



# Reaction Theory for Radioactive Isotopes

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# LANL Focus: Compound and Pre-Equilibrium Reactions

- **Nuclear reactions on medium to heavy nuclei in the fast to a few tens of MeV**
- **CoH<sub>3</sub> statistical Hauser-Feshbach code plays the central role at LANL**
  - Recent upgrade includes:
    - width fluctuation based on GOE (PRC92, 044617 (2015), PRC94, 014612 (2016))
    - unified description of direct and compound reactions (EPJA57, 16 (2021))
    - improved fission model (PRC107, 044610 (2024))
  - Statistical decay model extended to beta-delayed neutron emission, fission fragment decay
    - CGMF / BeoH codes produce FPY and other fission-related nuclear data
- **HF-BCS + QRPA with non-iterative Finite Amplitude Method (FAM) for nuclear reaction**
  - Neutron capture and photo-induced reactions
    - E1 and M1 GDR (PRC107, 054312 (2023))
  - Quantum mechanical direct and pre-equilibrium models
    - inelastic scattering data without adjustable parameters for direct and pre-equilibrium (PRC112,054607 (2025))

# Coupled-Channels and Hauser-Feshbach Code CoH<sub>3</sub>

- **Hauser-Feshbach-Moldauer theory for compound reaction**
  - 60k+ lines C++ code, including ~180 source and ~70 header files
  - written in OOP style, ~ 80 classes defined
  - GNU Autotools package for building
- **Some special features**
  - Internal optical model / coupled-channels solver
  - **Unified description of coupled-channels and statistical model**
  - Compound nucleus decay by deterministic or Monte Carlo method
  - Accurate exclusive reaction cross sections and spectra
  - Mean-field models included (**FRDM, Hartree-Fock-BCS**)
  - Subsidiary code **BeoH**
- **Open-source**
  - <https://github.com/toshihikokawano/coh3>

```
coh.cpp
/*****
/**
/**   C o H 3 : The Hauser-Feshbach Code                               **/
/**                                     Version 3.5 Miranda   (2015) **/
/**                                     T.Kawano                **/
/**   History                                                                **/
/**   3.0 Callisto : developing version for full Hauser-Feshbach (2009) **/
/**   3.1 Ariel   : fission modeling                                       (2010) **/
/**   3.2 Umbriel : COH + ECLIPSE unified version                         (2012) **/
/**   3.3 Titania : advanced memory management version                   (2013) **/
/**   3.4 Oberon  : mean-field theory included version                   (2015) **/
/**   3.5 Miranda : coupled-channels enhanced version                     (2015) **/
/**                                                                **/
/*****/
#include <string>
#include <iostream>
#include <sstream>
#include <iomanip>
#include <cstdlib>
#include <cstring>
#include <cmath>
#include <unistd.h>

using namespace std;
#define COH_TOPLEVEL
--:---- coh.cpp      Top (15,0)   Git-develop (C++// Abbrev)
```

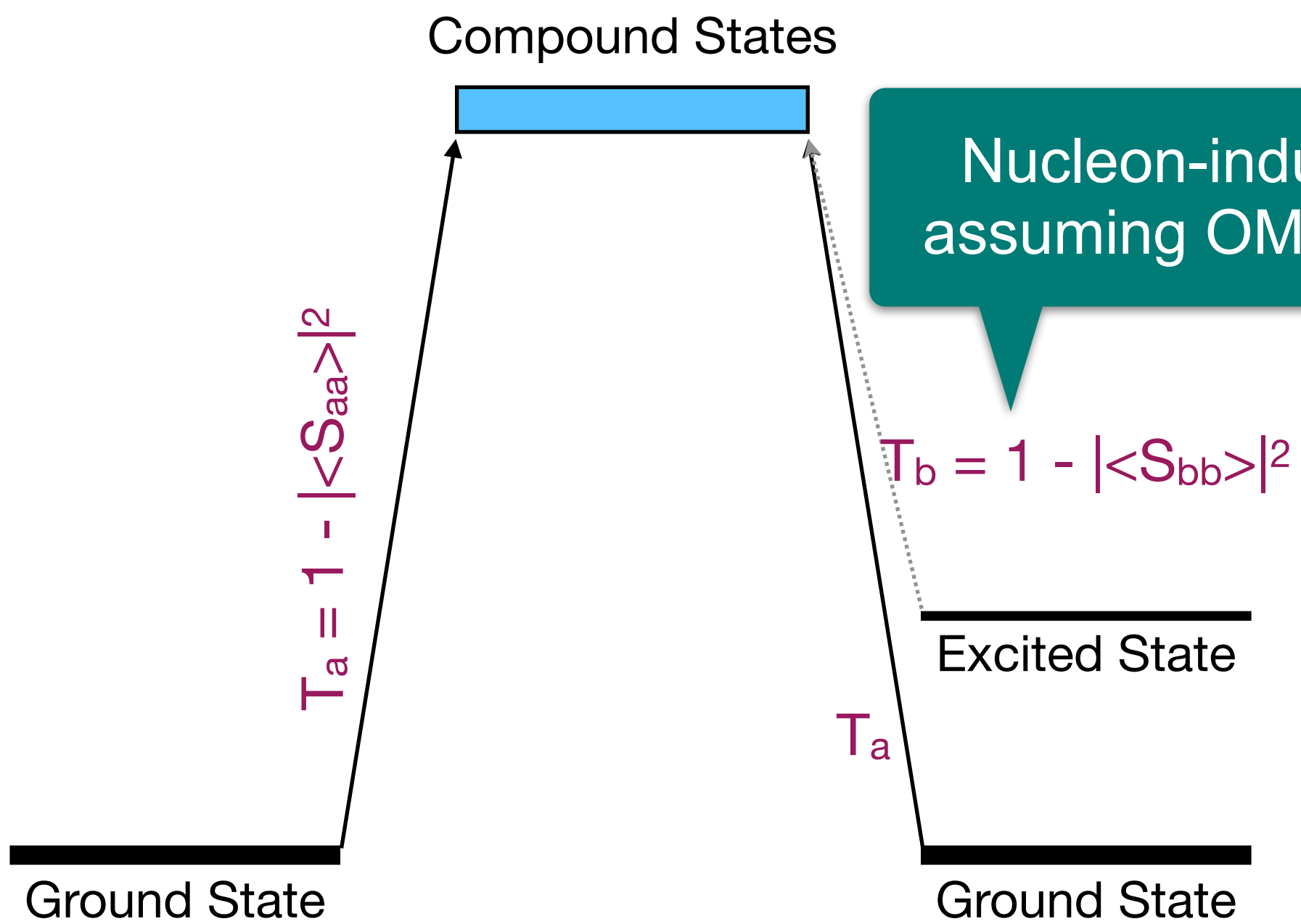


# Spherical and Deformed Targets

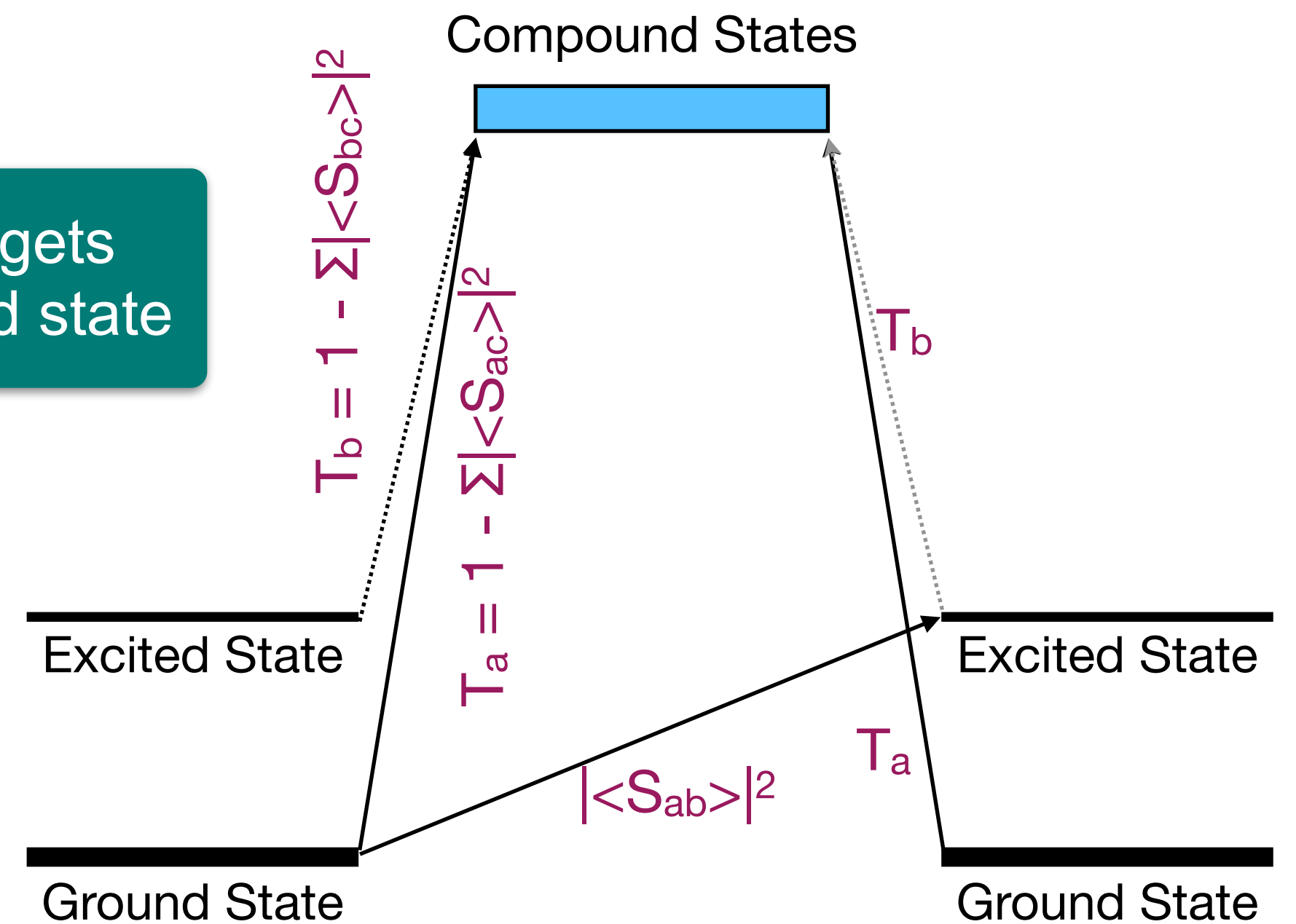
- **Single channel optical model**
  - target is spherical, S-matrix is diagonal
- **Coupled-channels optical model**
  - target is deformed, Include off-diagonal elements
  - generalized transmission coefficients (default)
  - or P-matrix in the EW transformation option

Generalized transmission coefficients in the coupled-channels formalism

$$T_{lj}^{(n)} = \sum_{J\Pi} \sum_a \frac{2s+1}{2j_a+1} g_J \left( 1 - \sum_b |S_{ab}^{J\Pi}|^2 \right) \delta_{n_a, n} \delta_{l_a, l} \delta_{j_a, j}$$

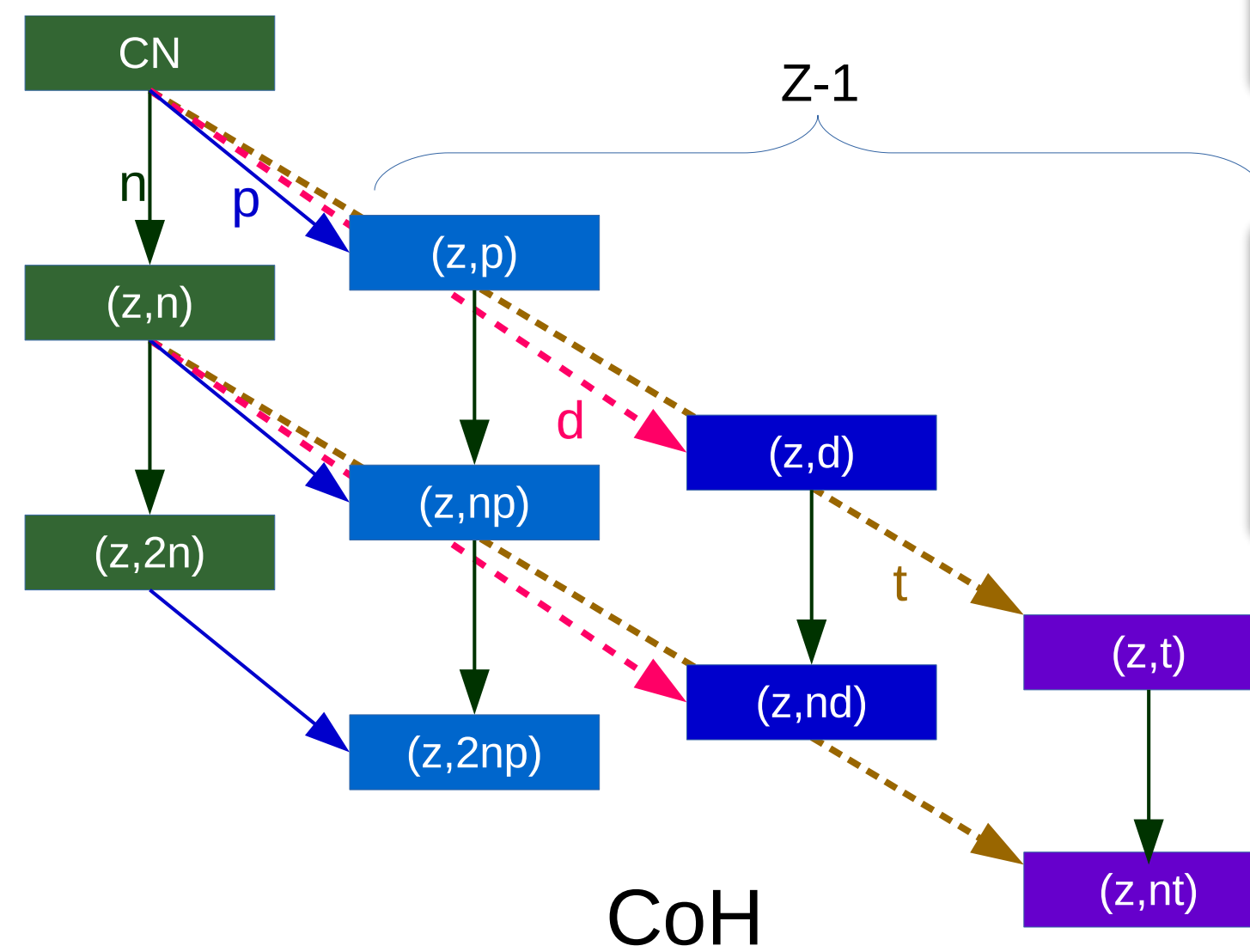
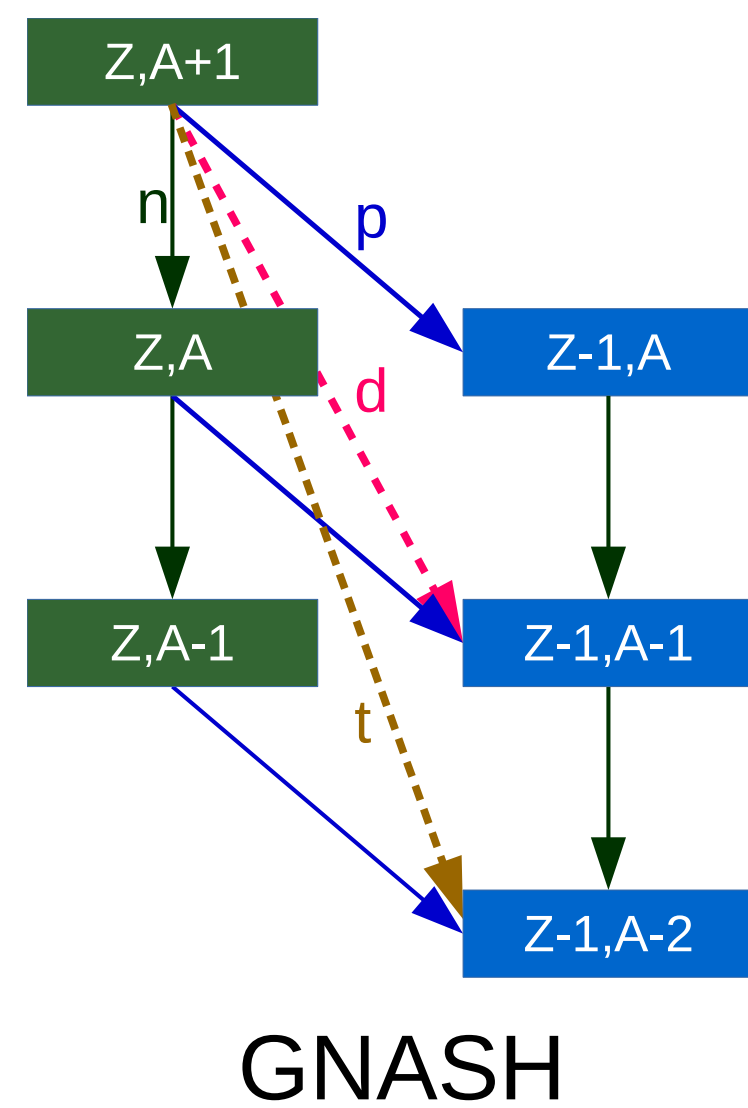


Nucleon-induced reaction on excited targets assuming OMP is the same as the ground state



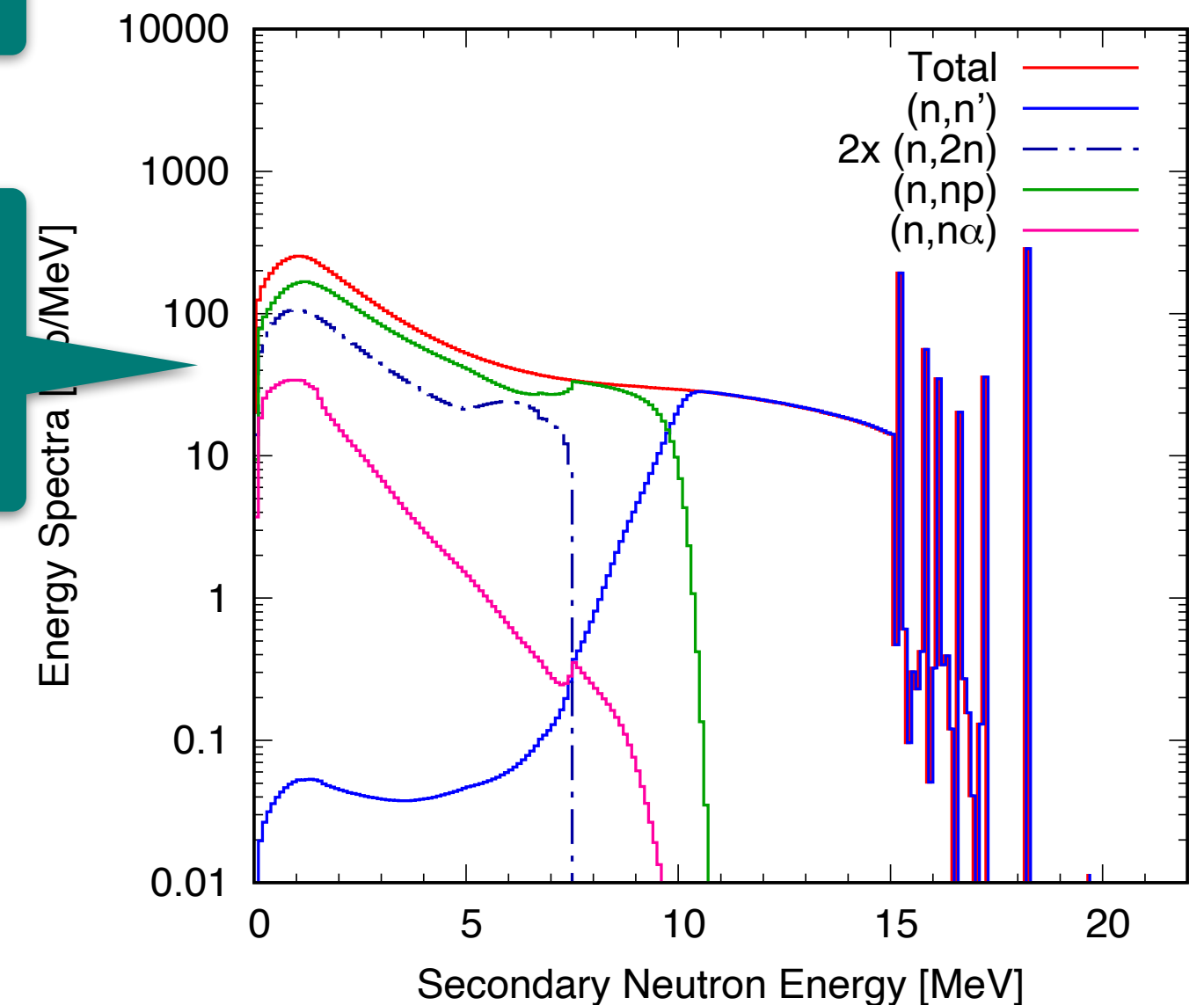
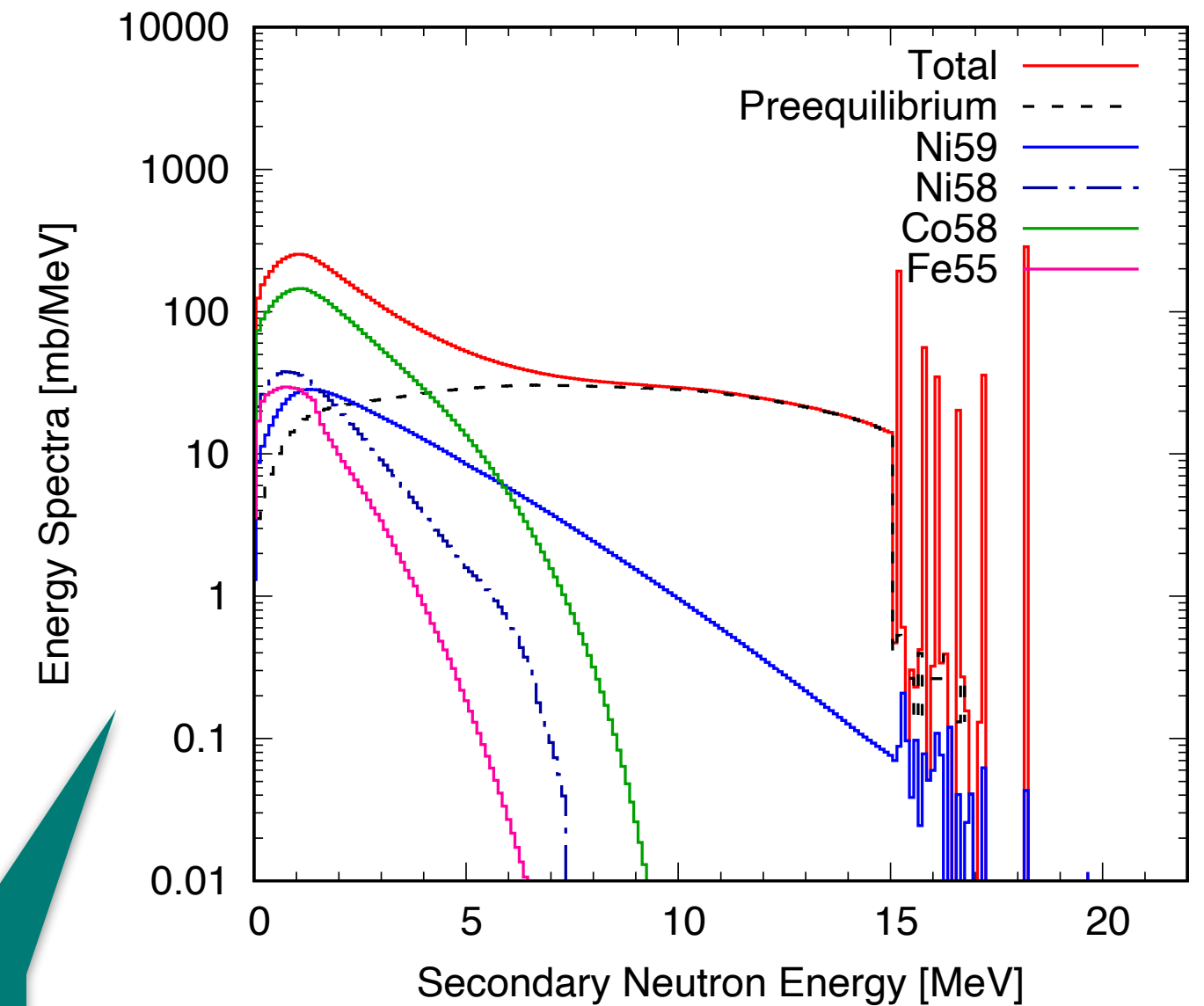
# Multi-Particle Emission and Exclusive Spectrum

- Historically Hauser-Feshbach codes lump the same residuals
  - can save memory, but needs some tricks to distinguish different reactions
- CoH creates independent objects for different reactions to disentangle individual reactions
  - each of reaction channels is clearly separated, but requires more memory



Model calculation

Special algorithm to decompose into exclusive spectrum

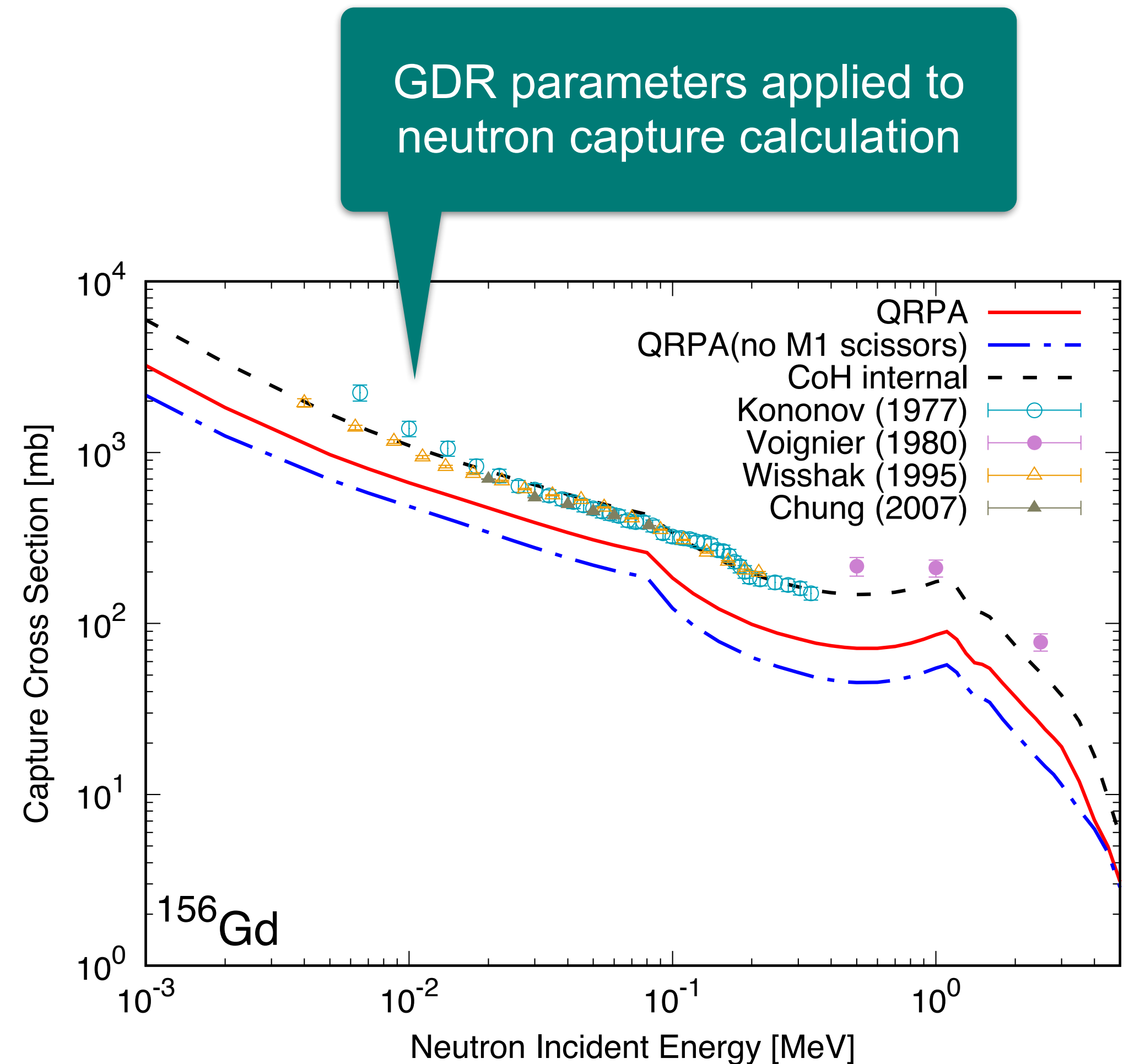
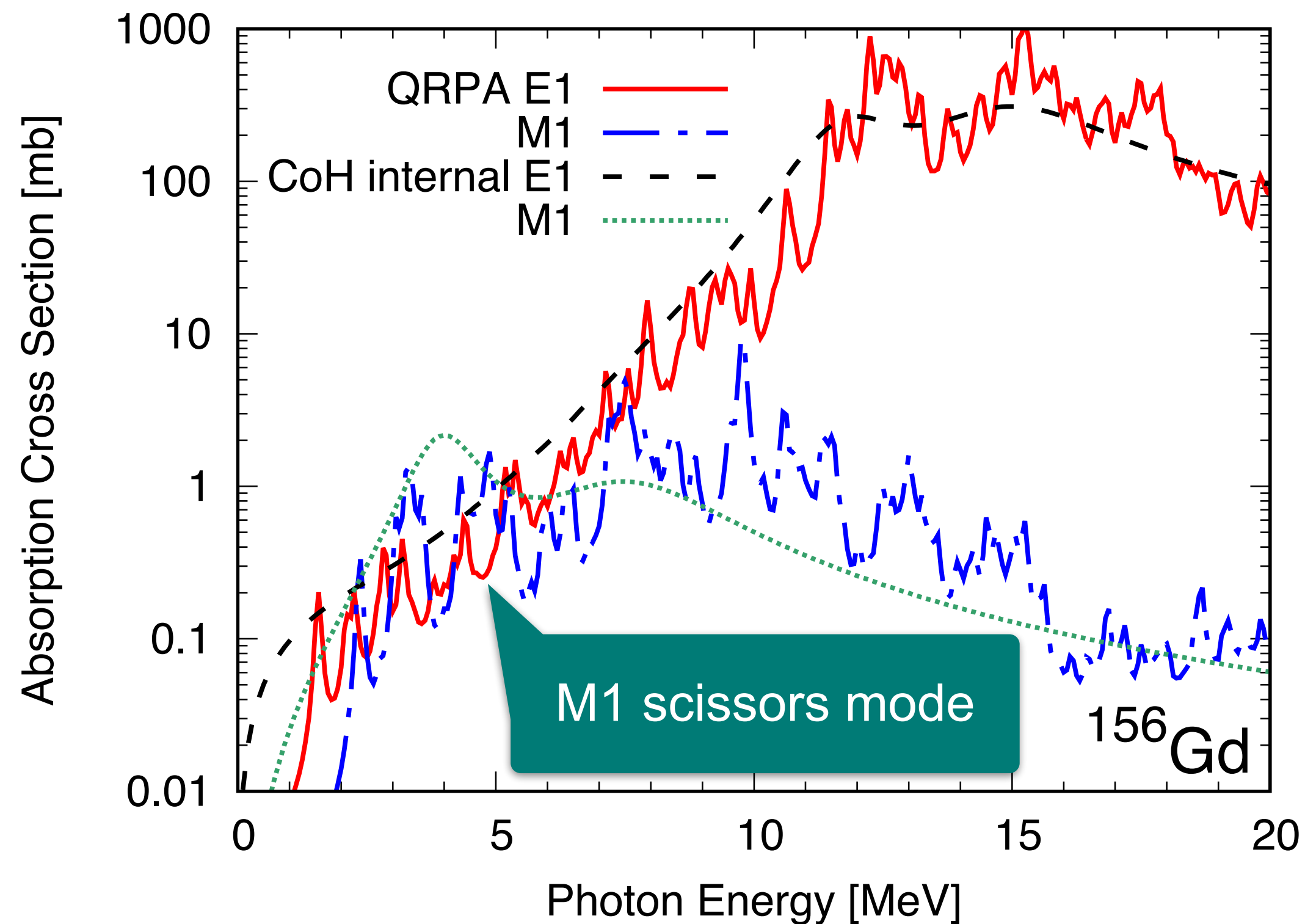


# Beyond Optical Model + Hauser-Feshbach Theory

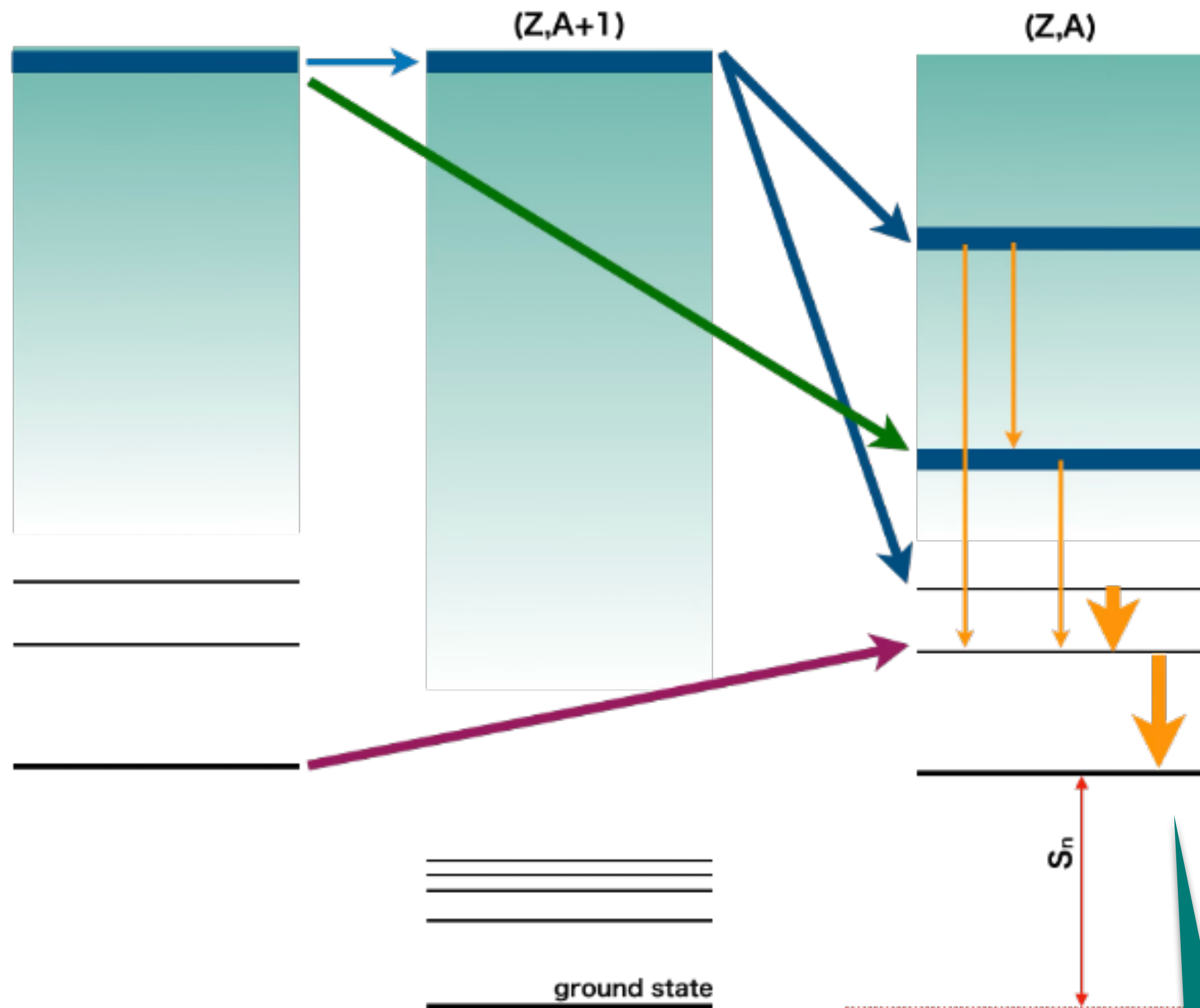
- **Photon channel**
  - Neutron capture reaction as an inverse process of photo-nuclear reaction
  - Transmission coefficient of photon is calculated by the photo-absorption cross section
    - Macroscopic Giant (Dipole etc) Resonances
    - Microscopic models - QRPA or FAM approaches
- **Fission channel**
  - Fission is not a simple inverse process of heavy ion fusion
  - Calculation of fission transmission coefficient strongly model dependent
- **Non-statistical reactions**
  - Coupled-channels, DWBA, Direct/SemiDirect capture, composite particle interactions, ...
  - Pre-equilibrium emission
    - Exciton model widely used, but no quantum mechanical effects
    - MSC/MSD calculation still expensive, but FAM approach is promising

# Non-Iterative Finite Amplitude Method (Photons and Pre-Equilibrium)

- **Fast calculation of QRPA developed by H. Sasaki**
  - Iteration procedure not required
  - So far applied to
    - photo-absorption (gamma-ray transmission coefficient)
    - Neutron inelastic scattering



# Impact of Initial Spin/Parity on Inelastic Scattering (Meta-Production)



- **Compound reaction**

- spin distribution in the (Z,A+1) CN is determined by the target spin and neutron transmission coefficients
- final state can be either in the continuum or discrete levels

- **Direct reaction**

- gamma-ray production = direct reaction cross section
- coupled-channels or DWBA

- **Pre-equilibrium process**

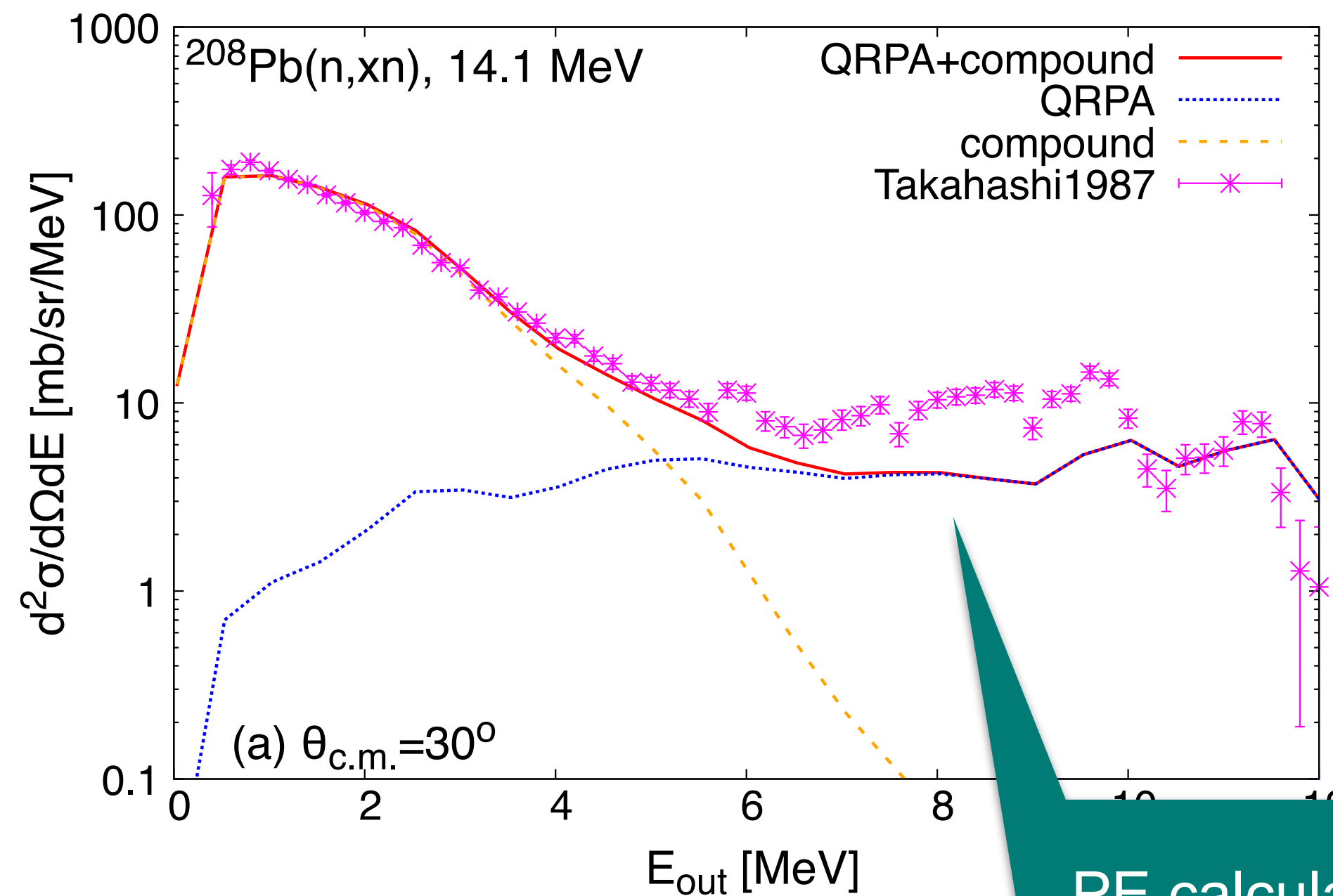
- populate the continuum directly
- smaller degree-of-freedom (limited spin transfer)

Gamma-rays are sensitive to spin/parity conservation

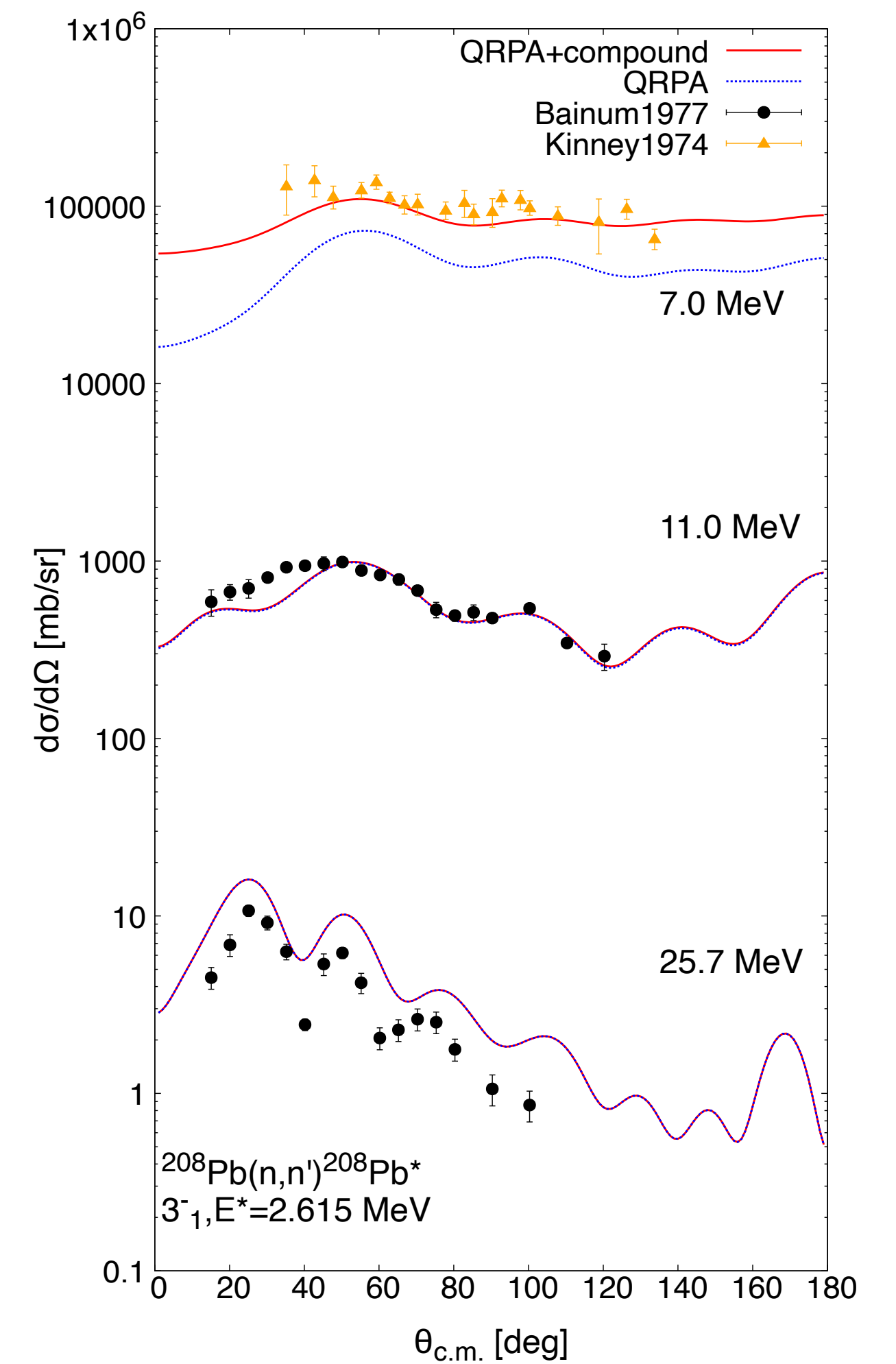
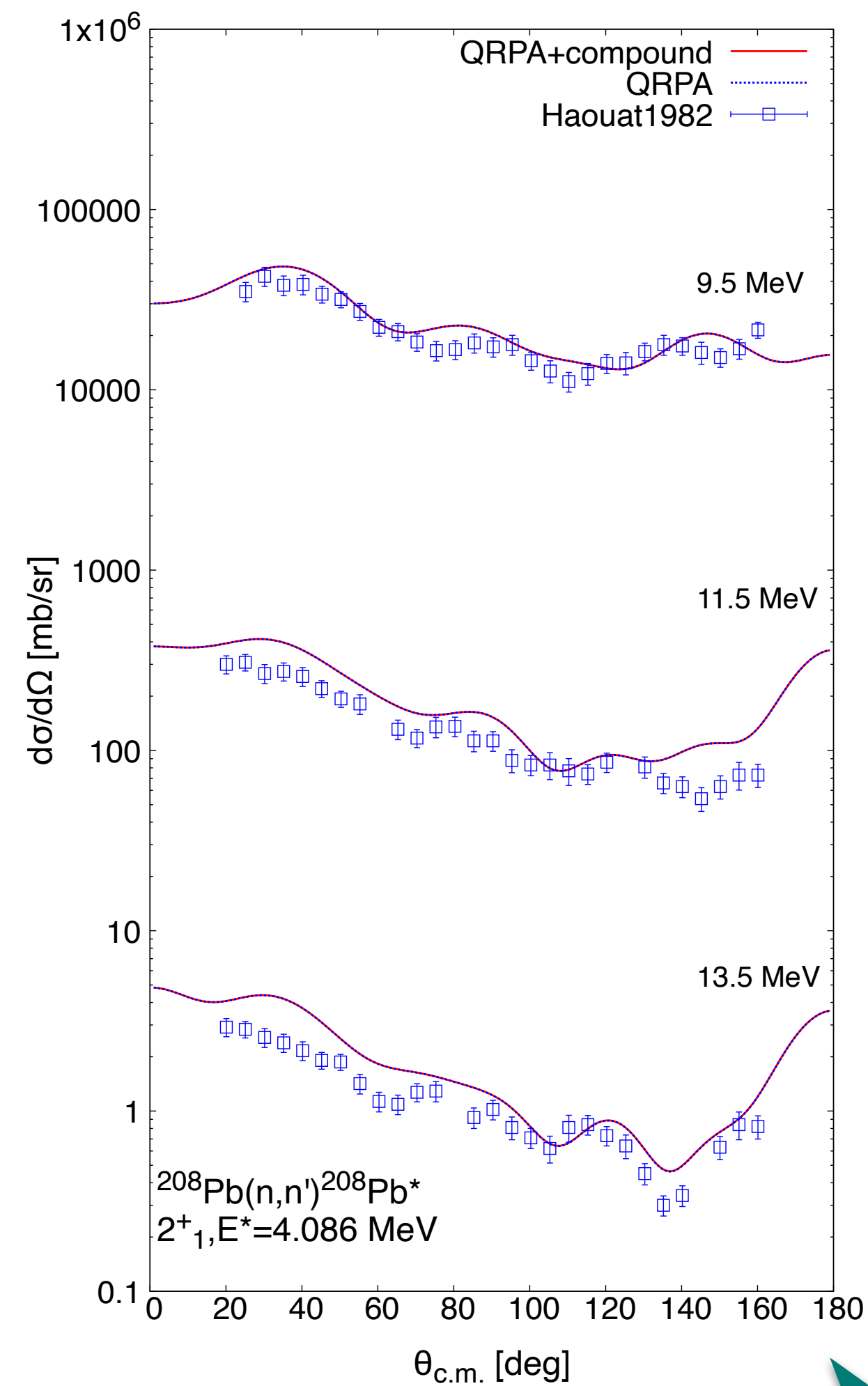
Microscopic approaches to DI and PE in a consistent manner

# Inelastic Scattering off $^{208}\text{Pb}$ , No Adjustable Parameters

- Microscopic approach to calculate  $(n,n')$  c.s. for both discrete and continuum final states
- Hartree-Fock BCS and Skyrme interaction
- non-Iterative Finite Amplitude Method (FAM) to solve Quasi-particle Random Phase Approximation (QRPA)



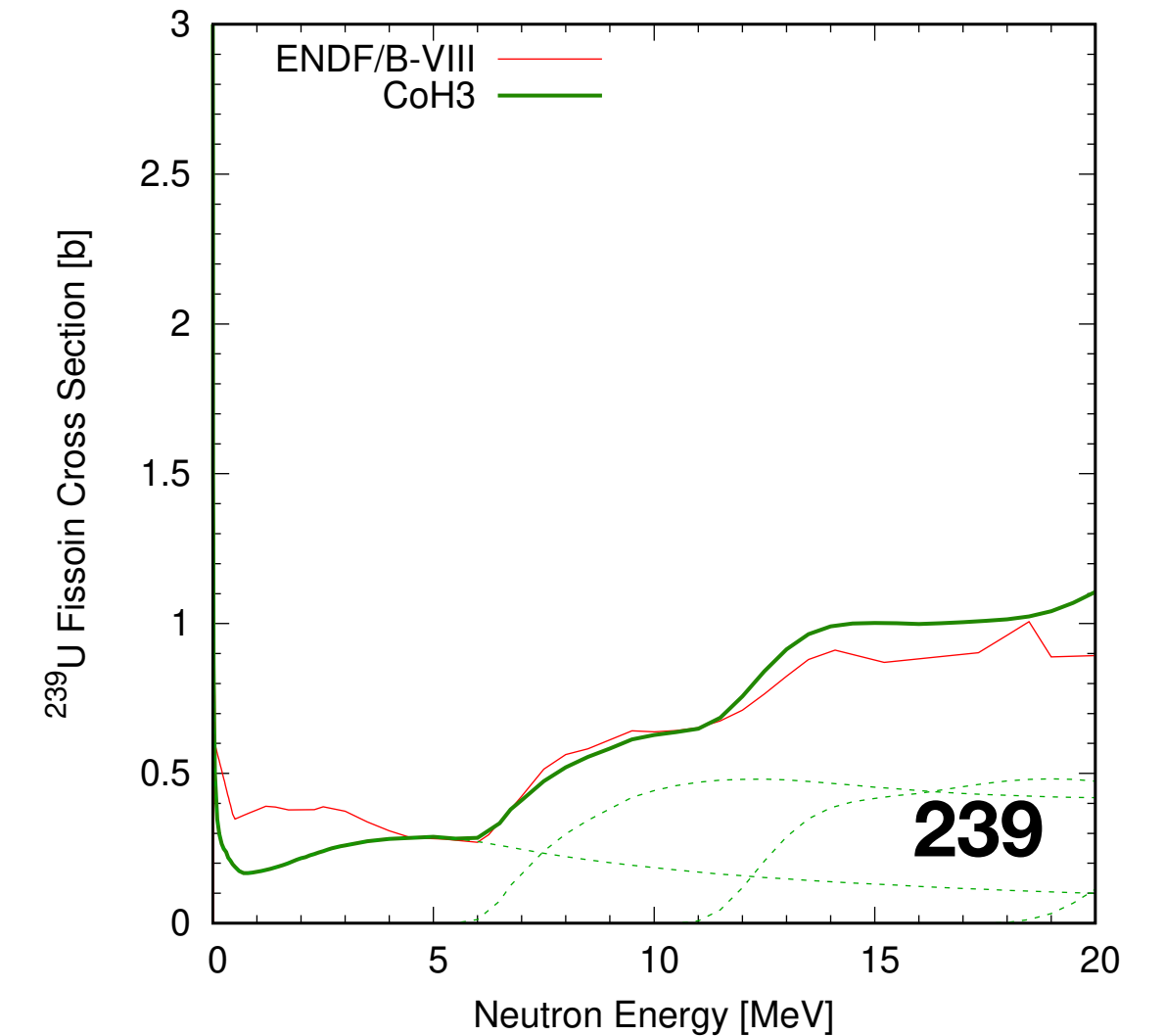
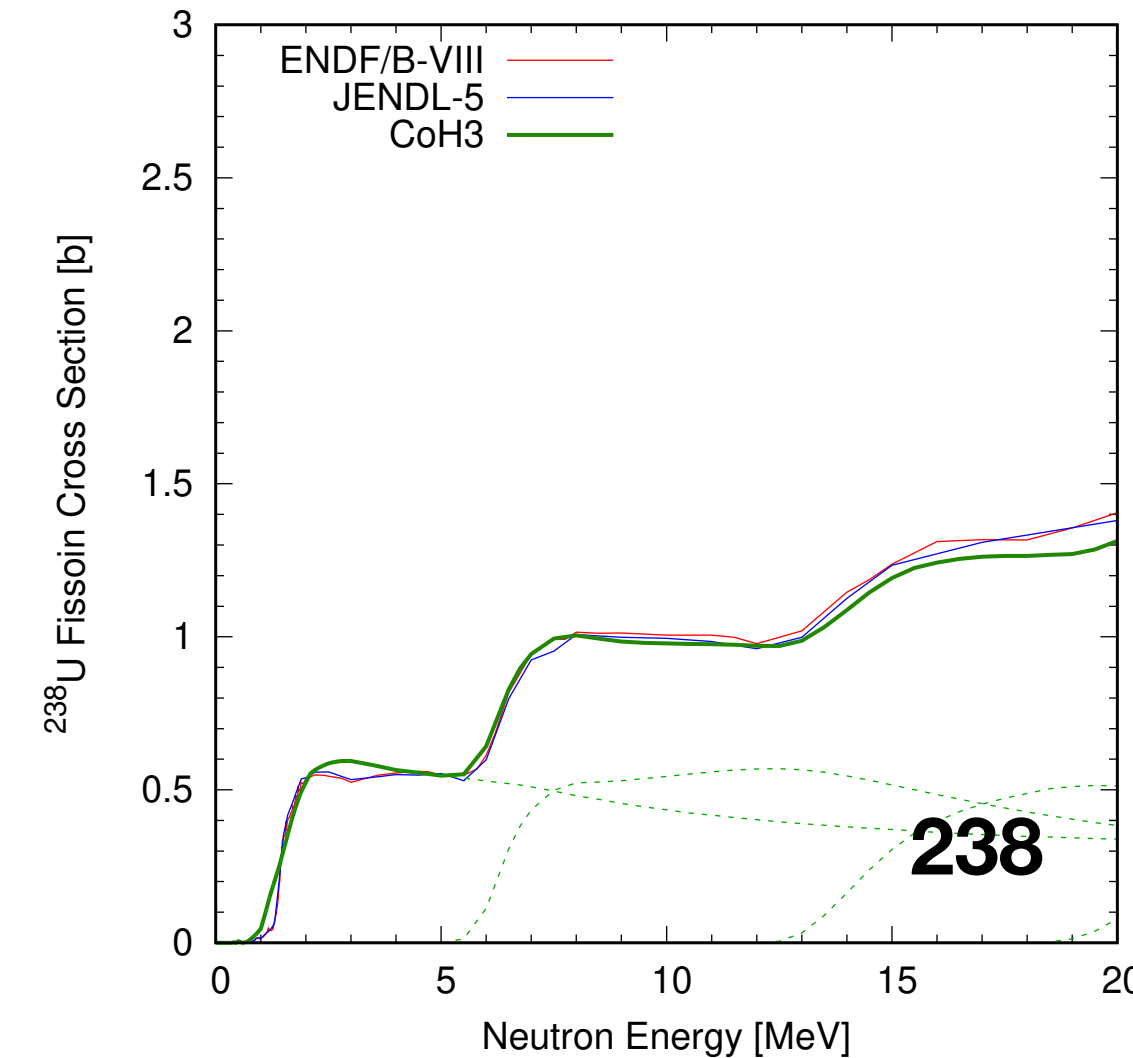
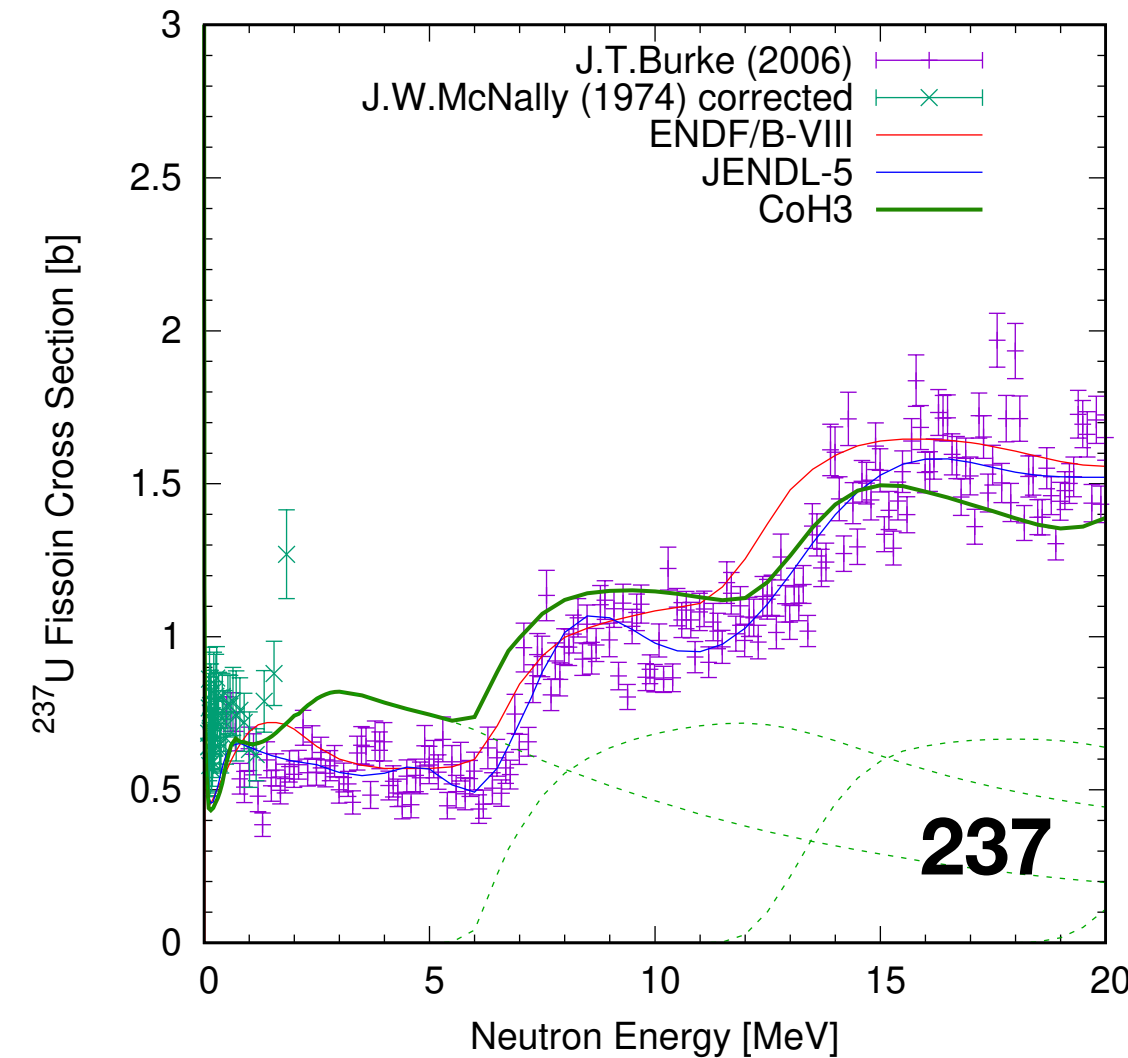
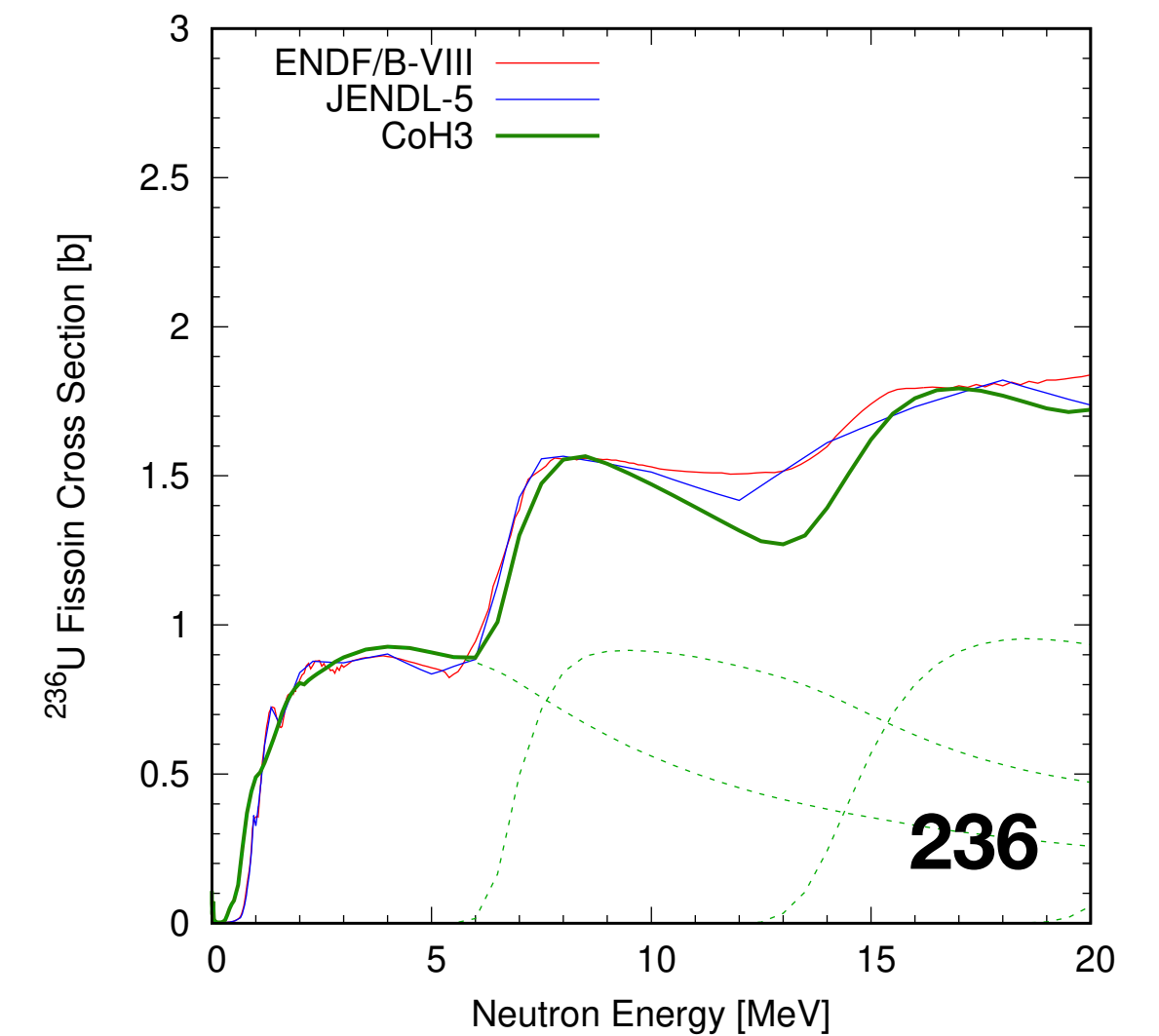
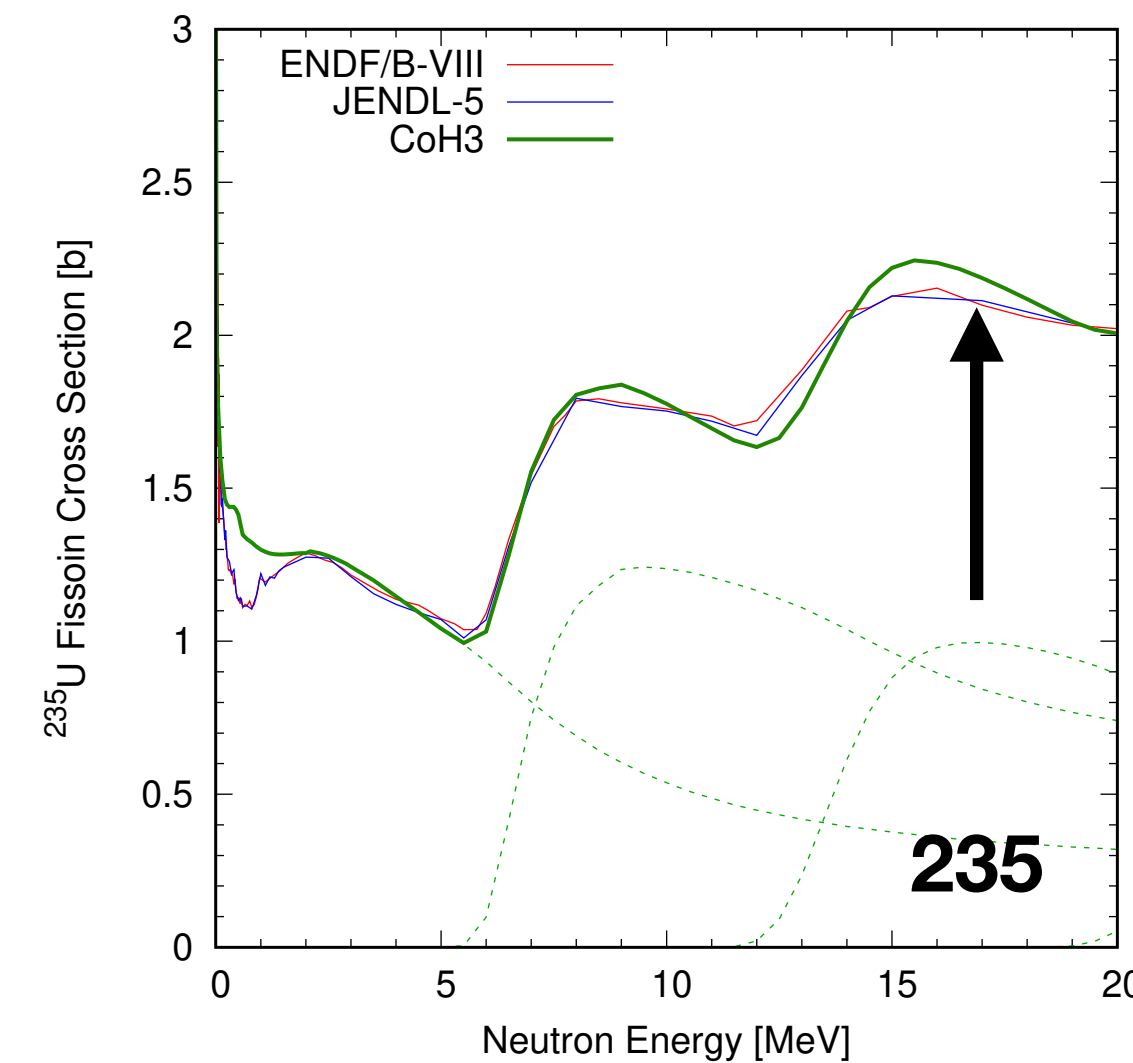
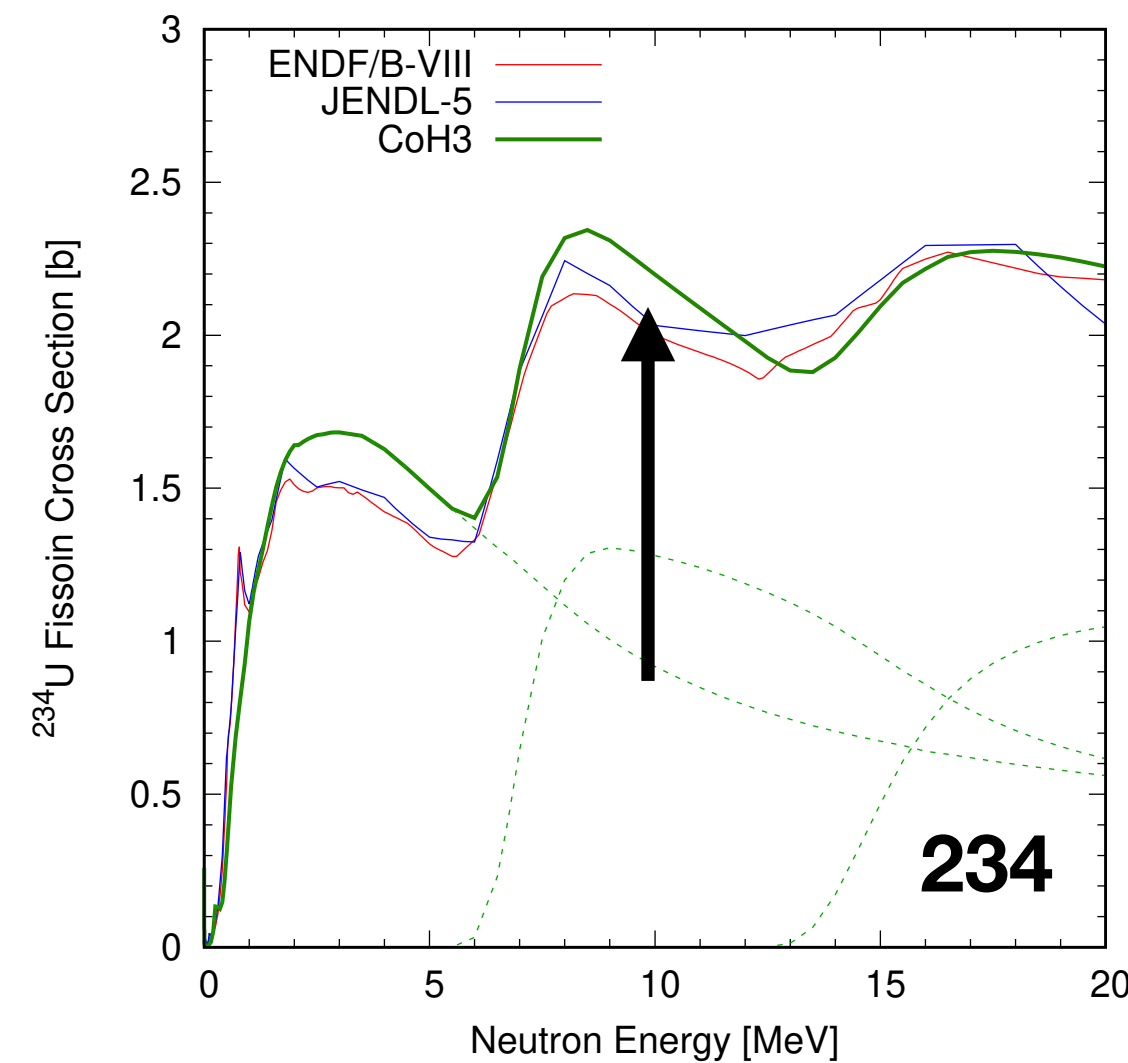
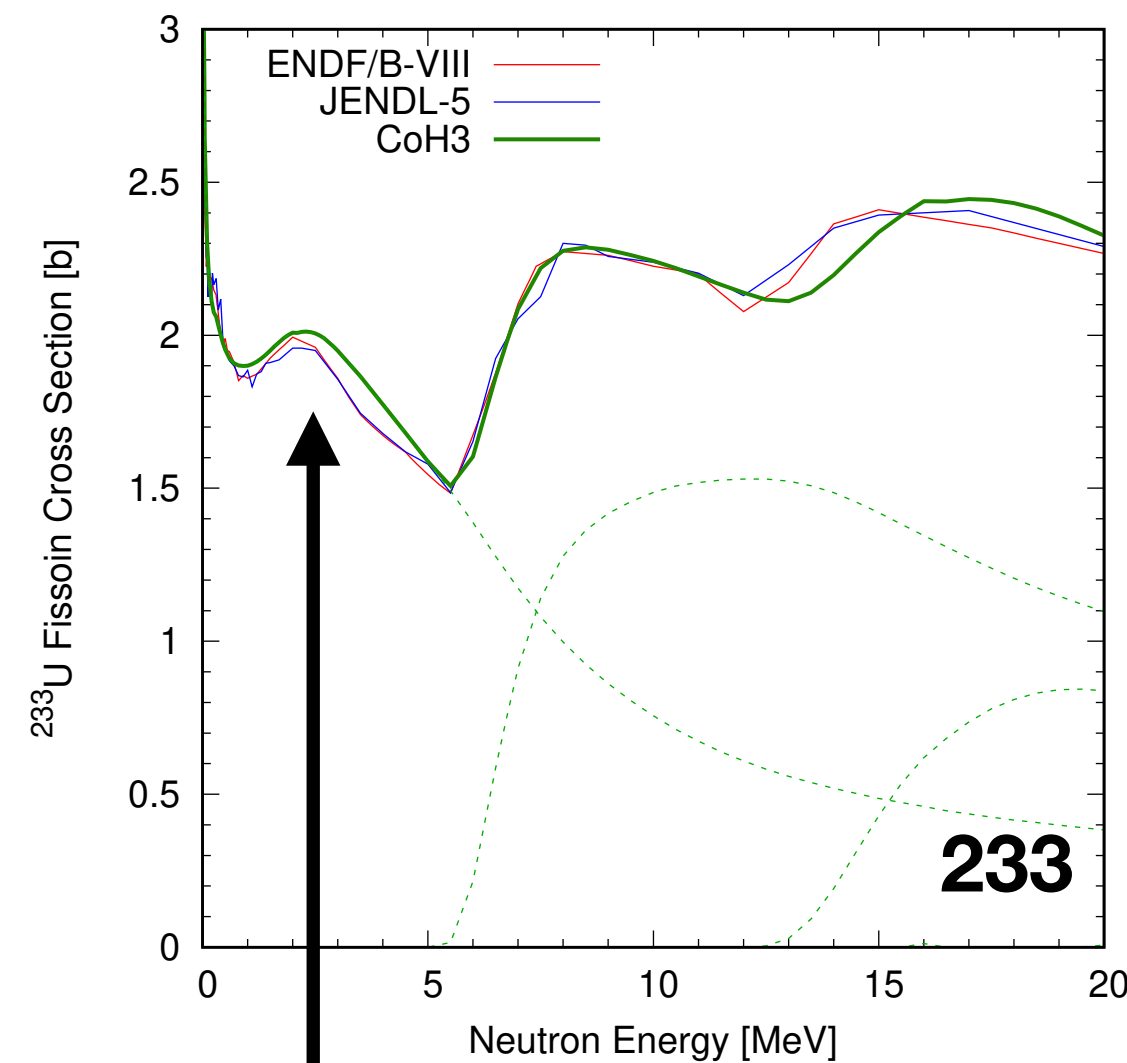
PE calculation, same basis as DI



No experimental deformation parameters needed

# Consistent Calculation of Fission Cross Sections (First Time!)

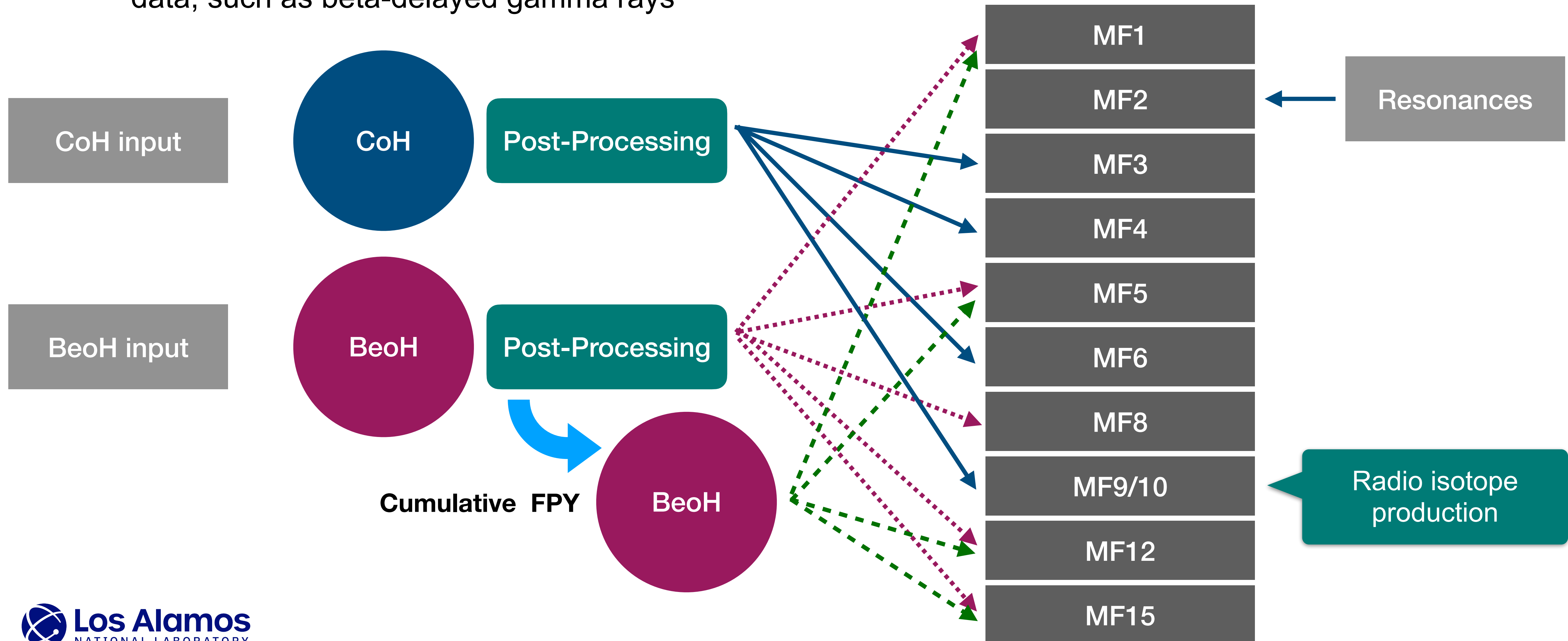
- Our new fission model applied to U isotopes from  $A = 233$  to  $239$ 
  - There is no direct measurement of  $^{237}\text{U}$  and  $^{239}\text{U}$  fission cross sections



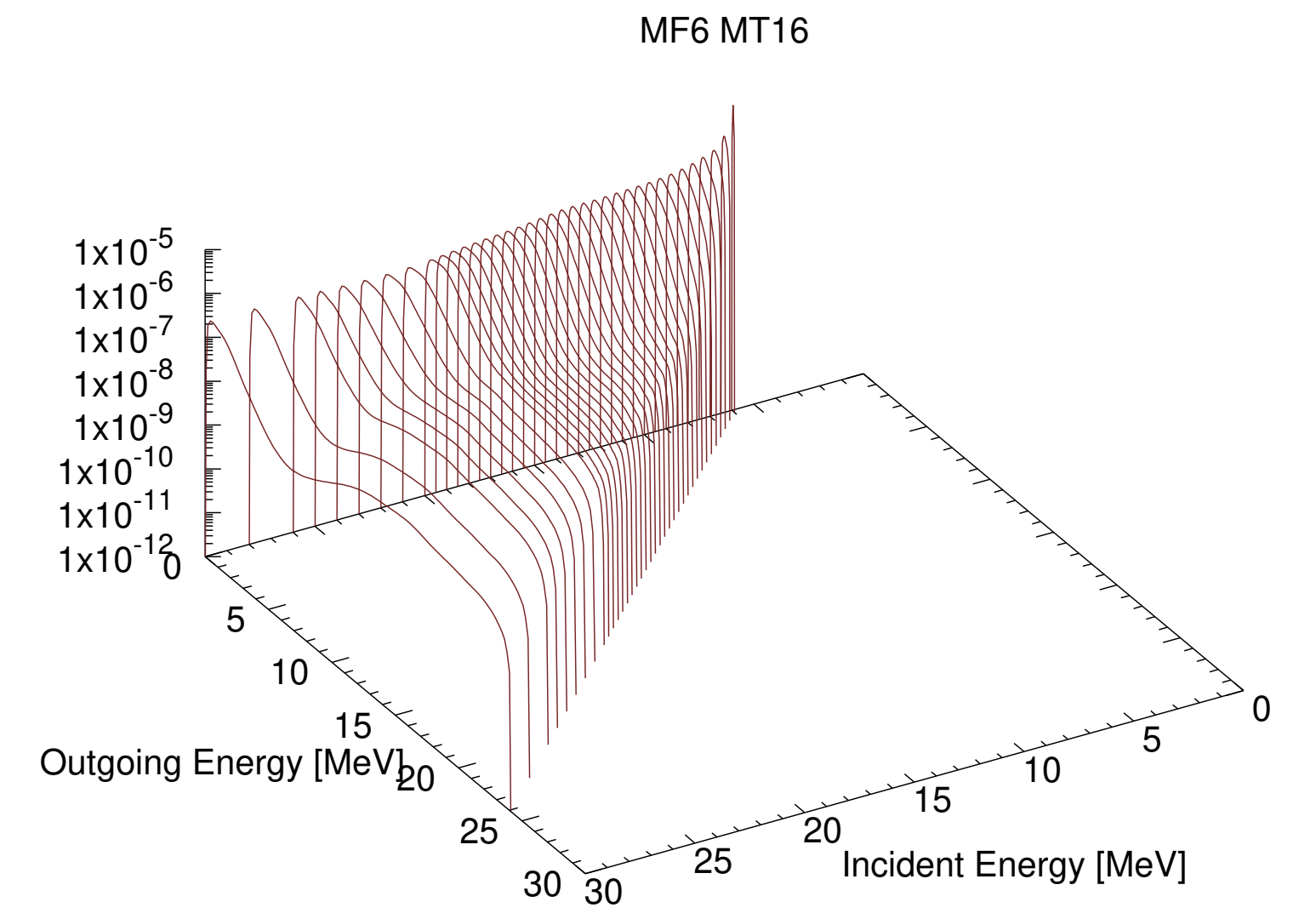
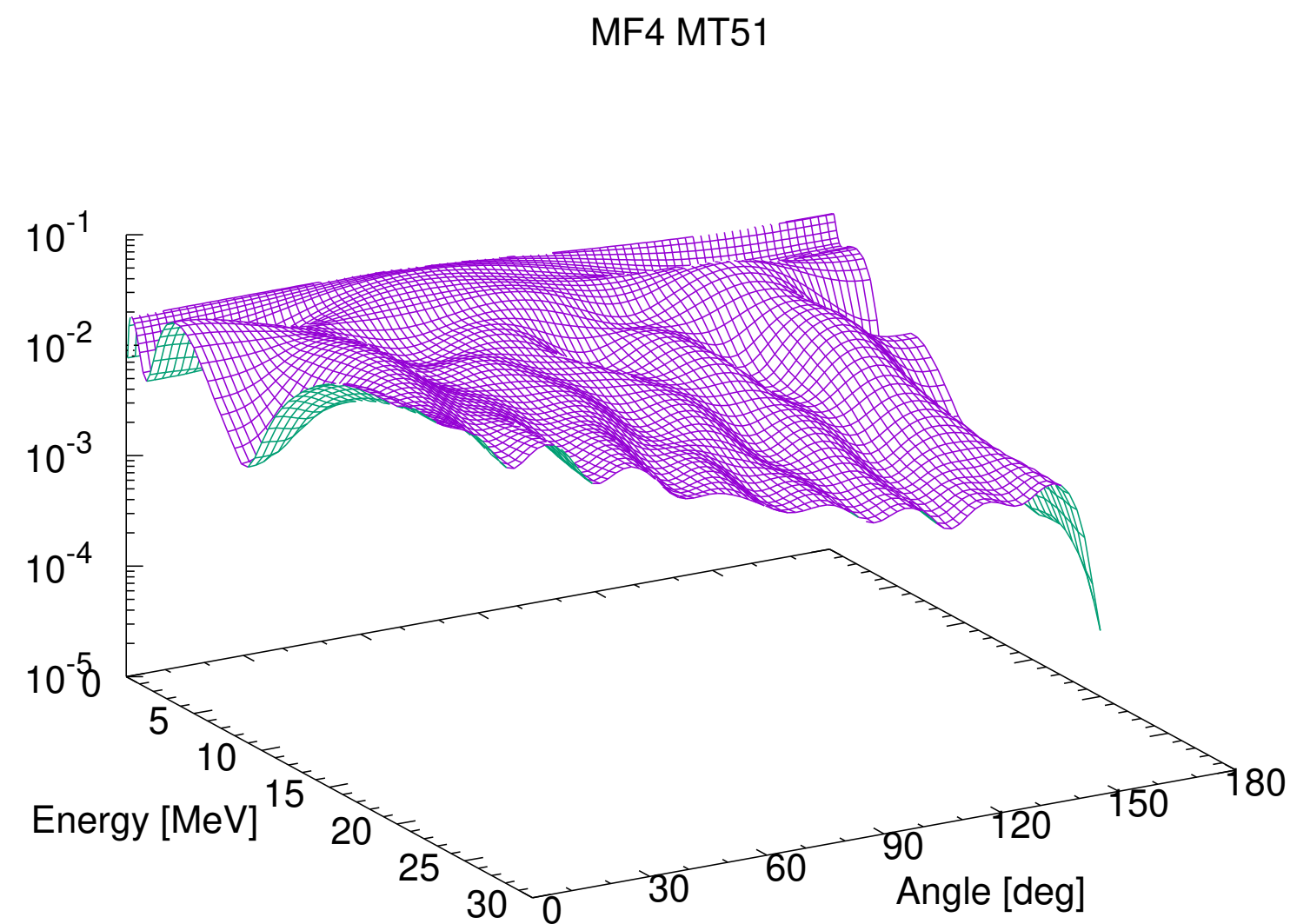
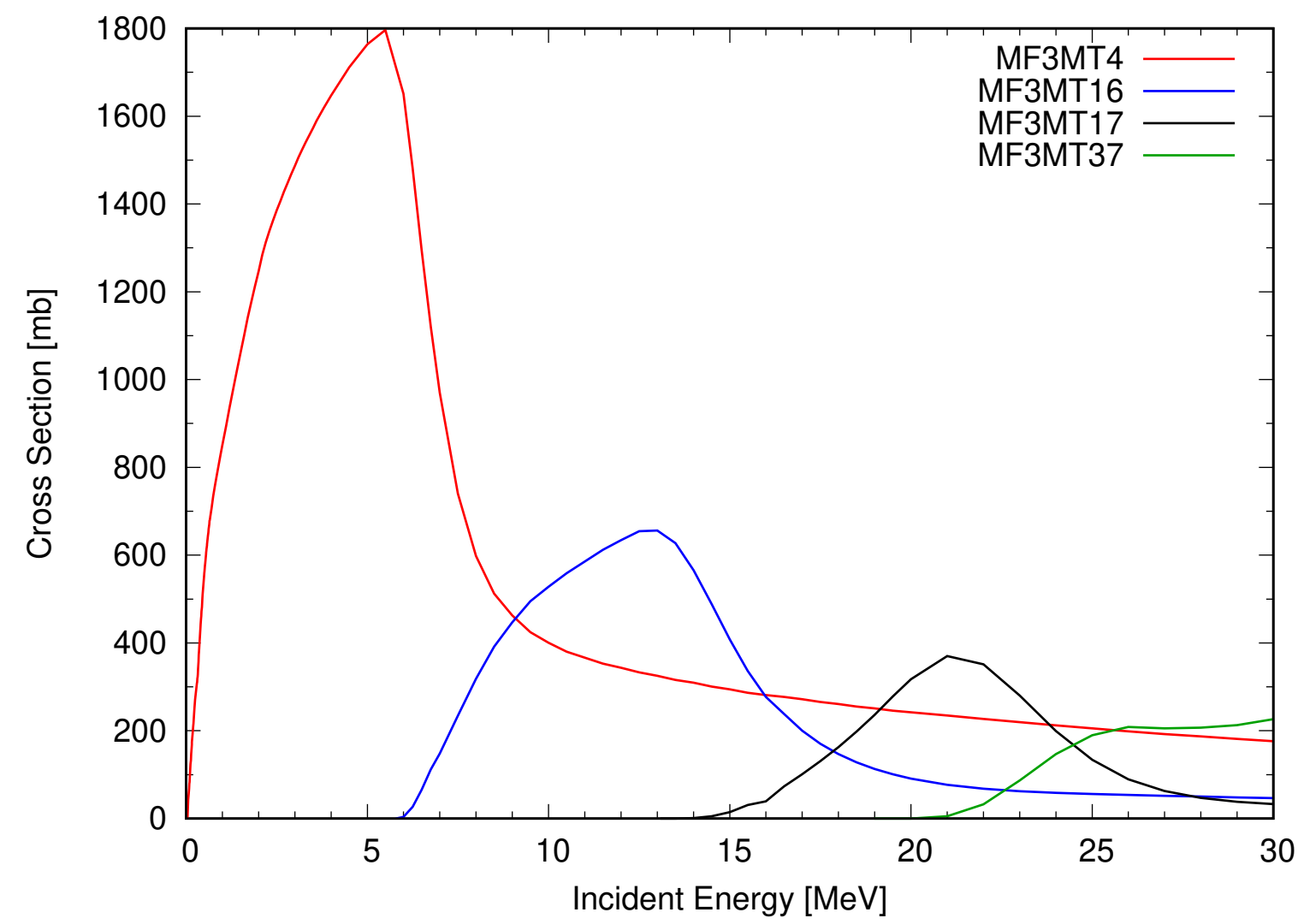
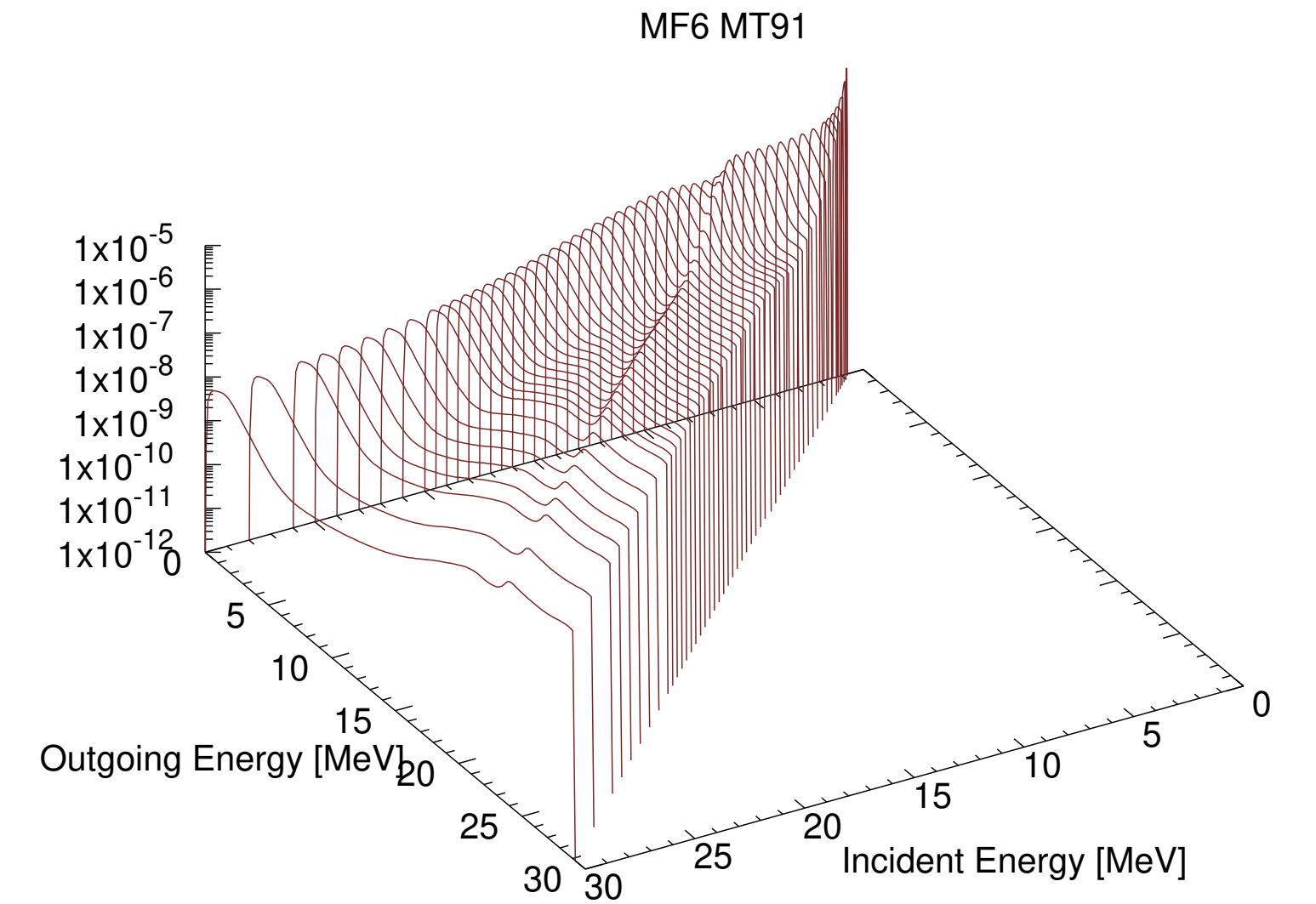
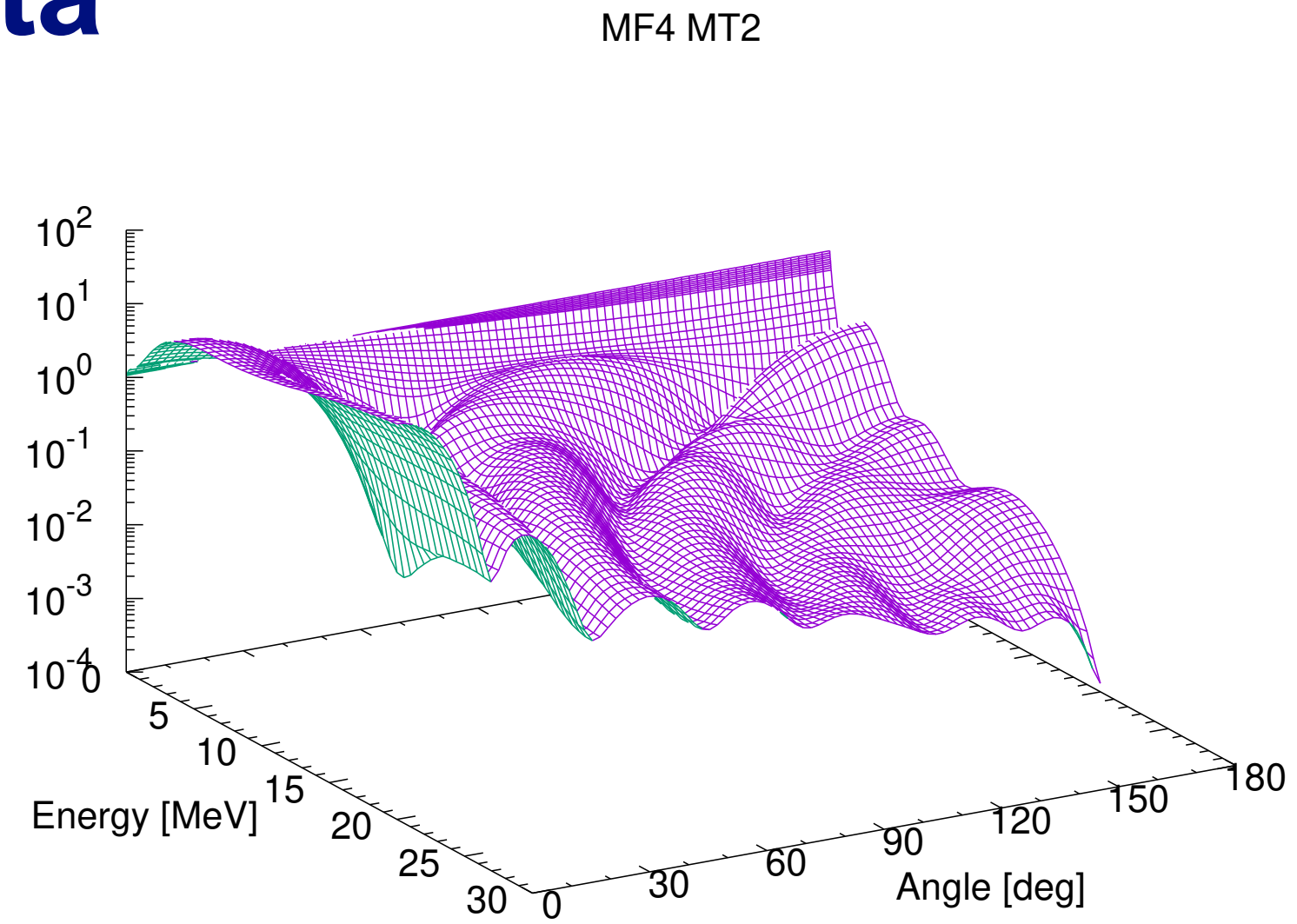
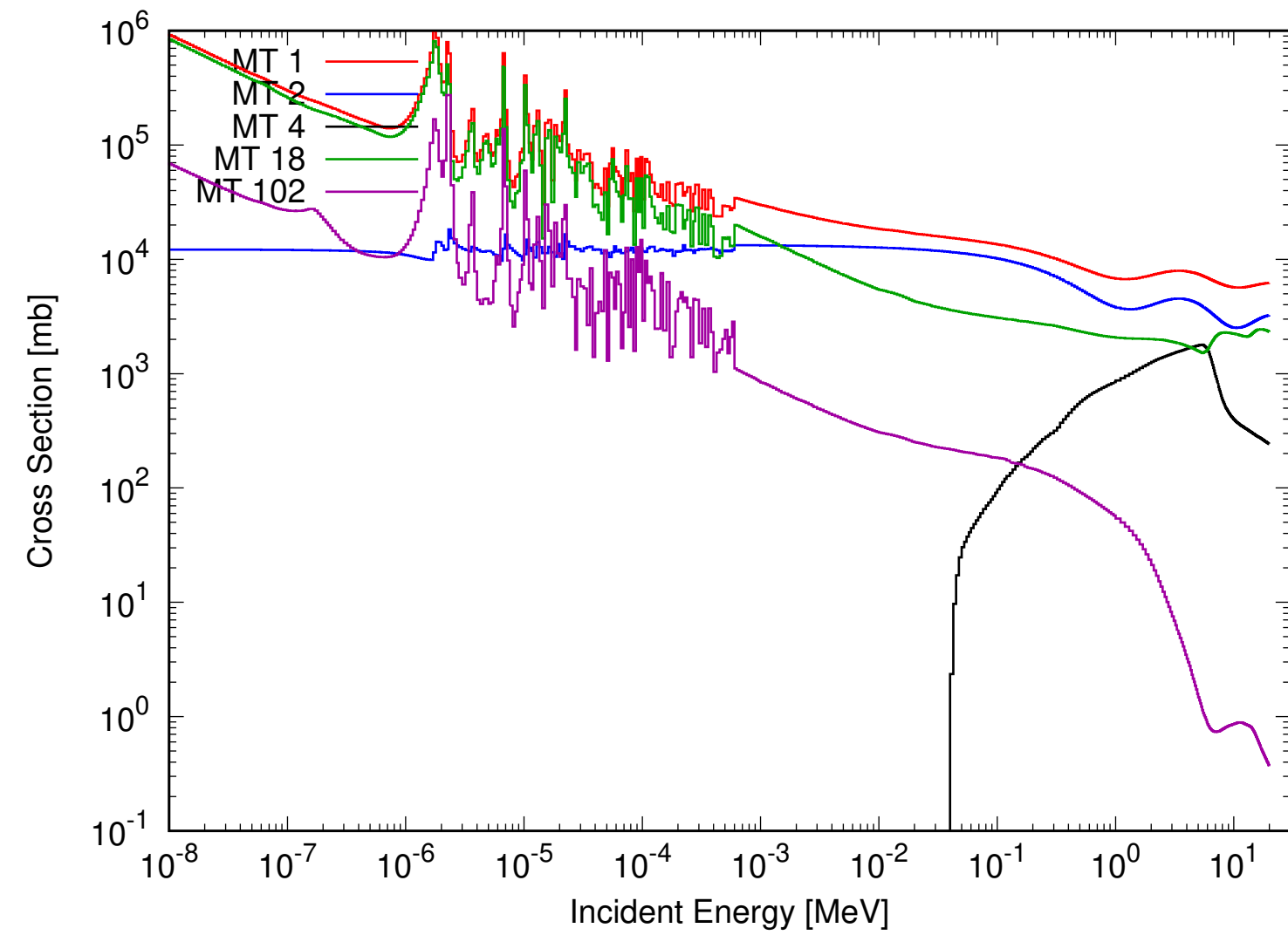
Same fission parameters for  $^{234}\text{U}$  used

# Los Alamos CoH<sub>3</sub>-based Evaluation: LACE

- **Production of all nuclear data using the CoH<sub>3</sub> and BeoH codes (with external resonance files)**
  - Facilitate to produce evaluated nuclear data files automatically, and provide not-so-commonly used data, such as beta-delayed gamma rays



# LACE Example $^{233}\text{U}$ Data



# Concluding Remarks

- **LANL nuclear reaction theory effort in the keV to 10x MeV region**
  - where many nuclear energy technologies, both fission and fusion, require accurate nuclear data
- **Microscopic nuclear structure theory for nuclear reaction calculation**
  - neutron capture with the GDR calculation by FAM
  - neutron direct and pre-equilibrium inelastic scattering with FAM
  - simultaneous calculation of fission cross section and fragment distribution (not in this talk)
- **Maintaining model codes essential to implement of advanced nuclear theories**
  - we try to make them open-source to stimulate the nuclear data community
  - just using existing codes as an evaluation tool does not have any scientific improvements
- **Nuclear data file production**
  - post-processing by the ENDF manipulation code DeCE available (open-source)
  - a new framework LACE to produce evaluated nuclear data at LANL, automates production of model-calculation-based evaluations