Nuclear reaction codes in data evaluation - case of EMPIRE

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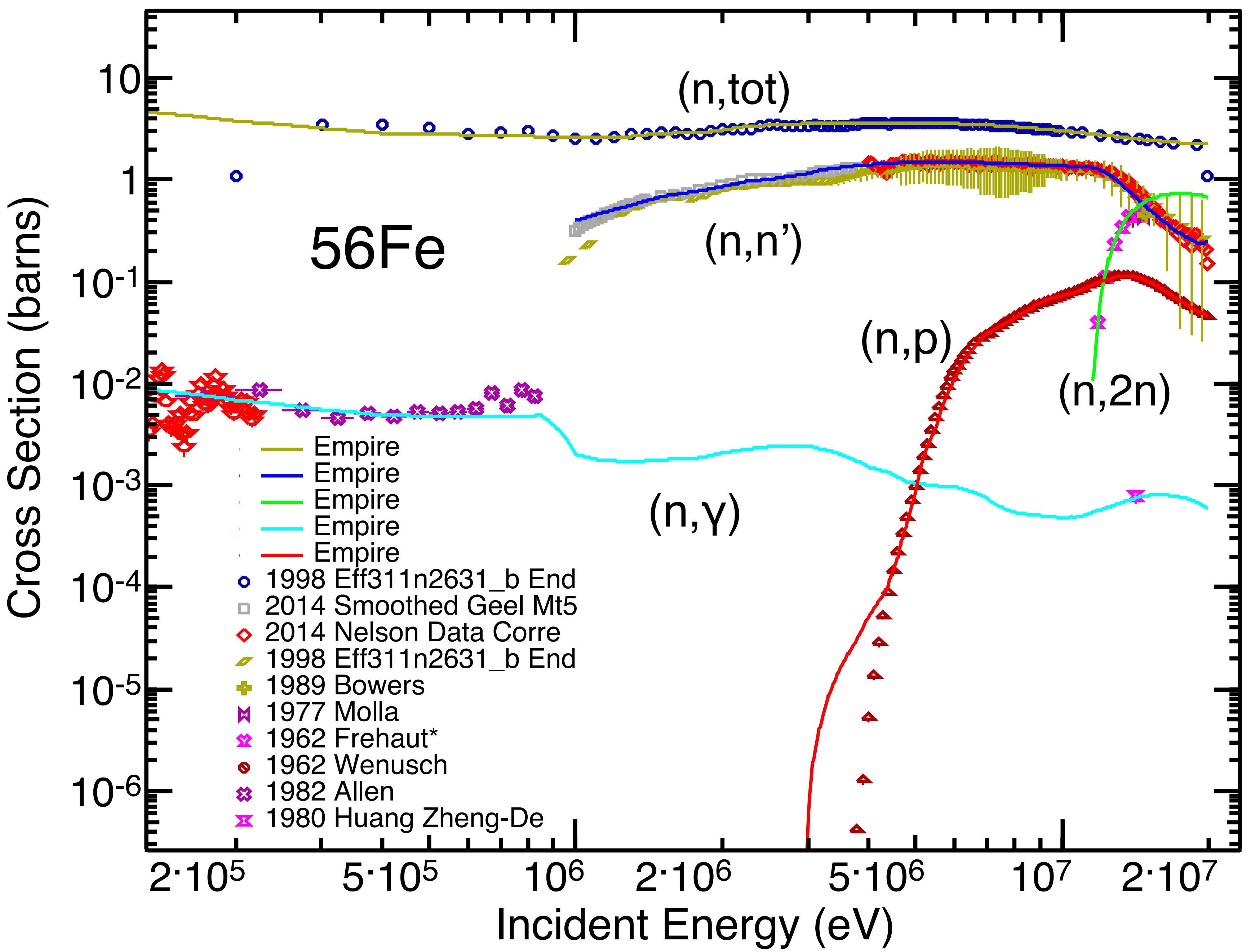
Why do we need reaction codes?



There are 4635 plots with experimental data for 56Fe+n; still:

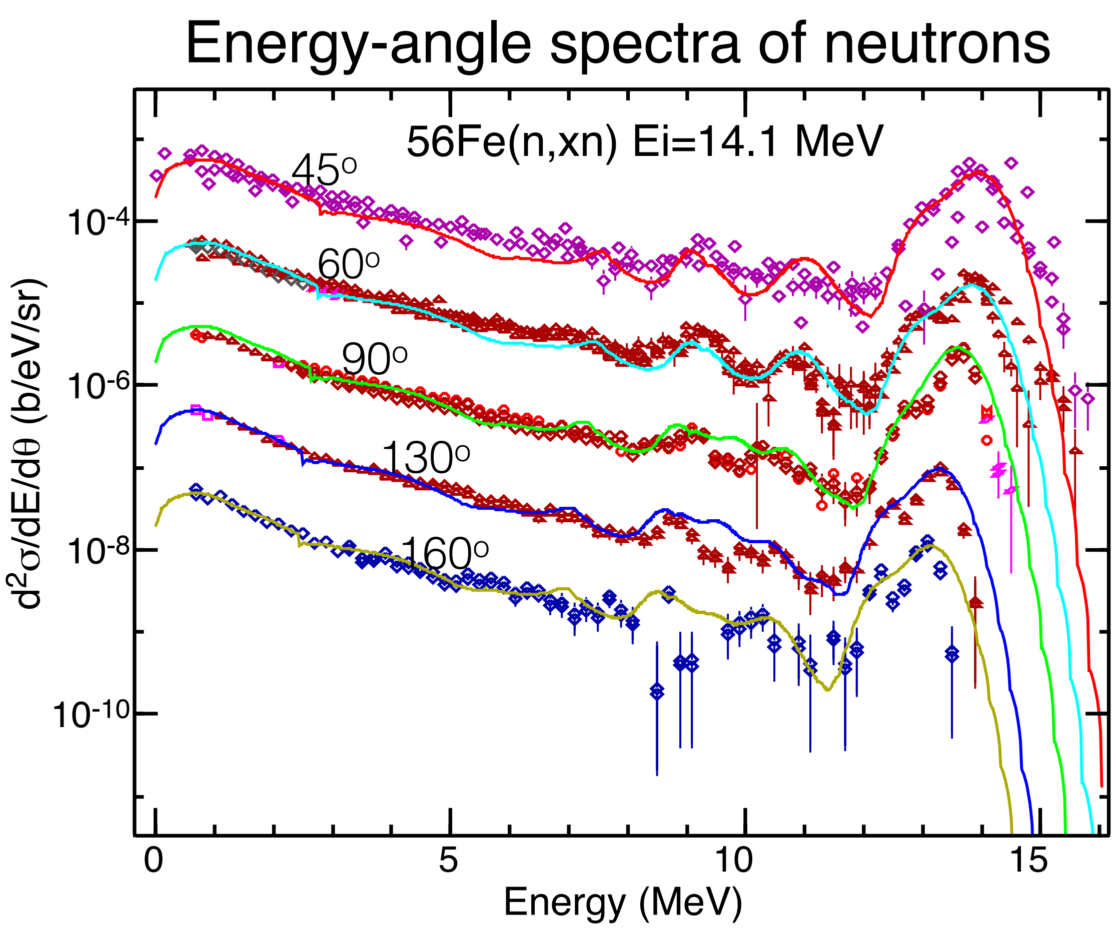
- single data points only available for: (n,np), (n,d), (n,t), (n,3He), (n, 4n), …
- …and for (n,γ) above 1 MeV
- DDX > 26 MeV: 60, 95, 150 MeV only

All nuclei, even the best measured, have gaps in data

Transport calculations require complete files

(these can be up to 30 Mb (~10^6 numbers) without covariances)

Reaction codes provide complete and consistent set of observables calculated using reaction physics models and constrained by exp. data.



Reaction codes allow to:

- maintain physically sound energy, angle, spin, parity, and mass dependencies of observables
- ensure unitarity and energy conservation
- fill gaps in the exp. data
- obtain exclusive spectra of ejectiles
- discriminate between discrepant data

Reaction codes are indispensable tools in modern data evaluation

Why EMPIRE?

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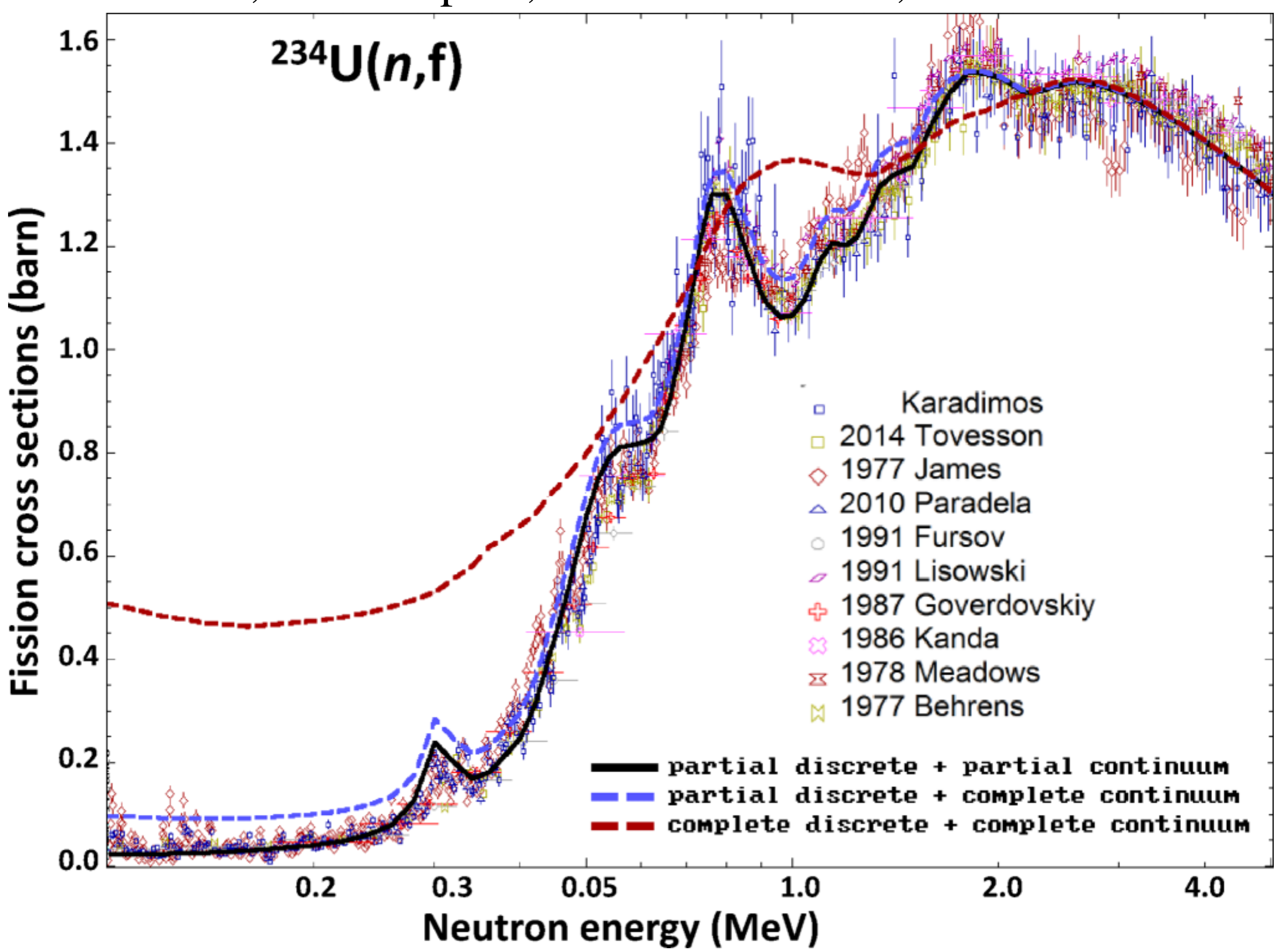


^{234}U(n,f) cross section calculated considering complete damping for class-II vibrational states and different degrees of damping for class-III vibrational states.

- Provided ~120 evaluations in ENDF/B-VIII.0b3; 75% full fast neutron evaluations including $^{\mathbf{238,235}}$**U**, ^{232}Th, $^{56,\mathbf{56},57,58}$**Fe**, $^{90\text{-}96}$Zr, ^{55}Mn
- Used for isotope production cross sections, including proton ones measured on BLIP
- Generated covariances
  - ENDF/B-VII
  - COMARA
  - Low-fidelity project

The major asset: **EMPIRE team** - 15 developers over 20 years (mostly **voluntary work!**), active core of 8 (3 BNL) contributing 300-1000 commits/year

EMPIRE-3.2 (Malta)

Nuclear Reaction Model Code

Neutron Resonances

Coupled Channels

DWBA

Optical Model

Multistep Direct

Multistep Compund

Exciton Model

Hybrid MC Simulation

HRTW

Hauser-Feshbach

Optical Model for Fission

ENDF Formatting

Verification

Kalman Filter

Covariances

EMPIRE-3.2 (Malta)

Nuclear Reaction Model Code

Atlas of n resonances

Neutron Resonances

Coupled Channels

DWBA

Optical Model

Direct reactions, absorption, T_{lj}

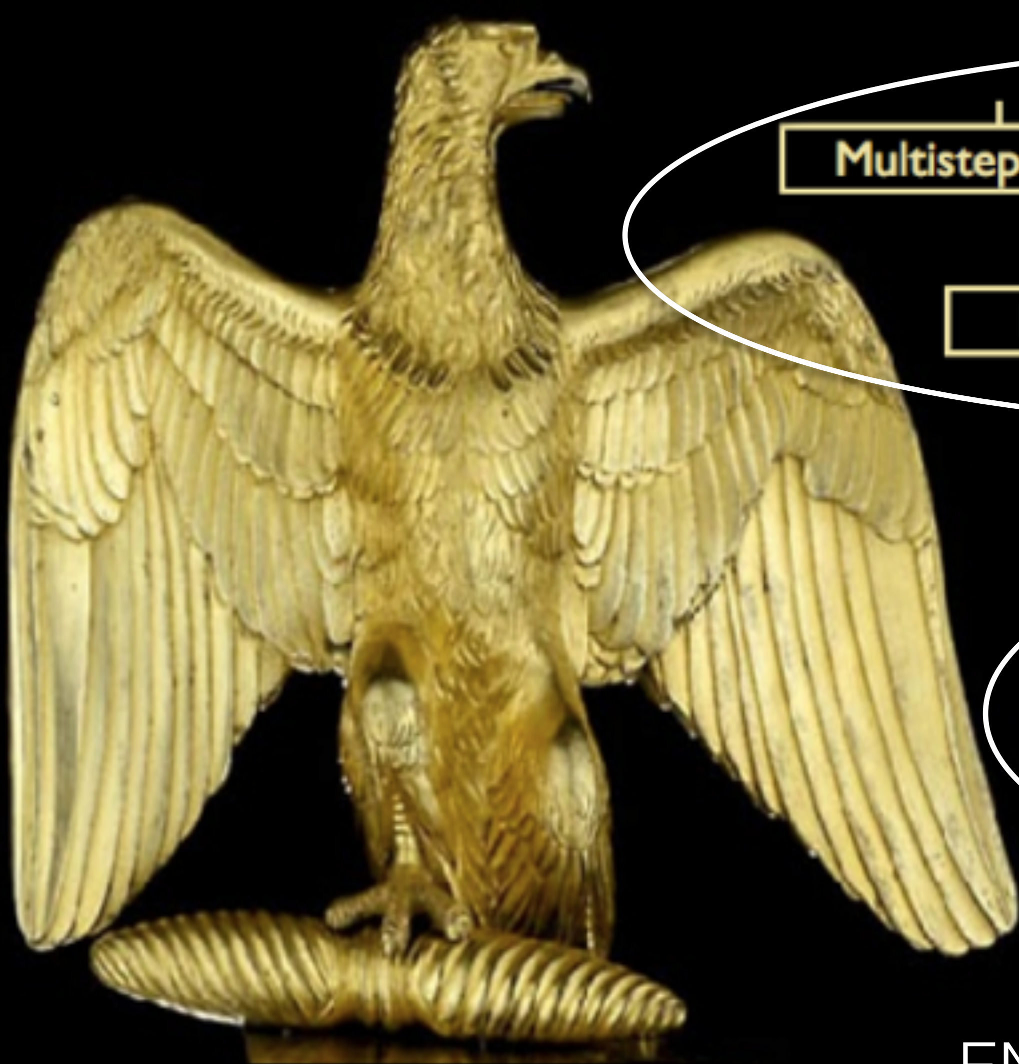
Multistep Direct

Multistep Compund

Exciton Model

Hybrid MC Simulation

Preequilibrium



HRTW

Hauser-Feshbach

Optical Model for Fission

Compound nucleus

ENDF

ENDF Formatting

Verification

Kalman Filter

Covariances

How big is EMPIRE?

- EMPIRE core: ~ 113 000 lines <= physics core
- utility codes: ~ 159 000 lines <= evaluation support
- 91 scripts: ~ 24 000 lines <= ‘framework’
- parameter library: 560 Mb <= input RIPL-3+
- EXFOR library: 1 Gb <= exp. data

For comparison:
NJOY ~110 000 lines
MCNP6.1 ~411 000 lines

What would EMPIRE benefit from?

Modernization

- Migration to Fortran90/95/…
- Implementation of unit-tests

Better physics

- Engelbrecht-Weidenmueller transformation (direct-compound interference)
- M1 scissor mode in γ-strength function (following T. Kawano)
- Direct-Semidirect capture
- K-dependent level densities (Grimes)

HPC (leverages ‘Computational Science Initiative’ thrust at BNL)

- Parallelization
- Adaptation to GPU

New features

- Support for the GND format
- Better parametrization for proton reactions - NNDC/BLIP collaboration in support of DOE isotope production
- MINUIT-based non-linear fitting and covariances