Reaction Theory Development at LANL

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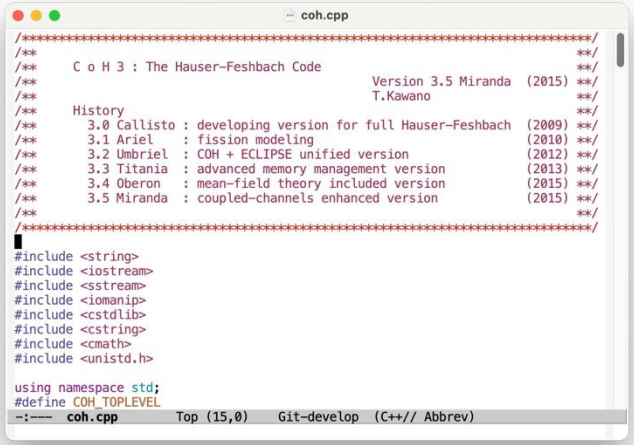
LANL focus: Compound and Pre-Equilibrium Reactions

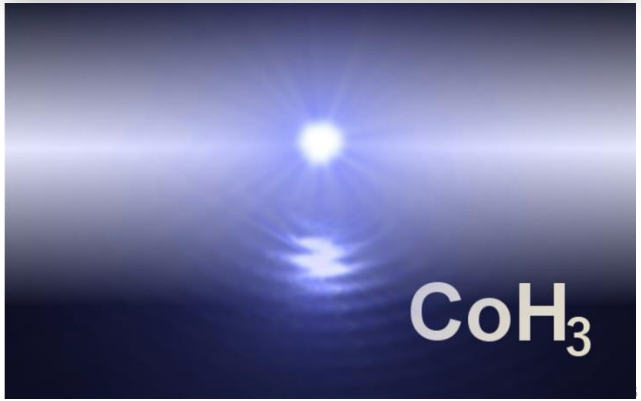
- Nuclear reactions on medium to heavy nuclei in the fast to a few tens of MeV
  - CoH_3 statistical Hauser-Feshbach code plays the central role at LANL
    - Recent upgrade include:
      - width fluctuation based on GOE (PRC**92**, 044617 (2015), PRC**94**, 014612 (2016))
      - unified description of direct and compound reactions (EPJA**57**, 16 (2021))
      - improved fission model (PRC**107**, 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 FAM for nuclear reaction
    - Neutron capture and photo-induced reactions
      - E1 and M1 GDR (PRC**107**, 044608 (2023)
    - Quantum mechanical direct and pre-equilibrium models
      - inelastic scattering data without adjustable parameters for direct and pre-equilibrium (PRC in press)

Coupled-Channels and Hauser-Feshbach Code CoH_3

- 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
- 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
  - Isotope production cross cross sections
  - Distinguish e.g. (n,d) and (n,np)
  - Mean-field models included (FRDM, Hartree-Fock-BCS)
  - Subsidiary code BeoH

https://github.com/toshihikokawano/coh3





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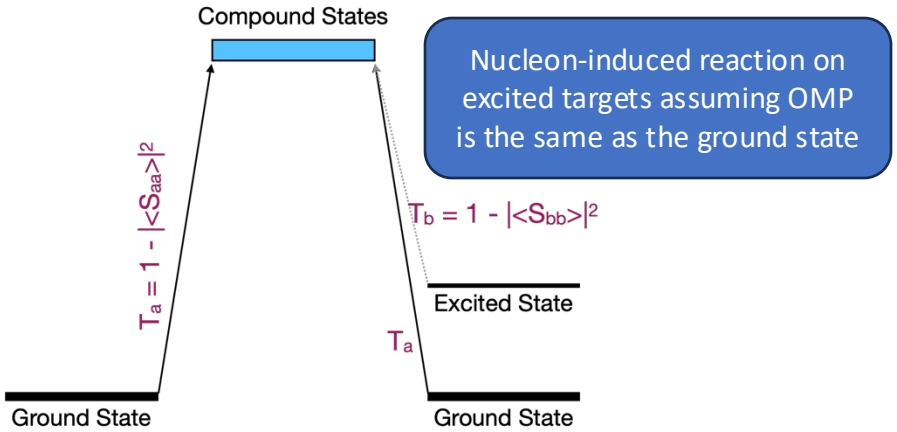
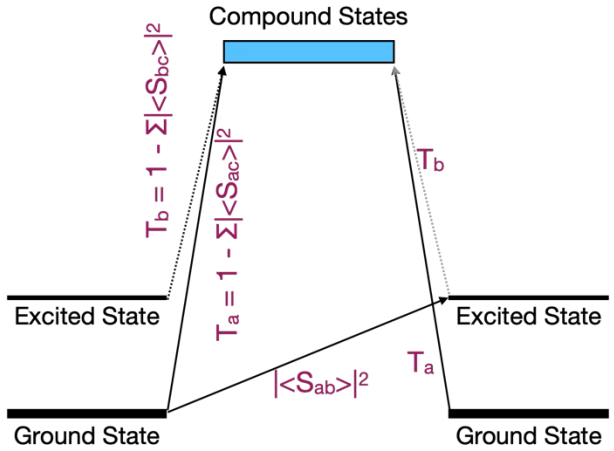
Spherical and Deformed Targets

- 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

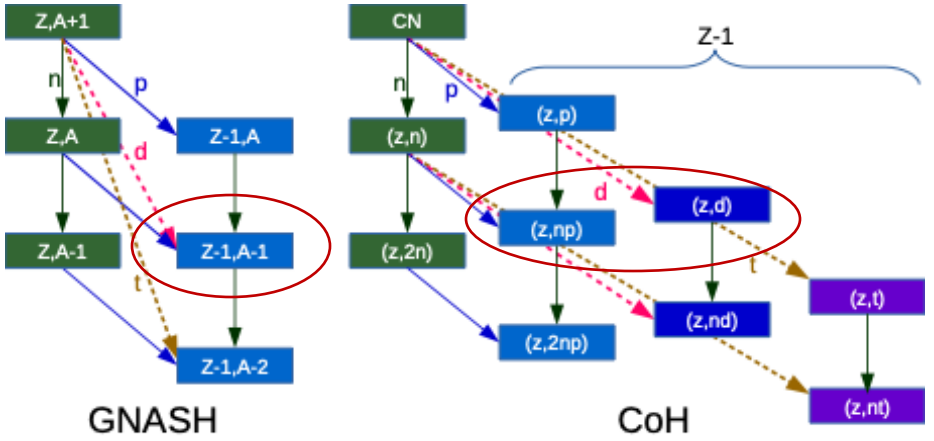
Generalized transmission coefficients in the coupled-channels formalism

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



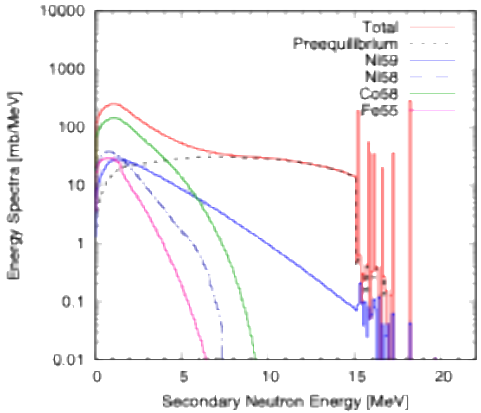


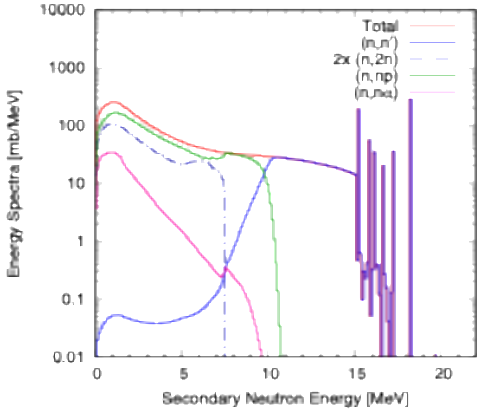
Multi-particle Emission and Exclusive Spectrum



The same (Z,A) nuclei are lumped

All CNs are treated separately to distinguish different reactions





Model calculation gives Inclusive Spectrum

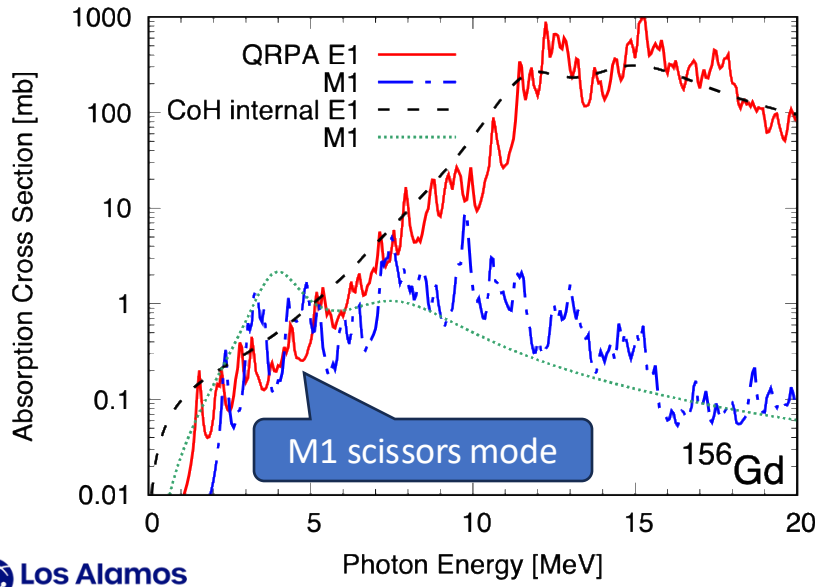
Special algorithm decomposes it into Exclusive Spectrum

Beyond Optical Model + Hauser-Feshbach Theory

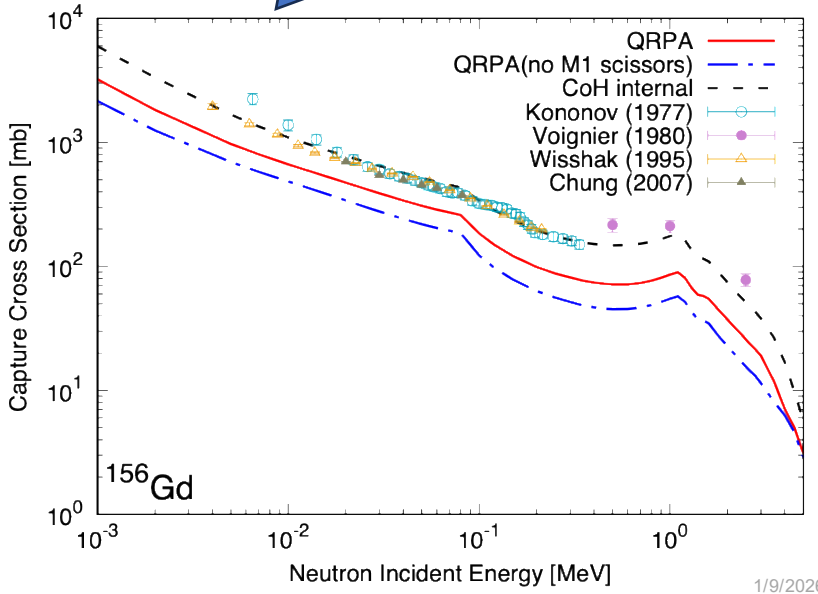
- Photon channel
  - Neutron capture reaction as an inverse process of photo-nuclear reaction
  - Transmission coefficient of photon is calculated by the photo-absorption cross section
    - Macroscopic Giant (Dipole etc) Resonances
    - Microscopic models - QRPA or FAM approaches
- Fission channel
  - Fission is not a simple inverse process of heavy ion fusion
  - Calculation of fission transmission coefficient strongly model dependent
- Direct 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

Non-Iterative Finite Amplitude Method

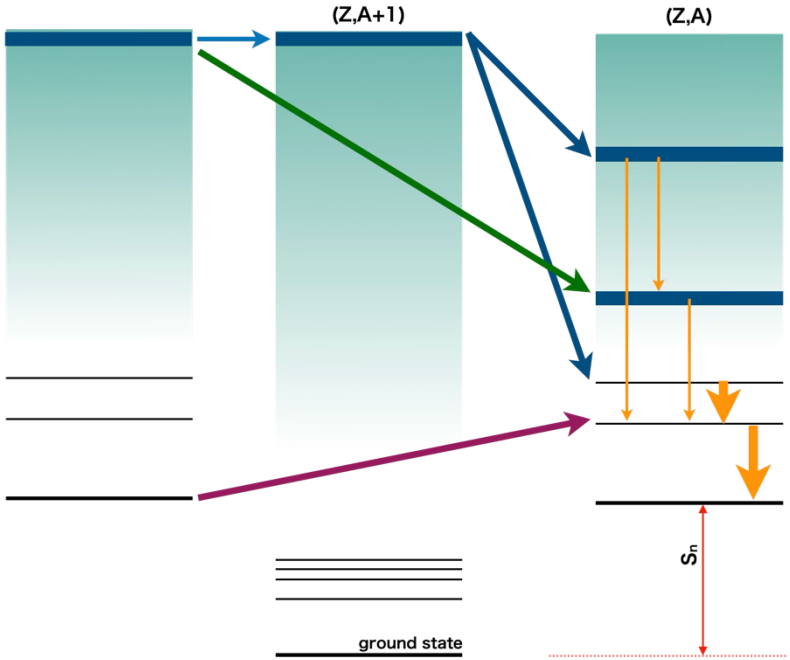
- Fast calculation technique developed by H. Sasaki
  - iterative procedure not required
  - so far applied to
    - photo-absorption (gamma-ray transmission coefficients)
    - neutron inelastic scattering



GDR parameters applied to neutron capture calculation



Impact of Initial Spin/Parity on Inelastic Scattering



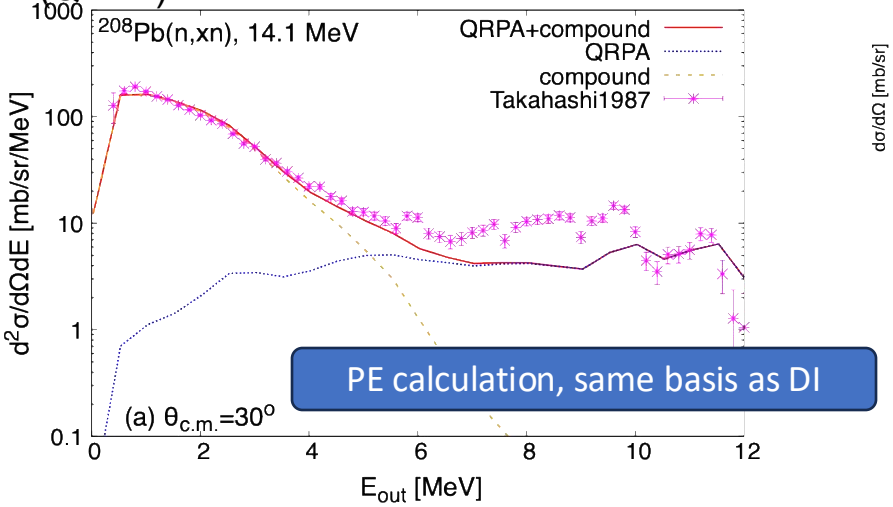
- Compound reaction
  - spin distribution in the (Z,A+1) CN is determined by the target spin and neutron transmission coefficients
  - final state can be either in the continuum or discrete levels
- Direct reaction
  - gamma-ray production = direct reaction cross section
  - coupled-channels or DWBA
- Pre-equilibrium process
  - populate the continuum directly
  - smaller degree-of-freedom (limited spin transfer)

Prompt gamma-rays are sensitive to spin/parity conservation

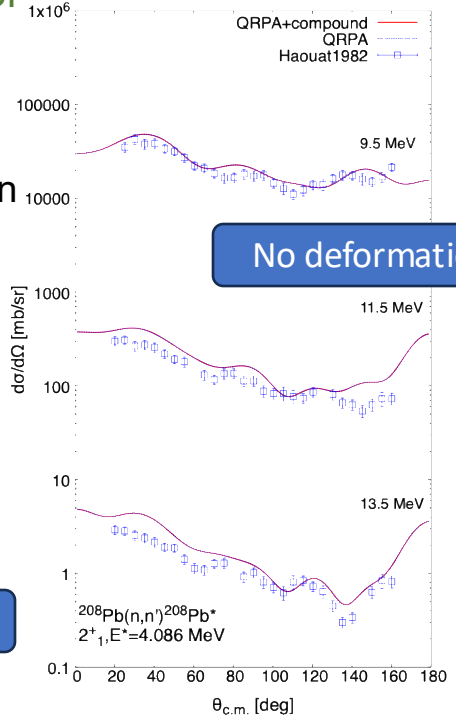
Microscopic approach to DI and PE in a consistent manner

Inelastic Scattering off ^{208}Pb, No Adjustable Parameters

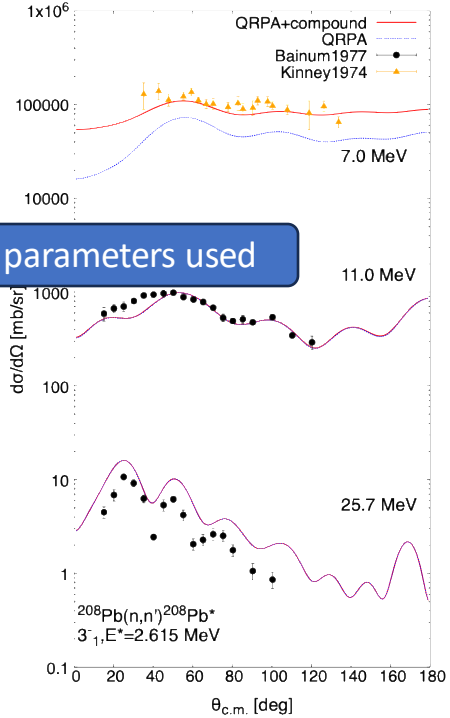
- Microscopic approach to calculate (n,n') c.s. for both discrete and continuum final states
  - Hartree-Fock BCS and Skyrme interaction
  - non-Iterative Finite Amplitude Method (FAM) to solve Quasi-particle Random Phase Approximation (QRPA)



PE calculation, same basis as DI



No deformation parameters used



Concluding Remarks and Perspective

- 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
- Nuclear data file production
  - post-processing by the ENDF manipulation code DeCE
  - a new framework to produce evaluated nuclear data at LANL (not in this talk) may automate production of model-calculation-based evaluations