR
- Will need the average cross sections either
  - from URR or
  - from Optical Model + Hauser-Feschbach calculation

What about angular dists?

Can't we just use EMPIRE's extensive collection of fudge factors?

- **TOTRED**: total XS multiplier
- **FUSRED**: reaction XS multiplier
- **FCCRED**: direct collective XS multiplier
- **FCORED**: DWBA collective XS multiplier
- **CINRED**: compound inelastic XS multiplier, reaction XS fixed
- **CELRED**: compound elastic XS multiplier, reaction XS floats
- **CELCOR**: compound elastic XS multiplier, reaction XS fixed
- **ELARED**: shape elastic XS multiplier

Maybe

EMPIRE's fudge factors can do almost anything we want to the average cross sections

- With all the fudge factors

$$\sigma_{el} = (\mathtt{ELARED})\sigma_{se} + (\mathtt{FUSRED})\sigma_{reac}(\mathtt{CELRED}) \times \frac{(\mathtt{CELCOR})T_{ce}}{(\mathtt{CELCOR})T_{ce} + (\mathtt{CINRED})T_{in} + \sum_{\text{rest of } c} T_c} W$$

Use this to put a fluctuation in the reaction cross section

Use this to adjust amount of fluctuation in compound elastic

What about angular dists?

After spinning my wheels over these resonances, I went back to basics

- Want the cross section

$$\sigma_{ab}(E)$$

- and angular distributions extracted from the differential cross section

$$\frac{d\sigma_{ab}(E)}{d\mu} = \sigma_{ab}(E)P(\mu|E), \text{ with } \mu = \cos\theta$$

- We can settle for just the P_1 term

$$\bar{\mu} = \int d\mu\mu P(\mu|E) = \int d\mu P_1(\mu)P(\mu|E)$$

For the angular distributions, let's go back to Blatt and Biedenharn

- Differential cross section is

$$\frac{d\sigma_{as;bs'}}{d\Omega} = \frac{\pi}{k_a^2} \sum_{L=0}^{\infty} P_L(\mu) B_L(as;bs')$$

- where

$$B_L(as,bs') = \frac{(-1)^{s'-s}}{4} \sum_{J_1 J_2 l_1 l_2 l'_1 l'_2} Z(l_1 J_1 l_2 J_2, sL) Z(l'_1 J_1 l'_2 J_2, s'L) \times$$
$$\Re\left[(\delta_{ab}\delta_{ss'}\delta_{l_1 l'_1} - S^{J_1}_{bs'l'_1;asl_1})^* (\delta_{ab}\delta_{ss'}\delta_{l_2 l'_2} - S^{J_2}_{bs'l'_2;asl_2}) \right]$$

Blatt and Biedenharn impractical for either RRR or URR

- We don't have the complete RRR set, so can't just write down the distribution

- A URR-like approach is unrealistic
  - For cross sections, have pdf

$$P(\sigma_{ab}|E)$$

  - Wouldn't an angular version be something like

$$P(\mu|\sigma_{ab}, E)P(\sigma_{ab}|E)$$

    no one has ever made such a thing and no code could use it

- So, must settle for average angular distribution

The average neatly separates into direct and compound parts

$$\langle B_L(as,bs')\rangle \equiv \left\langle B_L^{dir}(as,bs')\right\rangle + \left\langle B_L^{fl}(as,bs')\right\rangle$$

- Direct part computed in EMPIRE, TALYS, CoH

$$\left\langle B_L^{dir}(as,bs')\right\rangle = \frac{(-1)^{s'-s}}{4} \sum_{J_1 J_2 l_1 l_2 l'_1 l'_2} Z(l_1 J_1 l_2 J_2, sL) Z(l'_1 J_1 l'_2 J_2, s'L) \times$$

$$\Re\left[(\delta_{ab}\delta_{ss'}\delta_{l_1 l'_1} - < S^{J_1}_{bs'l'_1;asl_1} >)^* (\delta_{ab}\delta_{ss'}\delta_{l_2 l'_2} - < S^{J_2}_{bs'l'_2;asl_2} >)\right]$$

- Compound part not computed in EMPIRE yet *

$$\left\langle B_L^{fl}(as,bs')\right\rangle \frac{(-1)^{s'-s}}{4} \sum_{J_1 J_2 l_1 l_2 l'_1 l'_2} Z(l_1 J_1 l_2 J_2, sL) Z(l'_1 J_1 l'_2 J_2, s'L) \Re\left[< (S^{fl J_1}_{bs'l'_1;asl_1})^* S^{fl J_2}_{bs'l'_2;asl_2} >\right]$$

so, it is treated as isotropic in EMPIRE

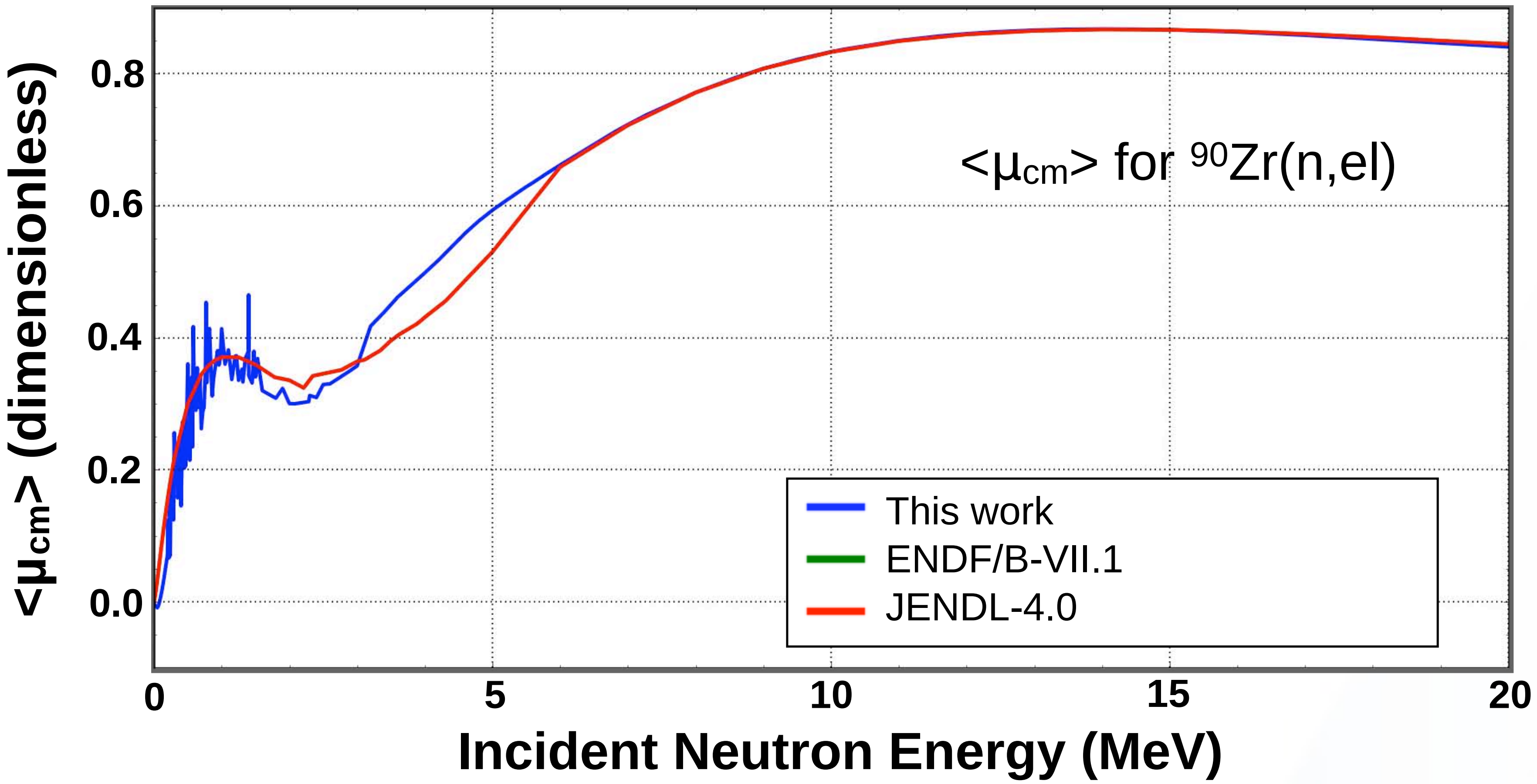
Given EMPIRE's limitations, we still get non-trivial angular distributions

$$P_{el}(\mu|E) = \frac{d\sigma_{el}/d\mu}{\sigma_{el}}$$

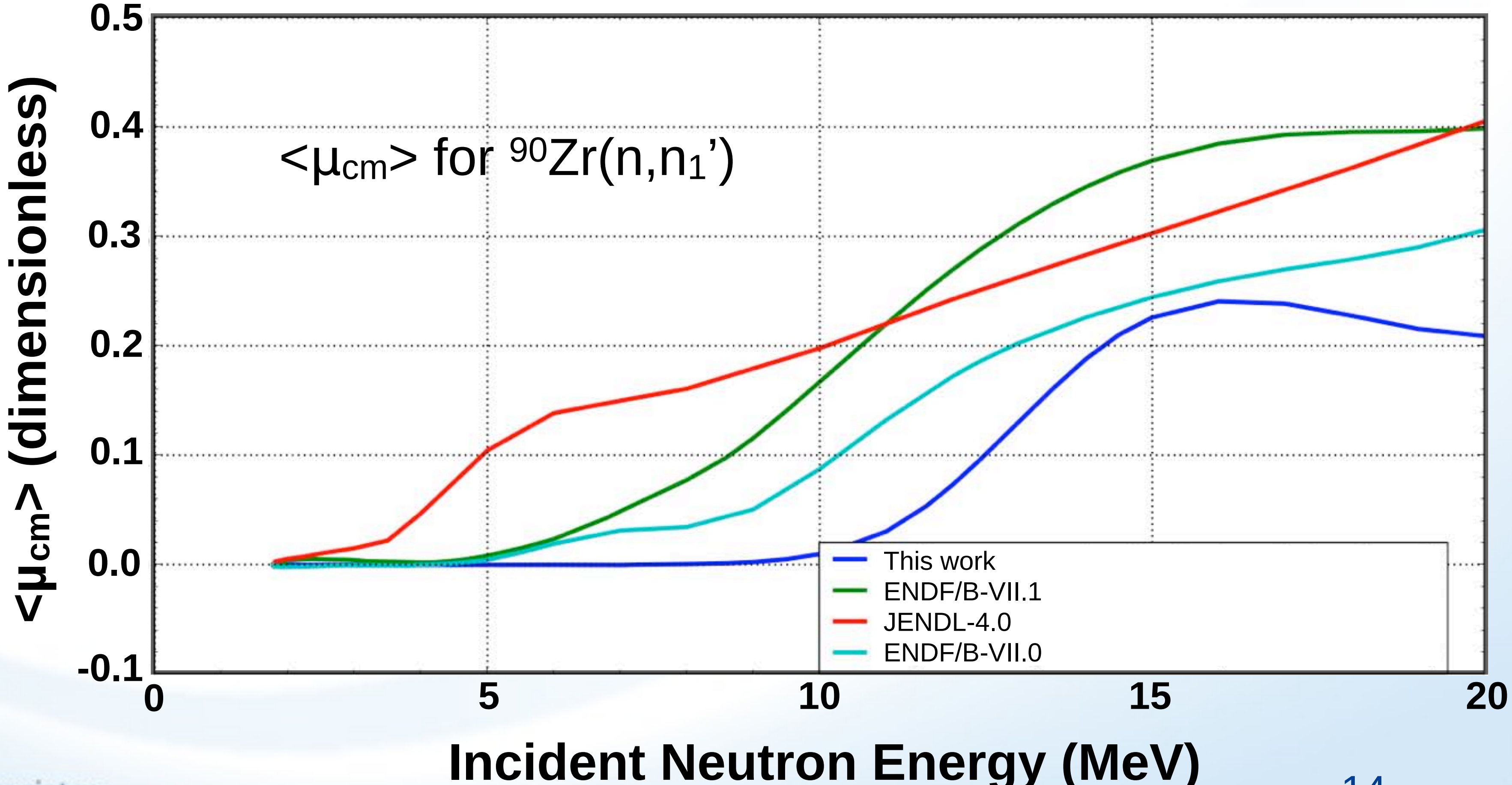
$$= \frac{\sigma_{se} P_{se}(\mu|E) + 0.5\sigma_{ce}}{\sigma_{se} + \sigma_{ce}}$$

Drives the shape of the angular distribution

Builds fluctuations into distribution



$<\mu_{cm}>$ for $^{90}Zr(n,el)$
This work
ENDF/B-VII.1
JENDL-4.0
$<\mu_{cm}>$ (dimensionless)
0.8
0.6
0.4
0.2
0.0
0
5
10
15
20
Incident Neutron Energy (MeV)



$<\mu_{cm}>$ for $^{90}Zr(n,n_1')$
This work
ENDF/B-VII.1
JENDL-4.0
ENDF/B-VII.0
$<\mu_{cm}>$ (dimensionless)
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
0
5
10
15
20
Incident Neutron Energy (MeV)

What next

- I've proved we can make an evaluation that
  - has fluctuations
  - has decent angular distributions
- The next step is to actually finish the evaluation!
  - Already have experimental database set up
  - Roberto Capote has been tweaked the OMP
  - Trying to get KALMAN and latest EMPIRE to cooperate
  - Then rework my Bayesian update code that folds in $^{nat}Zr(n,tot)$ data