Fe and EMPIRE-TENDL evaluations

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Brookhaven National Laboratory
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CIELO-Iron collaboration

BNL, CNDC, IAEA, IRM, JSI, LANL, ORNL, RPI, IRSN

- Exp. data analysis: CNDC
- Resonance range: ORNL & IRSN & BNL & IAEA
- Fast neutron range: EMPIRE (BNL, IAEA)
- File assembly: IAEA, BNL
- Testing: IAEA, RPI, BNL, LANL, JSI

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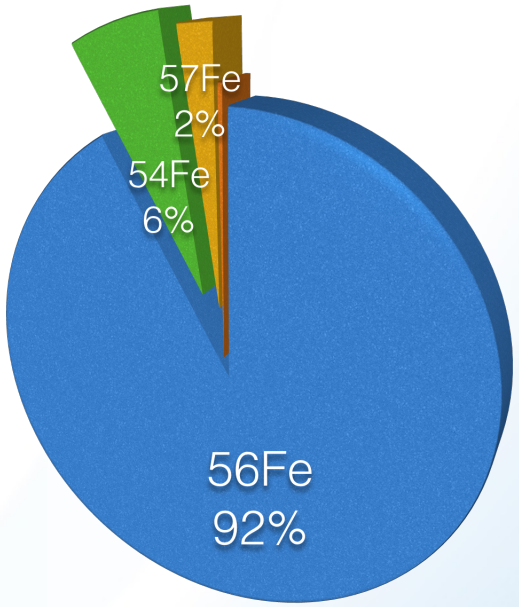
1. BNL, Upton, NY, USA
2. IAEA, Vienna, Austria
3. ORNL, Oak Ridge, TN, USA
4. EC-JRC-IRMM, Geel, Belgium
5. RPI, Troy, NY, USA
6. CNDC, Beijing, P.R.China
7. CIAE, Beijing, P.R.China
8. IRSN, Paris, France
9. ITA, Sao José dos Campos, Brazil
10. Bucharest University, Bucharest-Magurele, Romania

ENDF/B-VIII.0 release: Iron evaluation as part of the CIELO collaboration

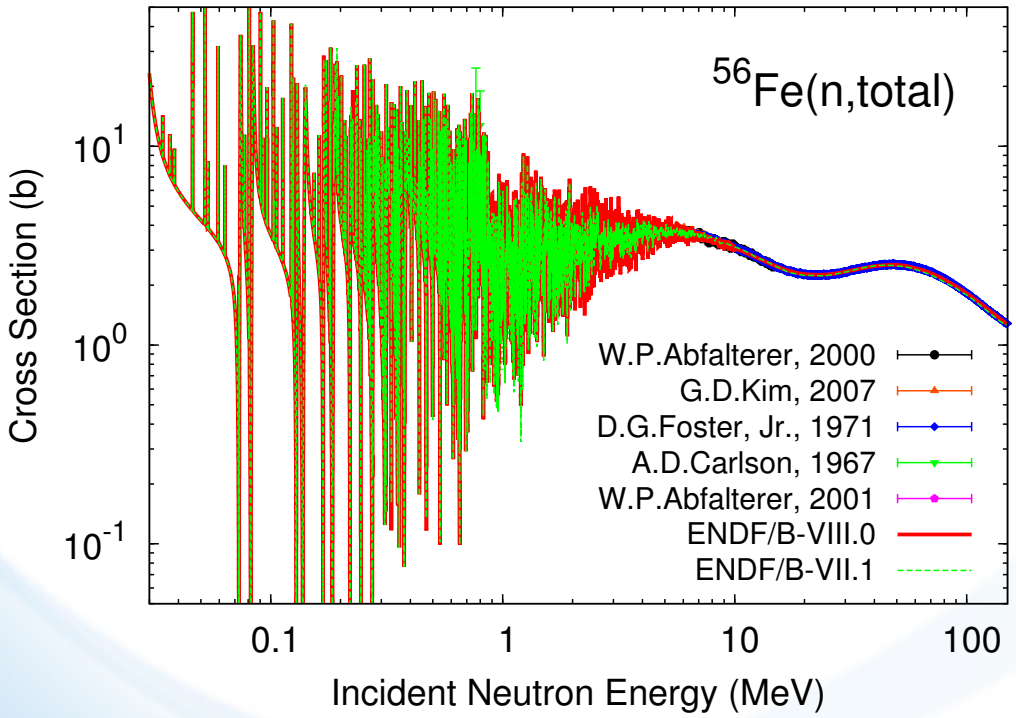
- Iron is a common structure material
- Difficult to evaluate: Strong resonances and fluctuations above inelastic threshold
- Deep interference minima: cross section near zero, which makes minor isotopes (and other steel components) relevant
- Validation tests in sync other major evaluations (^{235,238}U, ^{239}Pu)
- Strong reliance on experimental data including recent Geel, LANL and RPI
- IRDFF data adopted whenever available

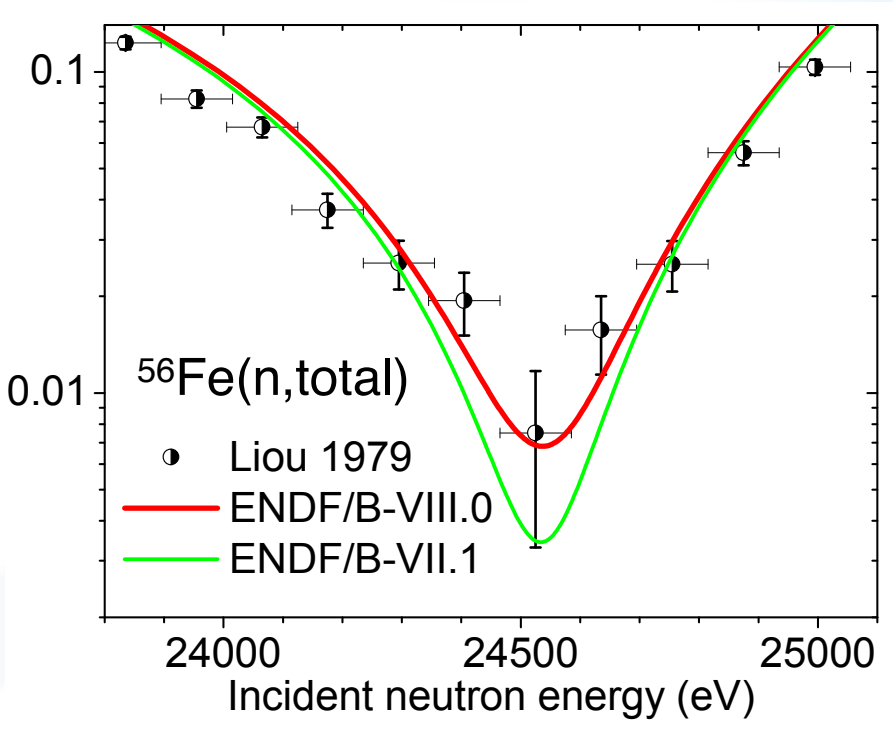


- Model calculations adjusted to reproduce IRDFF and exp. data
- Special attention devoted to angular distributions (AD)
  - AD derived from resonance parameters
  - Anisotropic AD compound nucleus inelastic scattering
  - Influence of AD on benchmark results

Resonances in ^{56}Fe

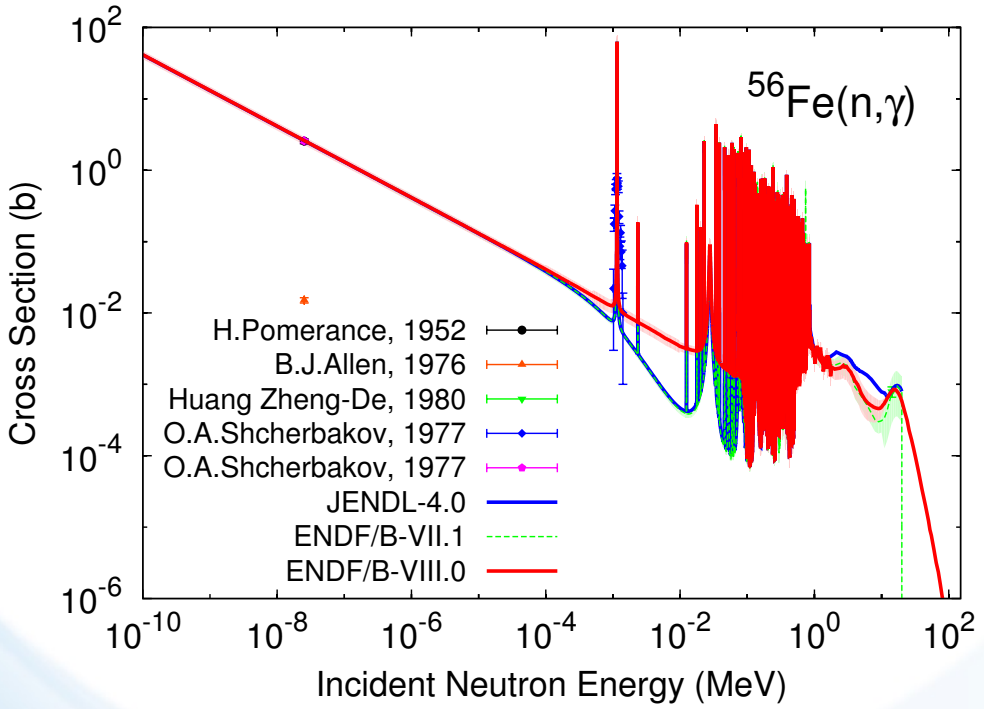
- Fluctuations extend high in energy
- Minor correction to previous evaluation (0.01 meV to 850 keV)

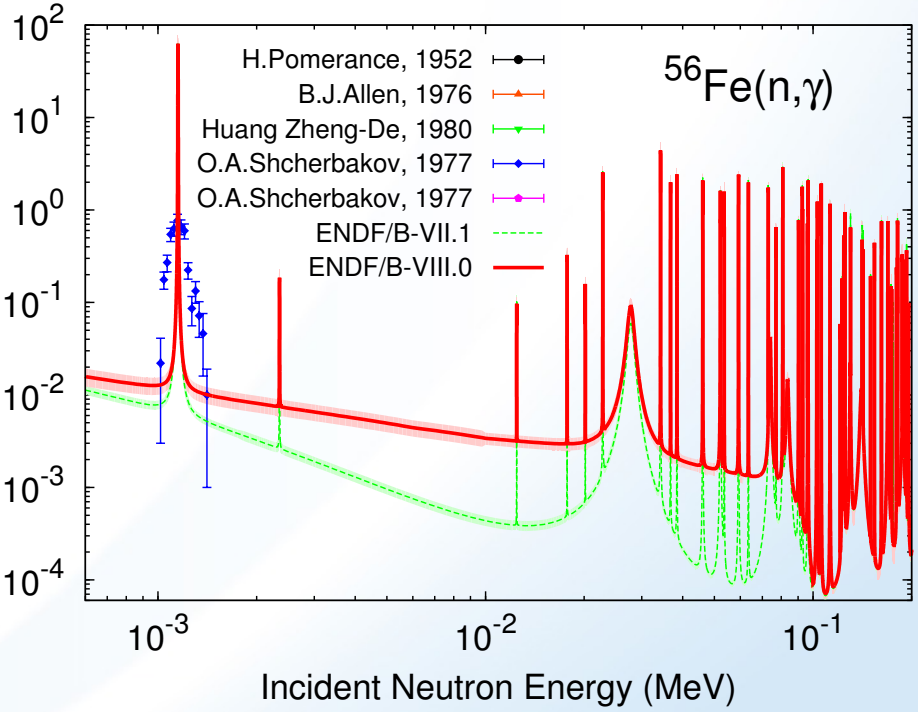




Resonances in ^{56}Fe

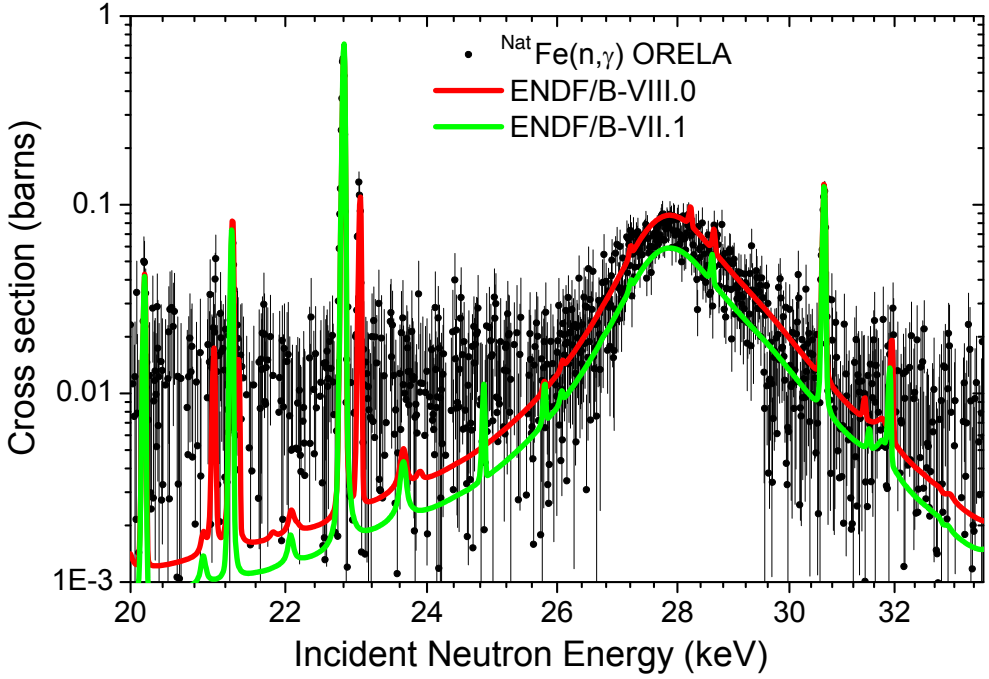
- ^{56}Fe(n,γ) background (10eV-100keV): HEU-MET-INT-001 (ZPR-34/9)

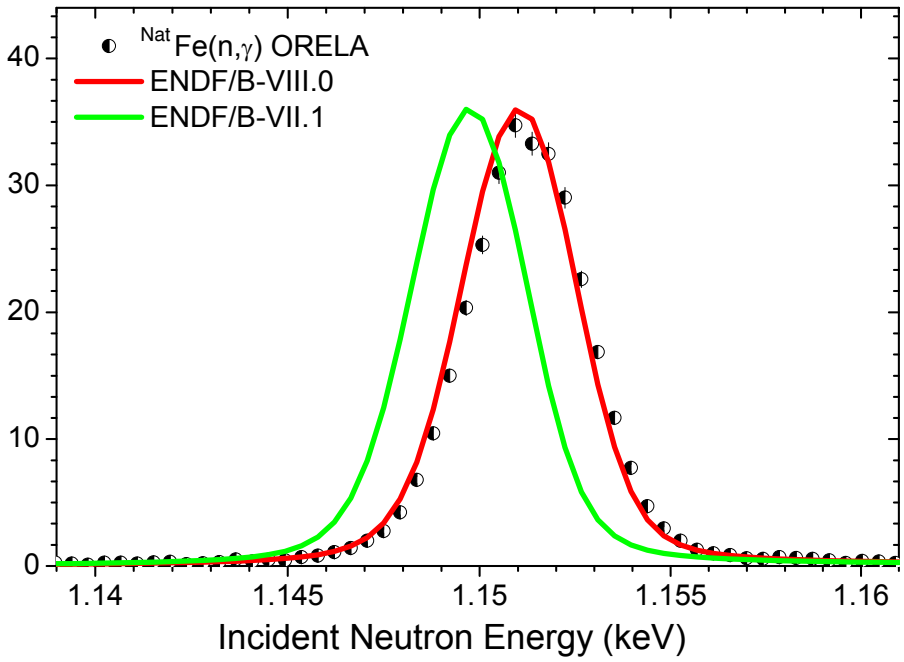




Resonances in ^{56}Fe against ^{Nat}Fe data

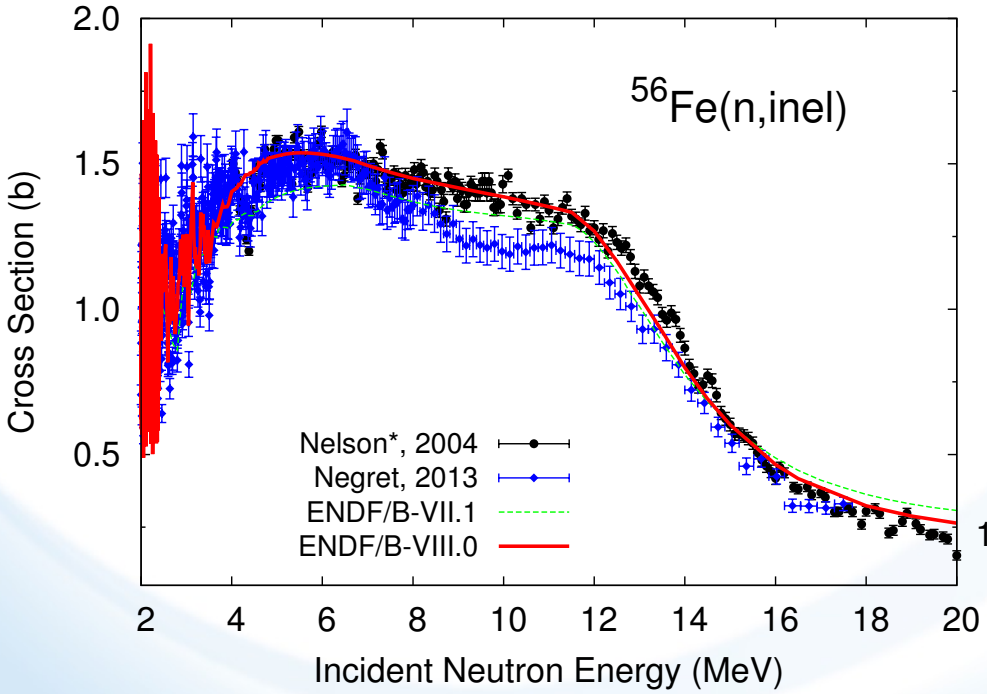
- Effect of added low-energy capture background and increased γ-width
- Shift on energy calibration

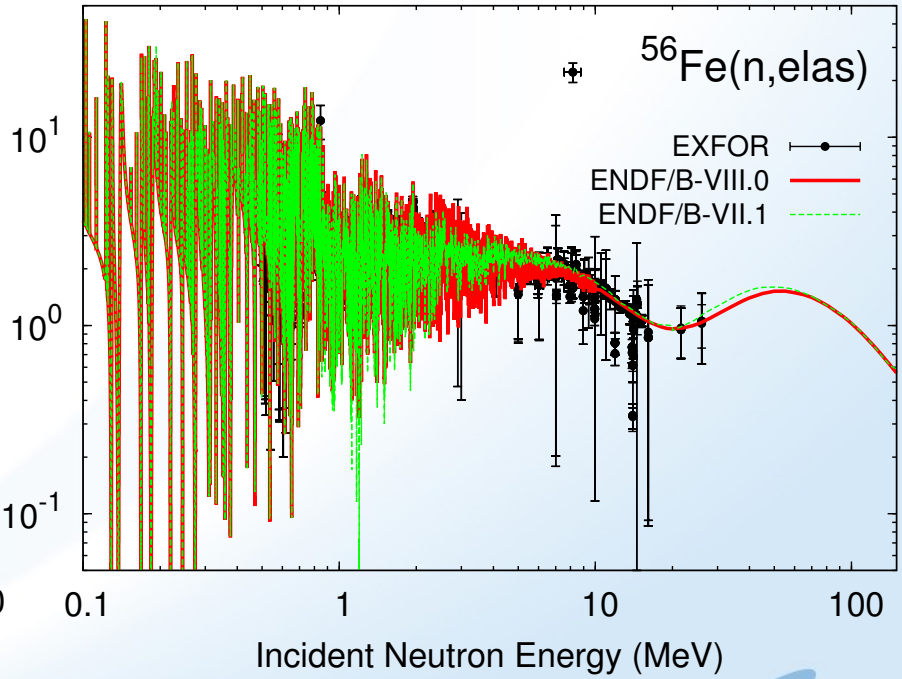




Elastic & inelastic for ^{56}Fe

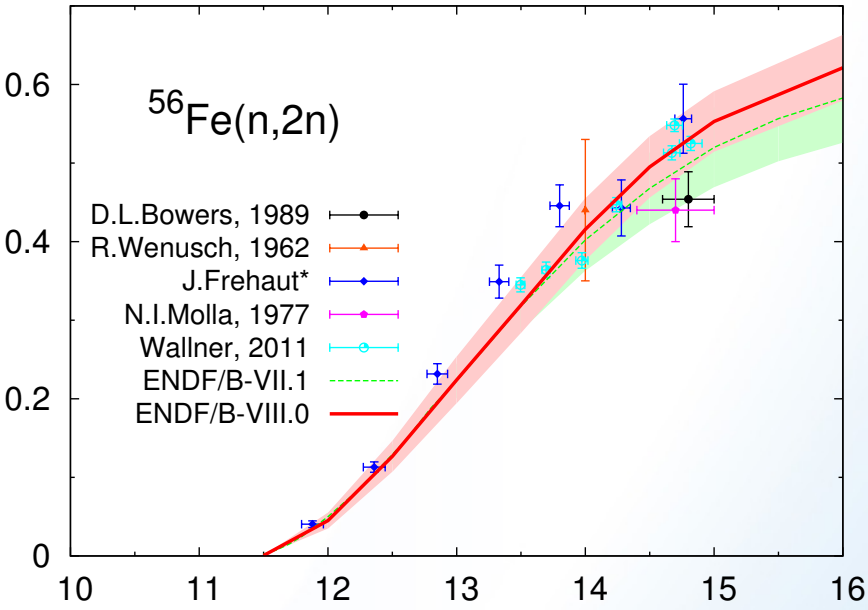
- Fluctuations imposed on inelastic scattering to the first and second excited states taken from experimental data
- Elastic obtained by subtraction of sum of all reactions from total

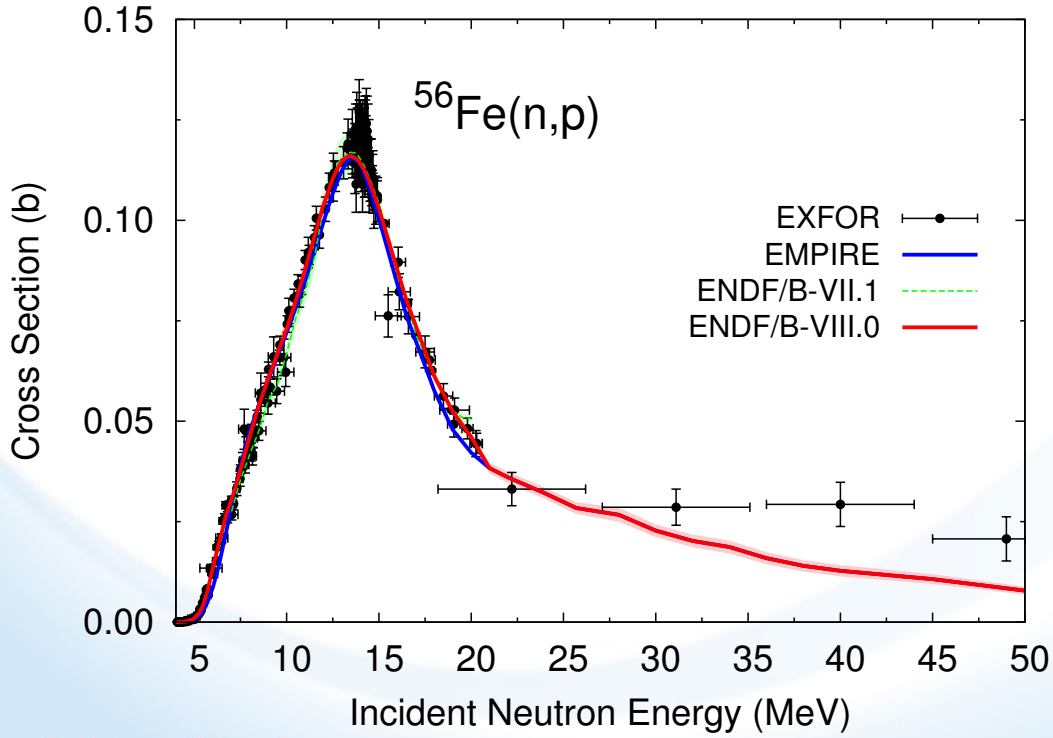


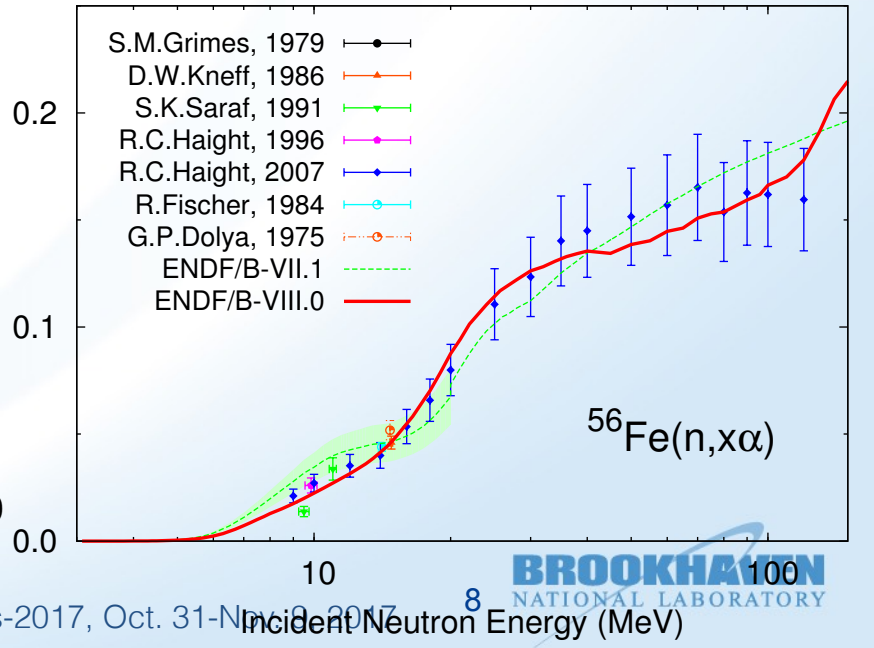


Fast neutron range

- EMPIRE
- Fitted model parameters to experimental data or IRDFF

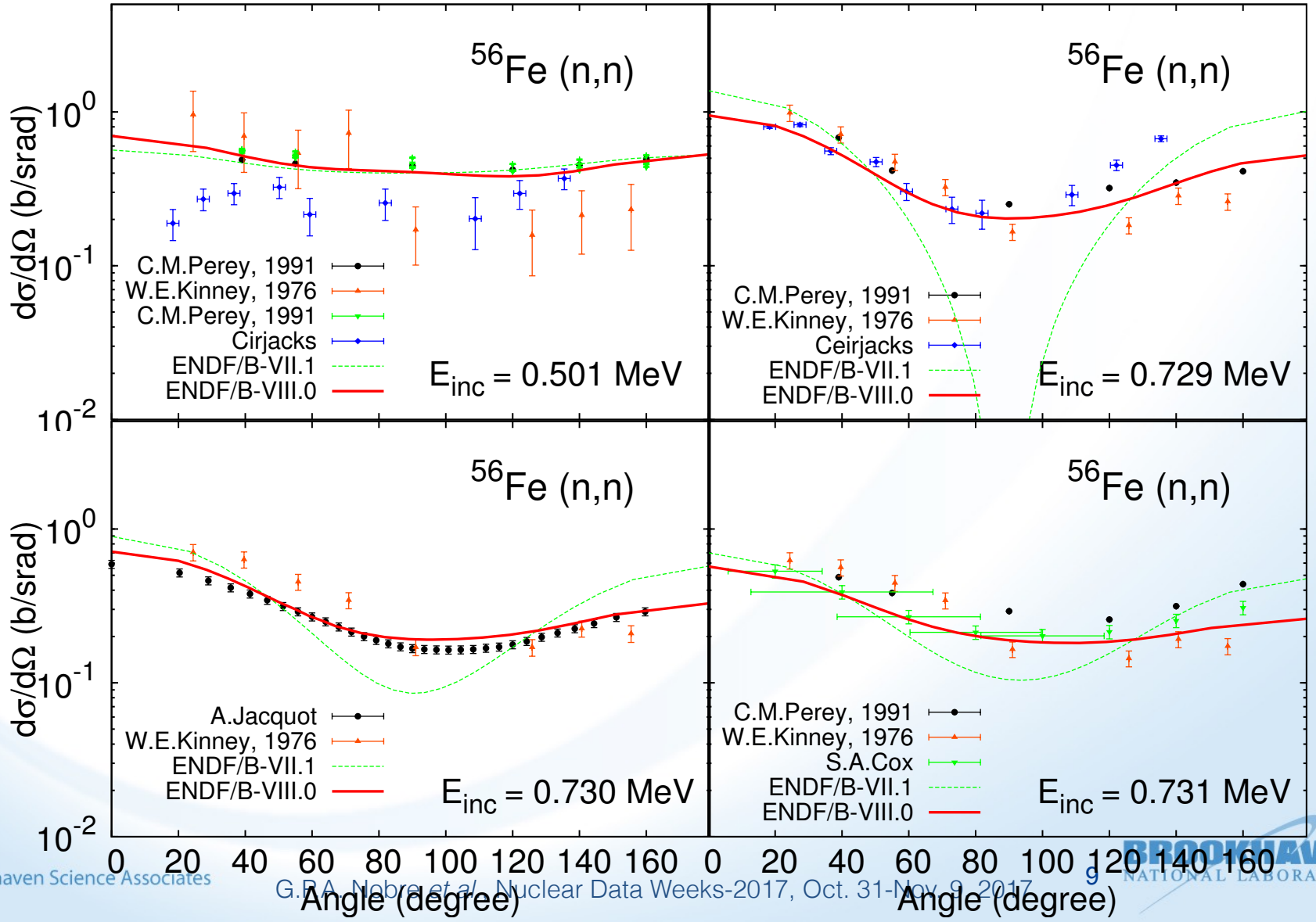






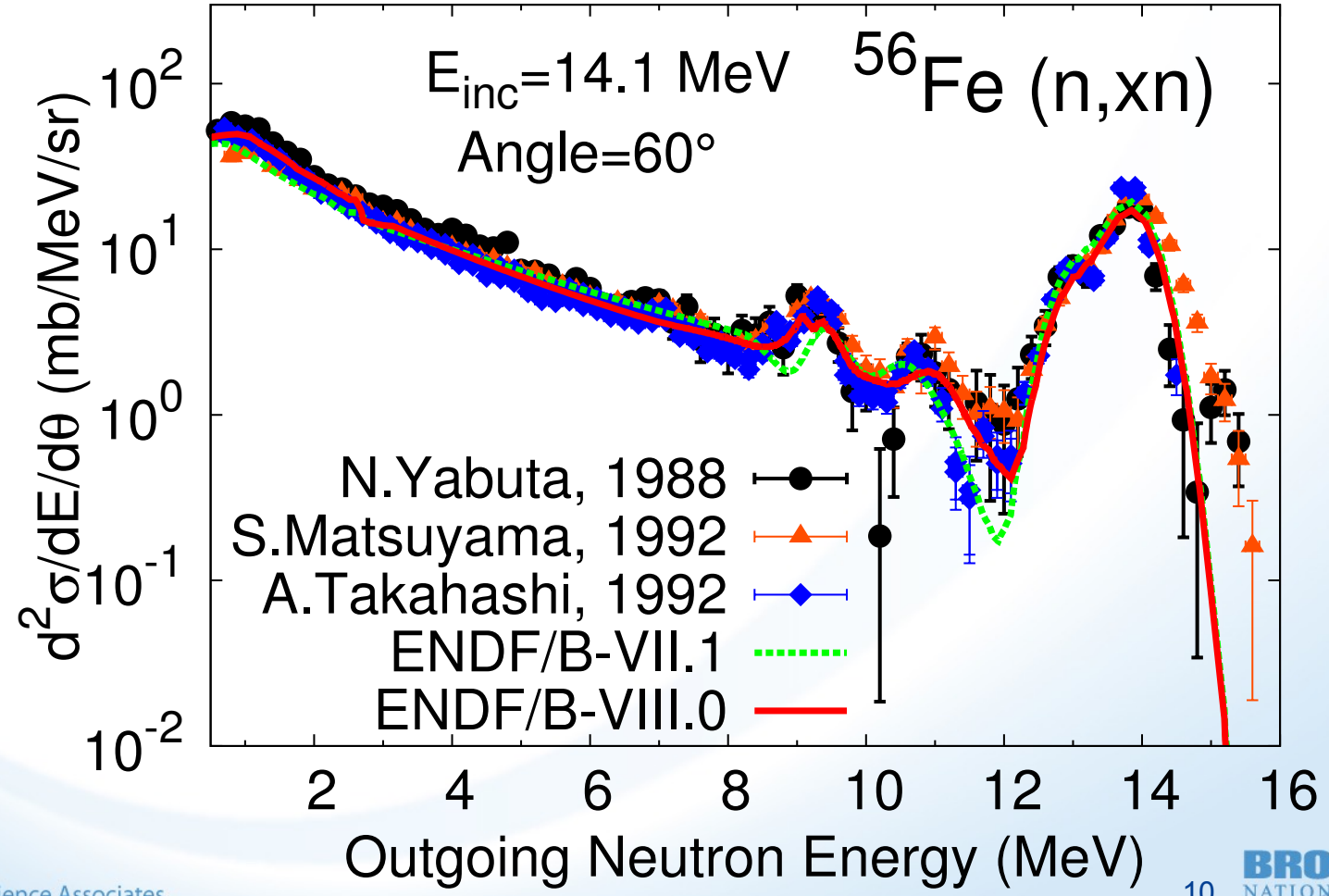
Angular distributions

Generally better agreement with Perey and Kinney data



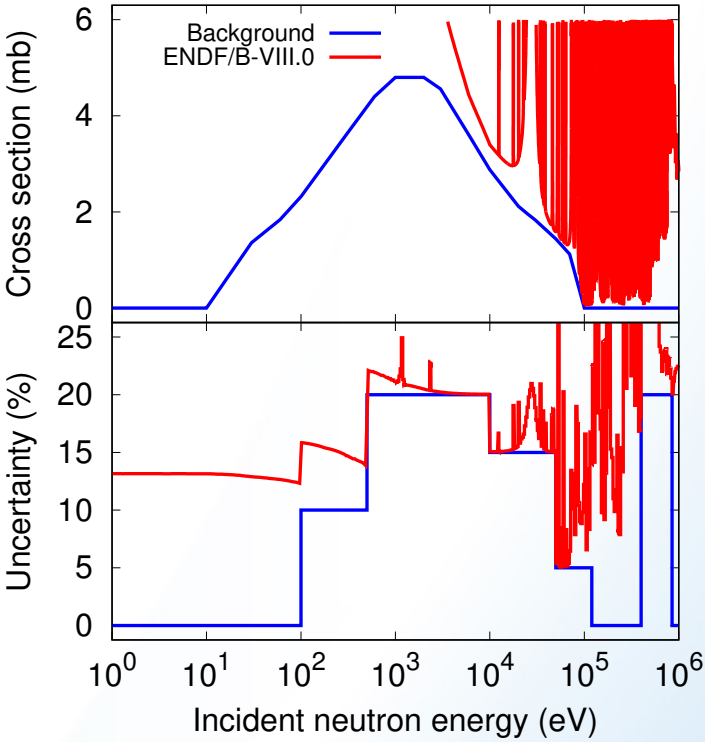
Double-differential spectra

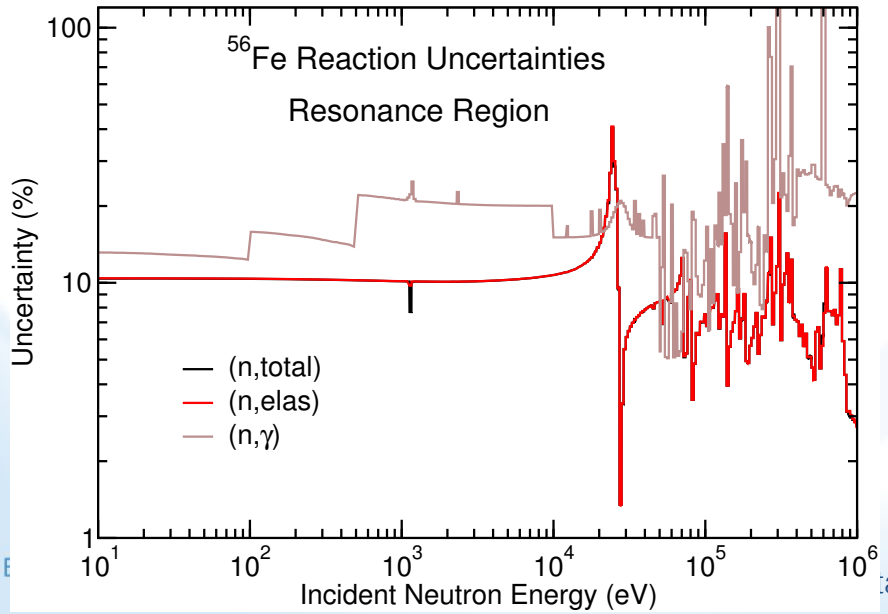
- In general, slightly better agreement with data

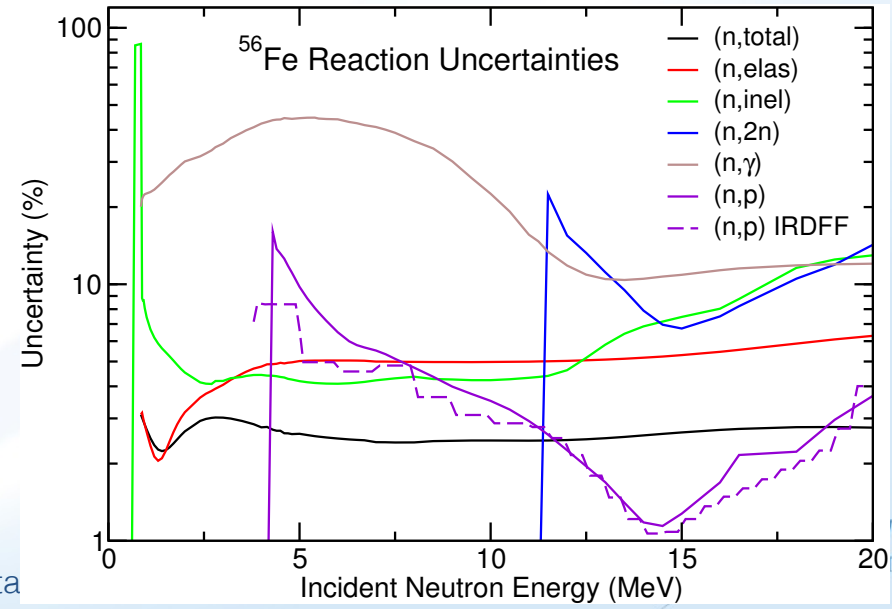


Uncertainty Quantification

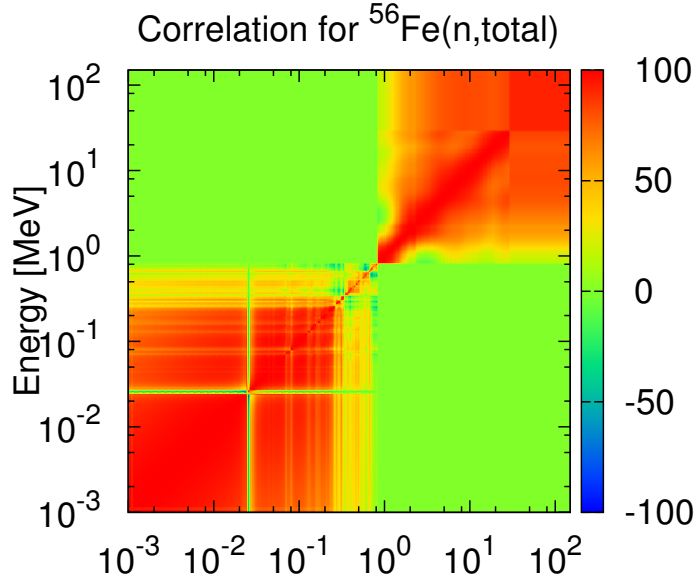
- Covariances for the RRR were generated from uncertainties in the Atlas (through EMPIRE res. module)
- Uncertainty background for (n,γ) needed between 100-840 keV
- In fast region, covariances were obtained from Kalman: experimental uncertainties and model constraints

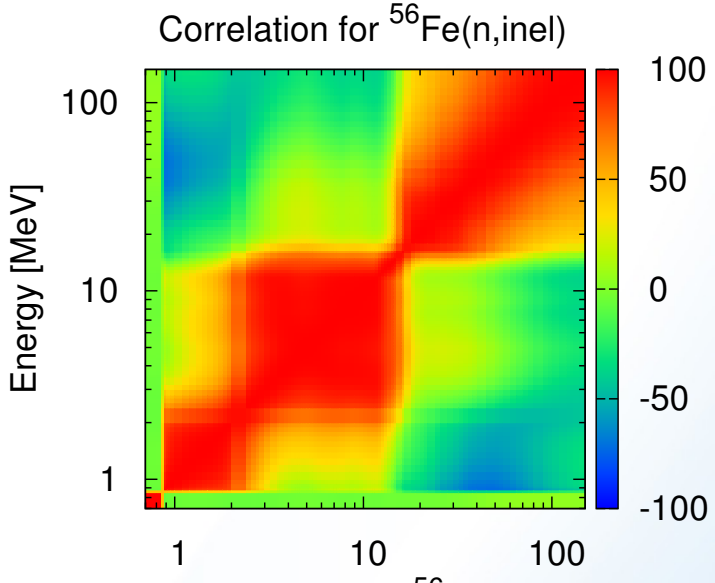


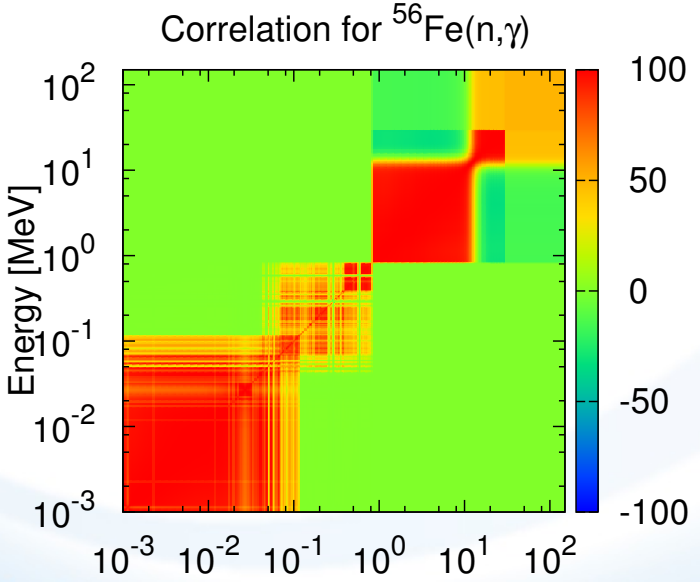


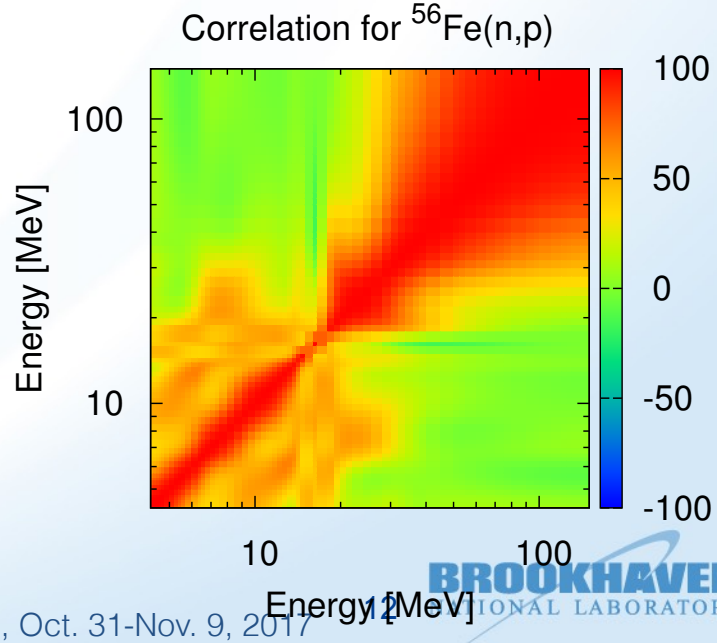


Covariances



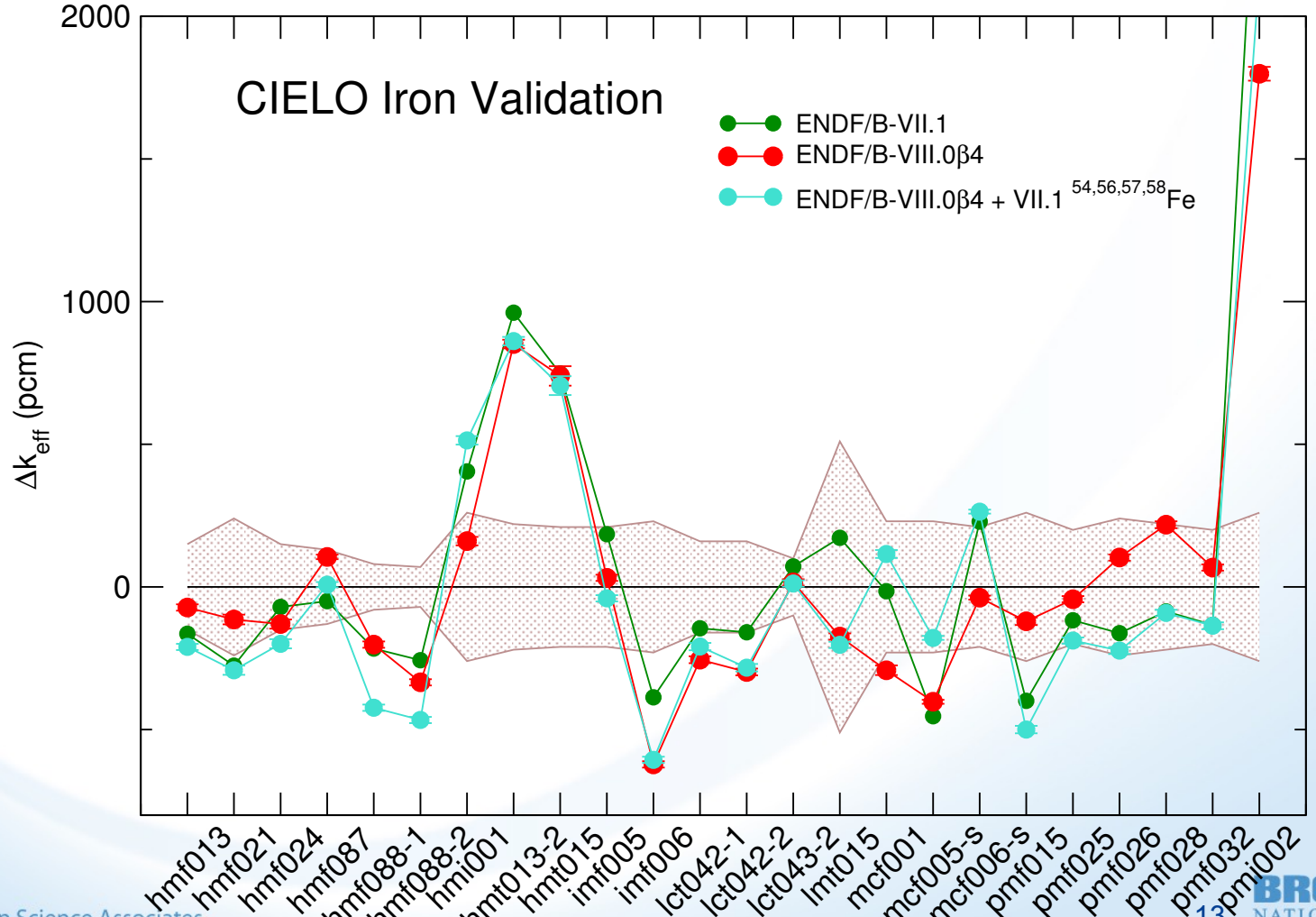






Validation

- Focused on benchmarks sensitive to Iron



Conclusions

- CIELO collaboration led to a new set of evaluations for main iron isotopes
- Recent measurements, state-of-the-art modeling, semi-integral data and integral benchmarks
- Our new results are generally better than ENDF/B-VII.1 (differential and integral testing)
- Experience with current efforts points direction for future improvements:
  - Re-evaluation of res. parameters
  - Reliable measurements of capture for minor isotopes (and other alloying elements)
  - Re-evaluation of ^{239}Pu, ^{52}Cr, and ^{58}Ni may allow reduction of background
  - …

New evaluations from EMPIRE & TENDL

- During last mini-CSEWG ~ 50 new evaluations of short/ long-lived isotopes were proposed from TENDL-2015
- We reviewed these evaluations, assessed their quality, and determined whether they should be included into the ENDF/B-VIII.0 release
- Added to the analysis all nuclides with $T_{1/2}$ > 1 day and nuclides that “bridges gaps” between nuclei
- Performed “default” EMPIRE calculations, formatted into ENDF-6 files and generated 800+ plots for main reactions for all > 103 nuclides
- Compared with TENDL files
- Ran checking codes

Conclusions

- TENDL: Problems at low energies for scattering on excited targets
- ENDF-6 format: encoding of “superelastic” is unclear
- EMPIRE vs. TENDL:
  - EMPIRE does proper deformed coupled-channel calculations: better results for rare-earths
  - Codes make different choices of levels to couple
  - Resonance data are normally inexistent: TENDL creates realistic-looking resonances which can be misleading (format does not distinguish between “artificial” and “real” ones
  - Resonances from TENDL are extrapolated: 3-4 orders of magnitude too high
- Incorporated: 28 from TENDL, 74 from EMPIRE