ENDF Updates for Structural Materials Data, Evaluation and Reaction Modeling

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in collaboration with

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Highlights

Nuclear Data Upgrades for Structural Materials in ENDF/B-VII.0

- Relatively modest effort was made for ENDF/B-VII.0
  - Problem reported by D. Smith for V(n,np) data.
    — fixed by D. Rochman by an EMPIRE calculation
  - Energy conservation problem in LA-150 (a bug in GNASH) was fixed
    — Cr, Fe, Ni, Cu.
  - Some data were taken from other libraries — Ti (JENDL), Zn (JEFF)

New High Energy Experimental Data from LANSCE

- Gas production cross section measurements at LANSCE (R.C. Haight).
- proton and α-particle production data for Fe and Ni.
- ^{56}Fe α production was adjusted to reproduce the LANSCE data.

Plans for ENDF/B-VII.1

- New evaluations for Ti isotopes available, including covariances.
- V data will be reviewed, and covariance data will be added.
- Upgrades Fe and Ni high energy data based on LANSCE experimental data.

Recent Improvement in Nuclear Reaction Modeling at LANL

- Direct / Semidirect (DSD) capture with the Hartree-Fock BCS theory
  L. Bonneau, TK, T. Watanabe, S. Chiba, Phys. Rev. **C** 75, 054618 (2007).
- Impact of spin distribution in the pre-equilibrium process
  D. Dashdorj, TK, et al., Phys. Rev. **C** 75, 054612 (2007).
- Effects of direct reaction coupling in compound reactions (KKM)
  TK, L. Bonneau, A. Kerman, Proc. in ND2007.
- β-delayed neutron emission
  TK. P. Möller, W.B. Wilson, Phys. Rev. **C** 78, 054601 (2008).
- Monte Carlo Hauser-Feshbach calculation
  TK, P. Talou, M.B. Chadwick, in progress.

Ti Evaluation Overview

Resonance Region

- New resonance parameters adopted
  - from Atlas by Mughabghab, fixed some parameters by Oh
  - resonance energy range extended, upper limit from 300 keV to 367 keV (^{48}Ti)
- Fictitious levels added with Fröhner's method

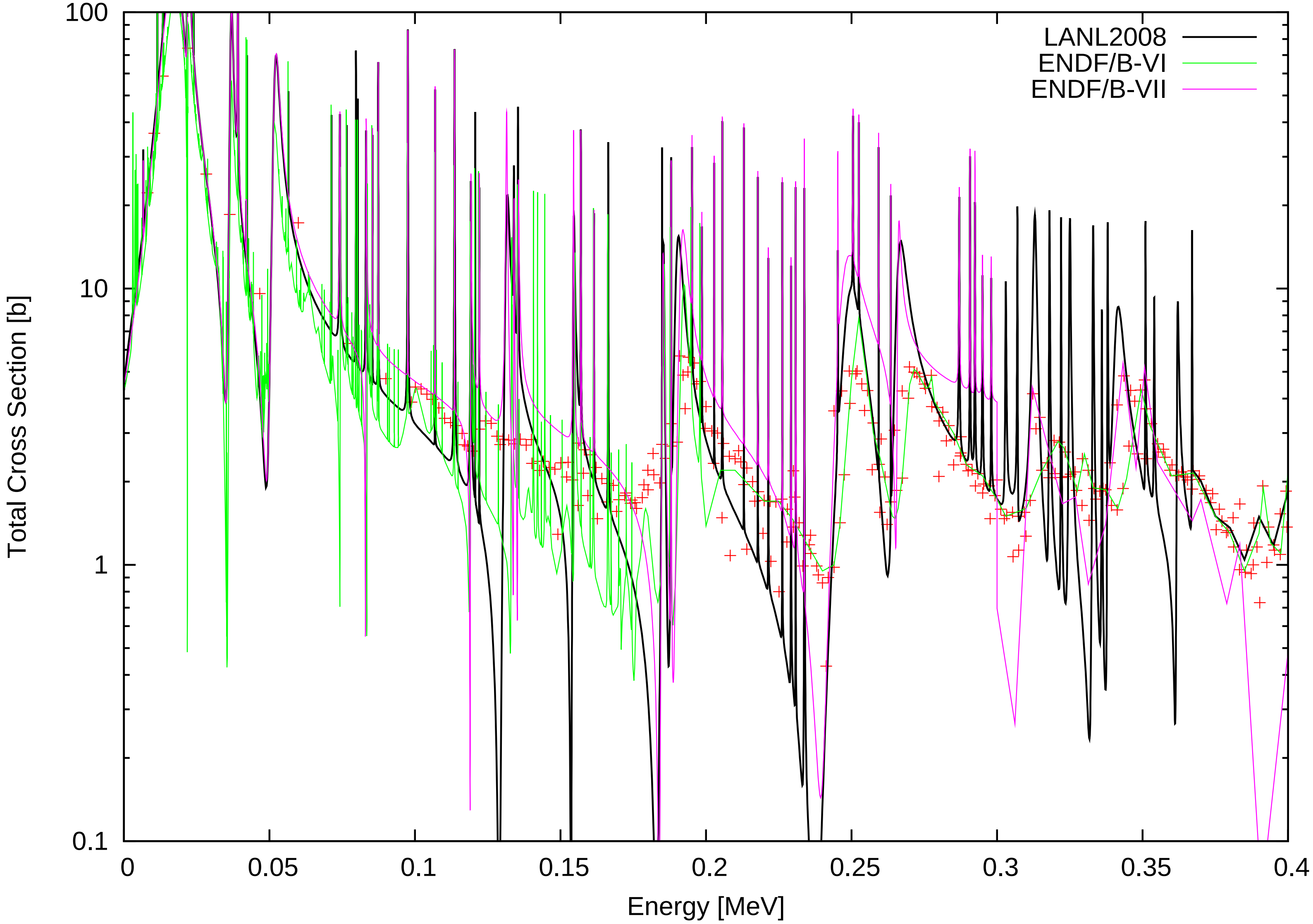
High Energy Range

- Total cross section from 367 keV to 6 MeV, least-squares fitting to experimental data
- New GNASH calculations, based on calculations by D. Dashdorj et al.
  Phys. Rev. **C** 75, 054612 (2007)

Elastic Scattering Angular Distribution

- ENDF/B-VI adopted up to 4 MeV
- Above 4 MeV, optical model calculation

New Resonance Parameters, Total Cross Section



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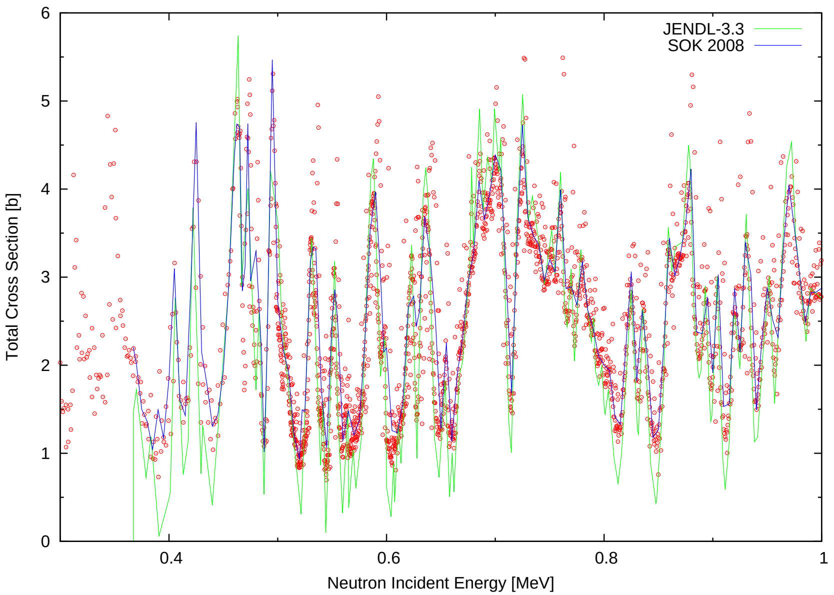
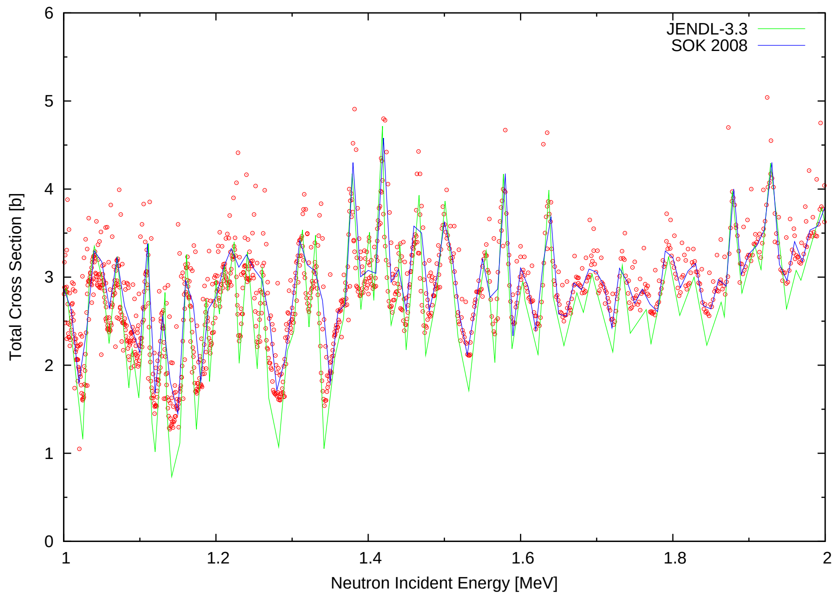
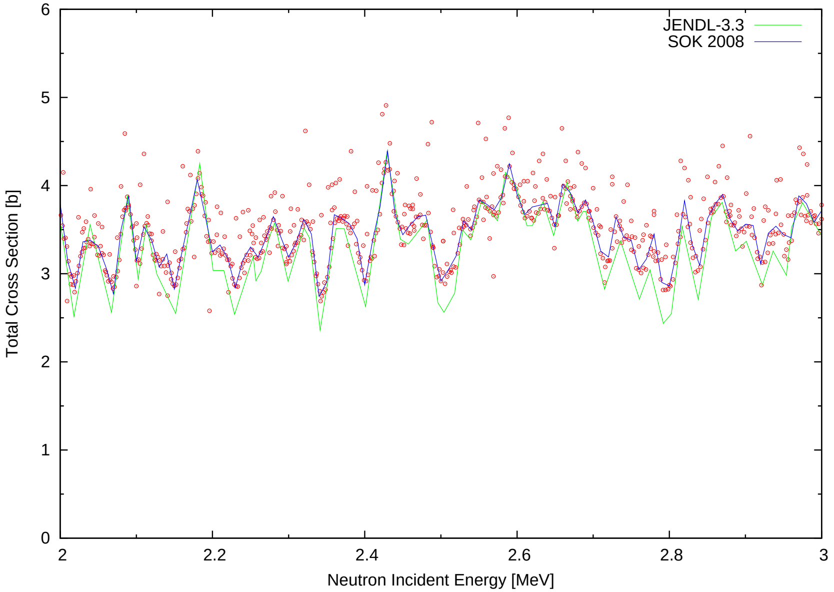
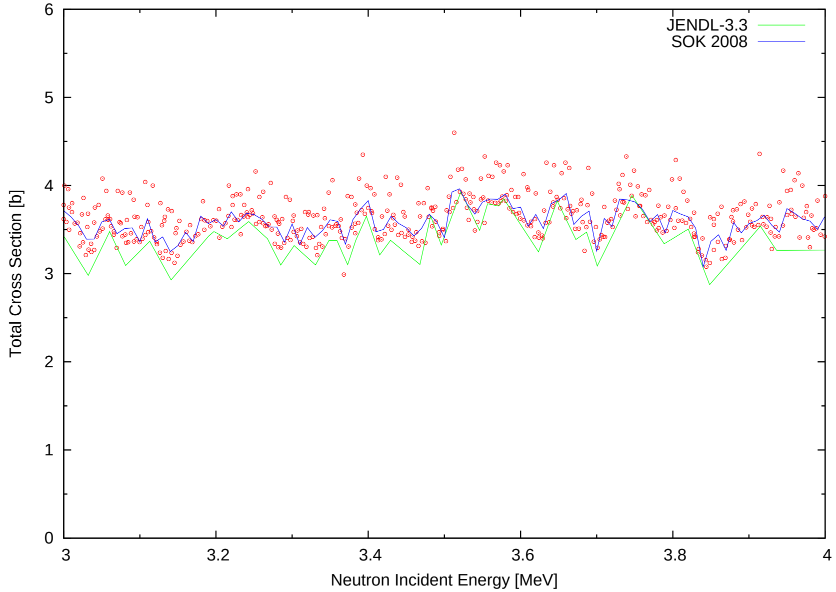
SOK, Least-Squares Fitting to Total Cross Section









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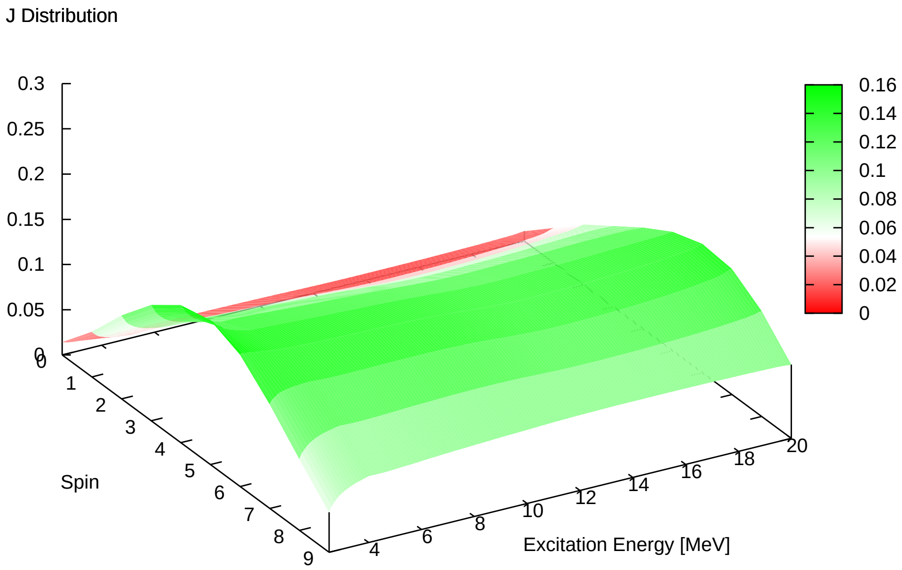
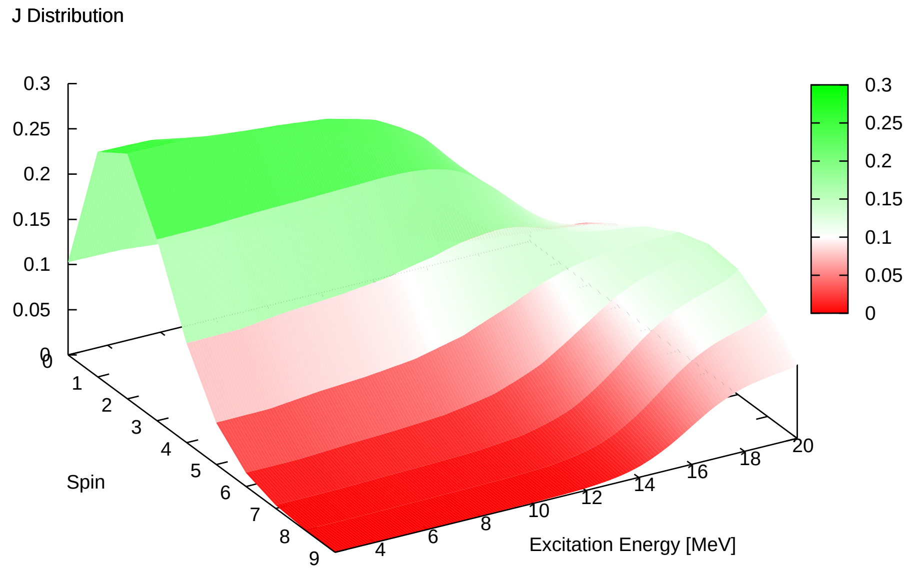
Spin Distribution in the Continuum

Analysis of GEANIE Data Requires a New Spin Physics in HF

CN Reaction Only



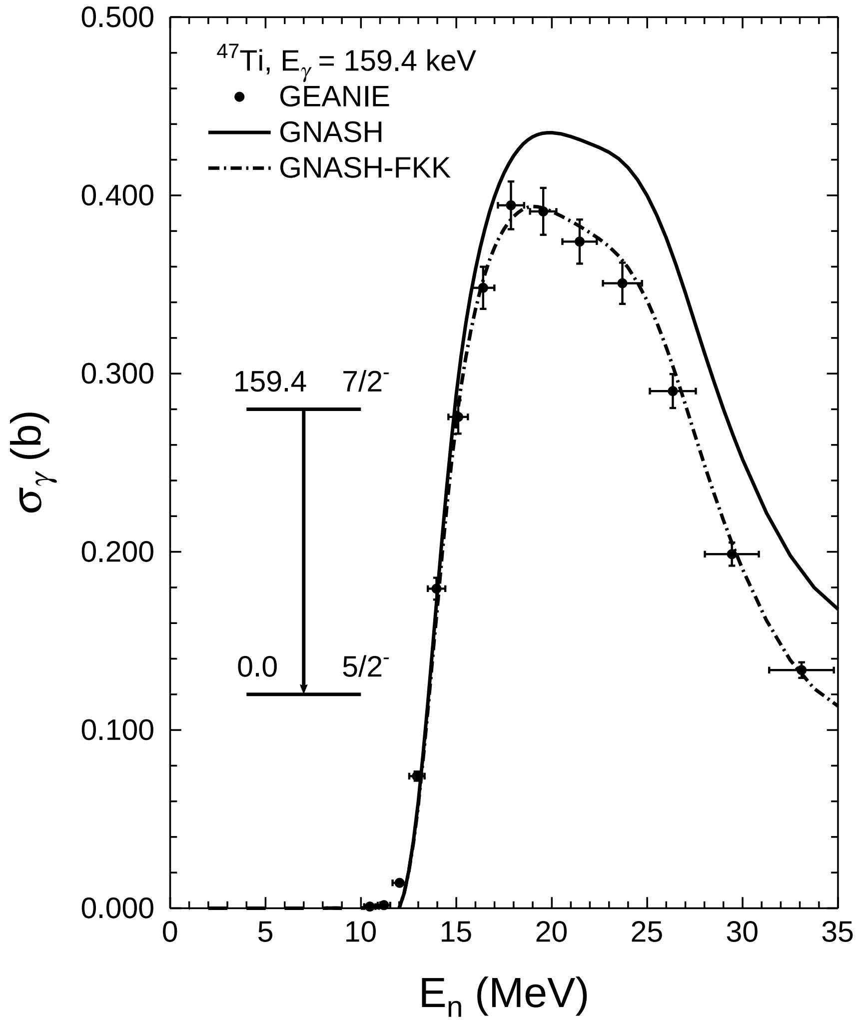
CN + FKK



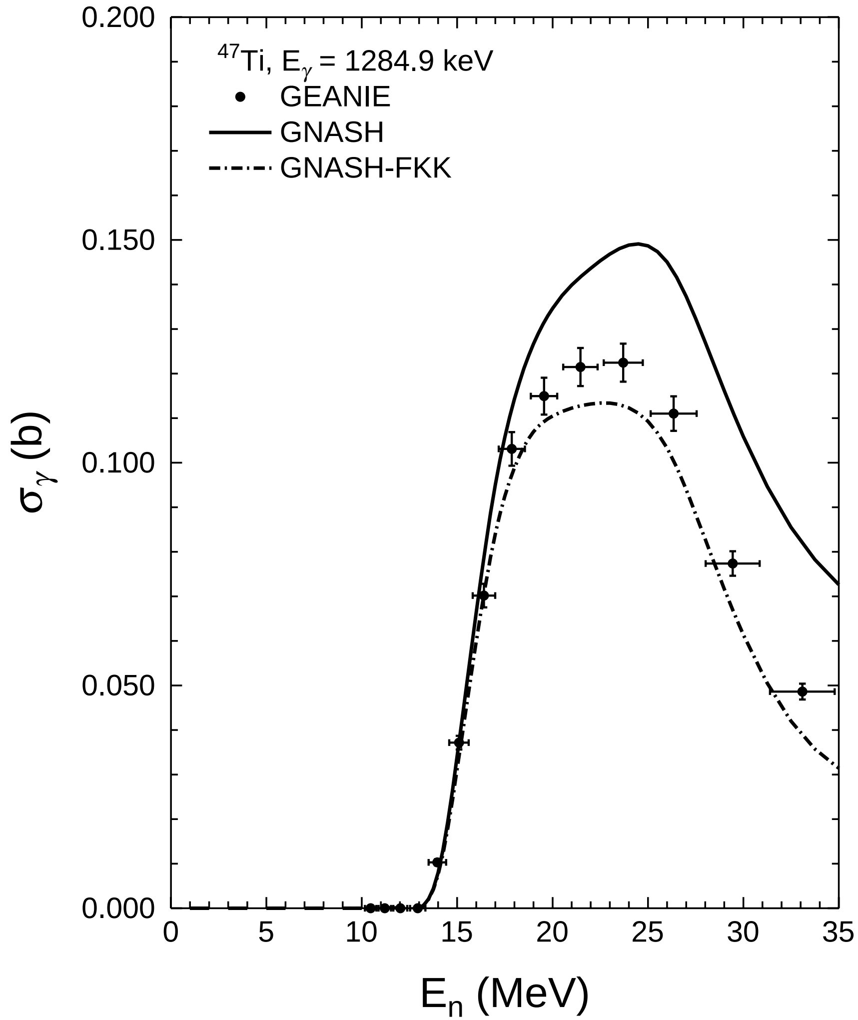
- The FKK calculation suppresses the high-spin state population in the continuum because its angular momentum transfer is not so large.
- We expect that transitions from the higher spin-state become smaller.

Ti-48 (n,2n)

D. Dashdorj et al., Phys. Rev. C **75**, 054612 (2007)

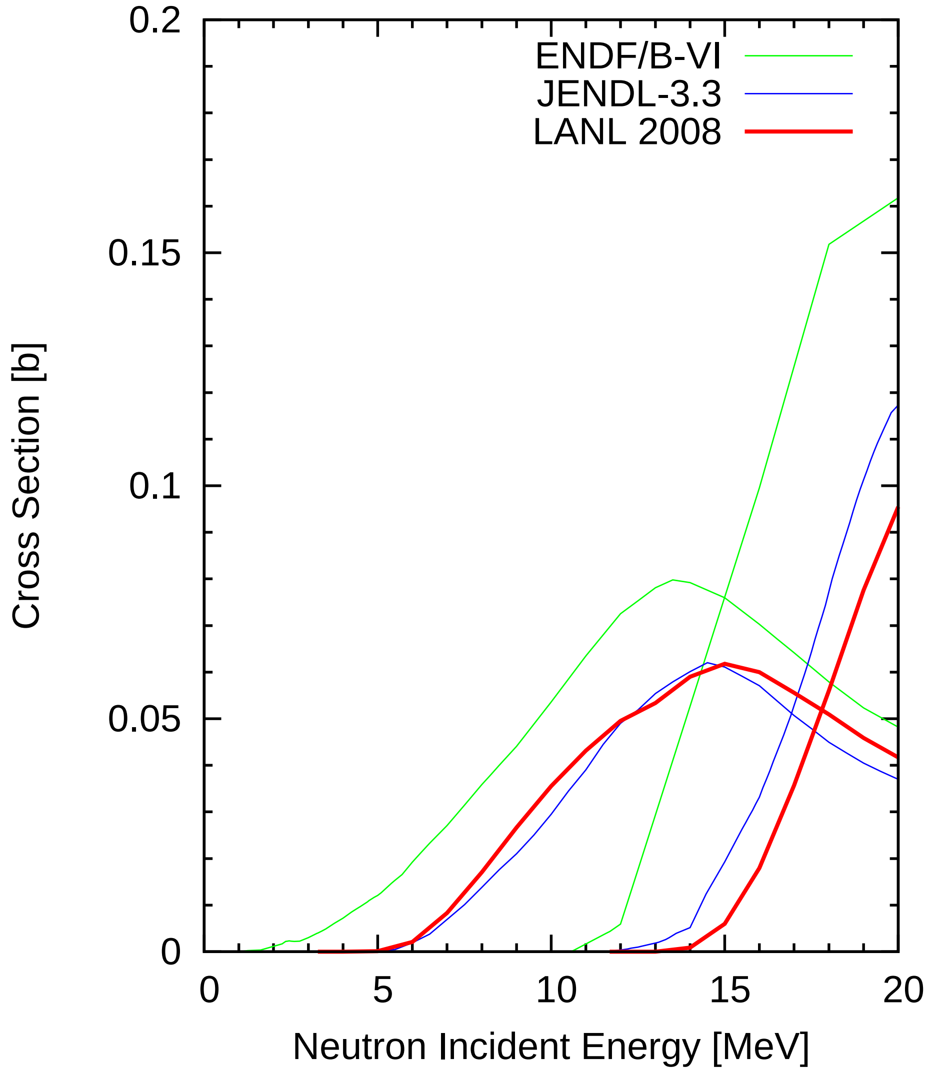


159.4 keV $(7/2^-)$ to GS

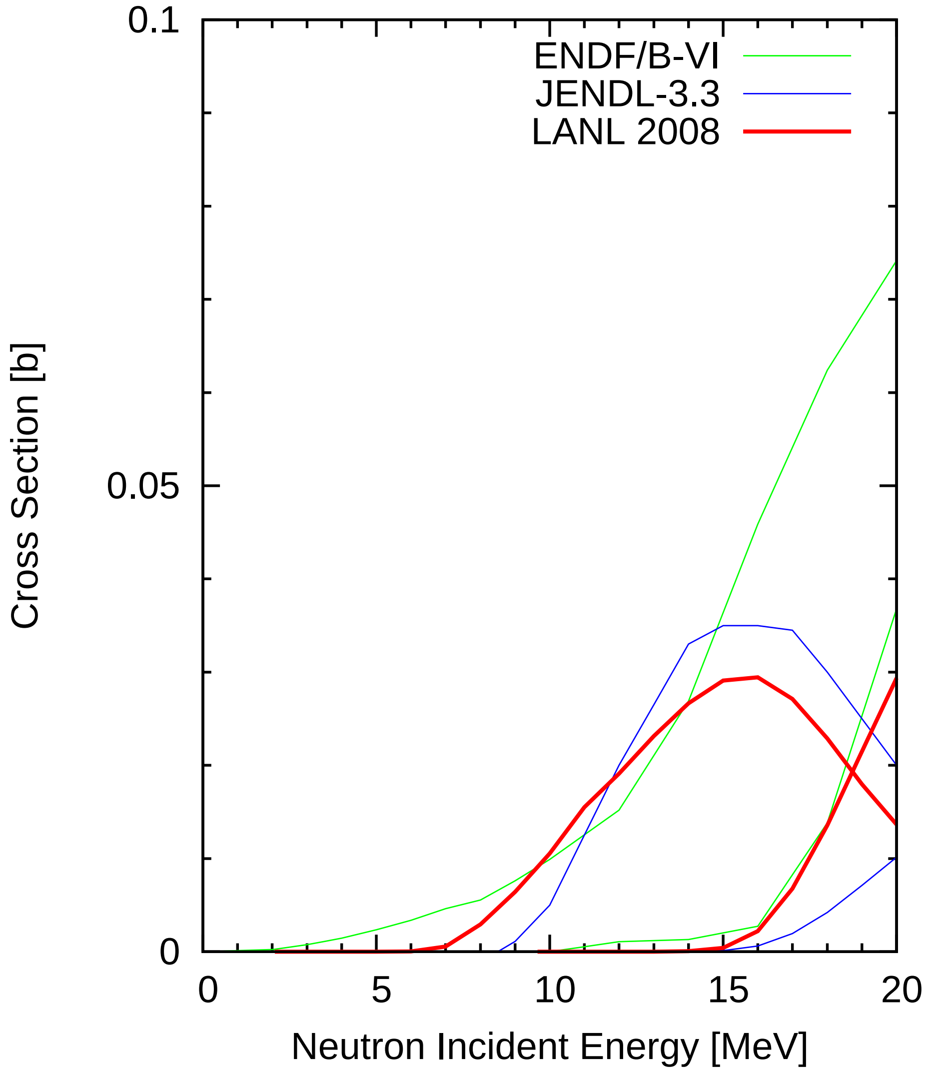


1444.3 keV $(11/2^-)$ to 159.4 keV $(7/2^-)$

Ti-48 Charged Particles



(n,p), (n,np)



(n,α), (n,nα)

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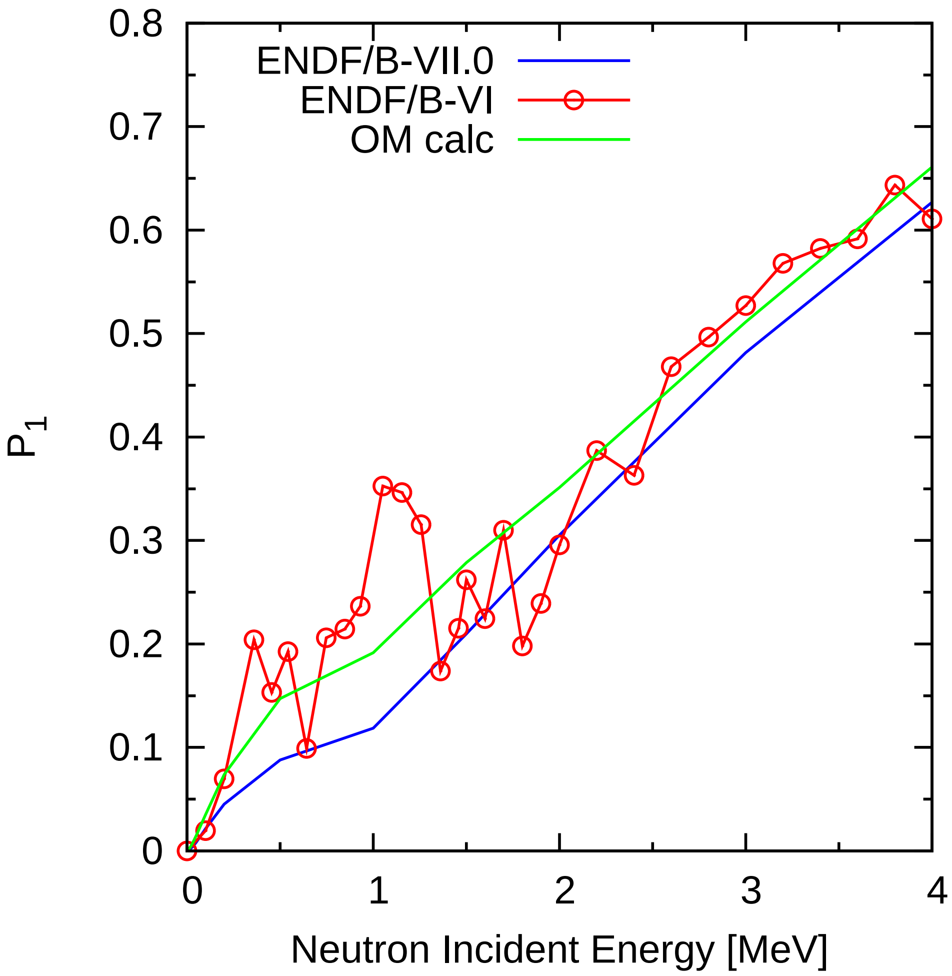
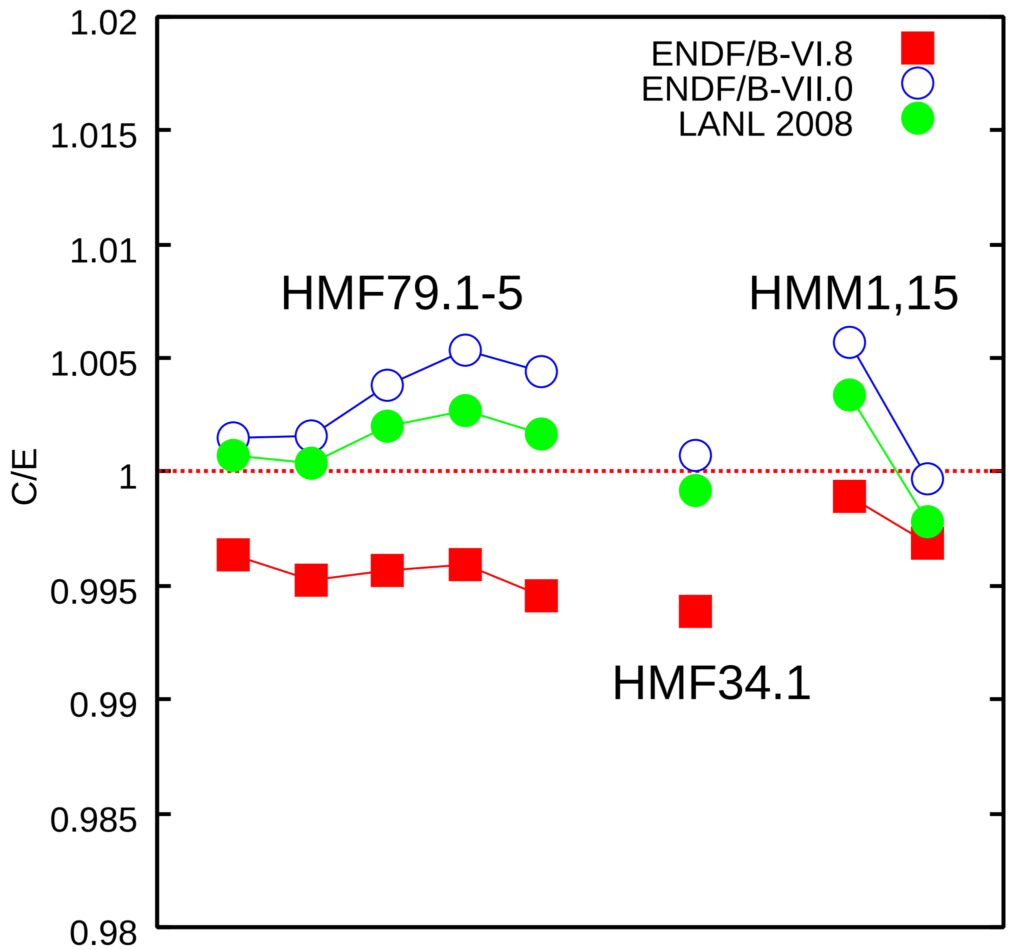
Elastic Scattering Angular Distribution and Keff

P_1 Legendre Coefficient and $k_{\rm eff}$





We adopted P_ℓ from ENDF/B-VI up to 4 MeV.

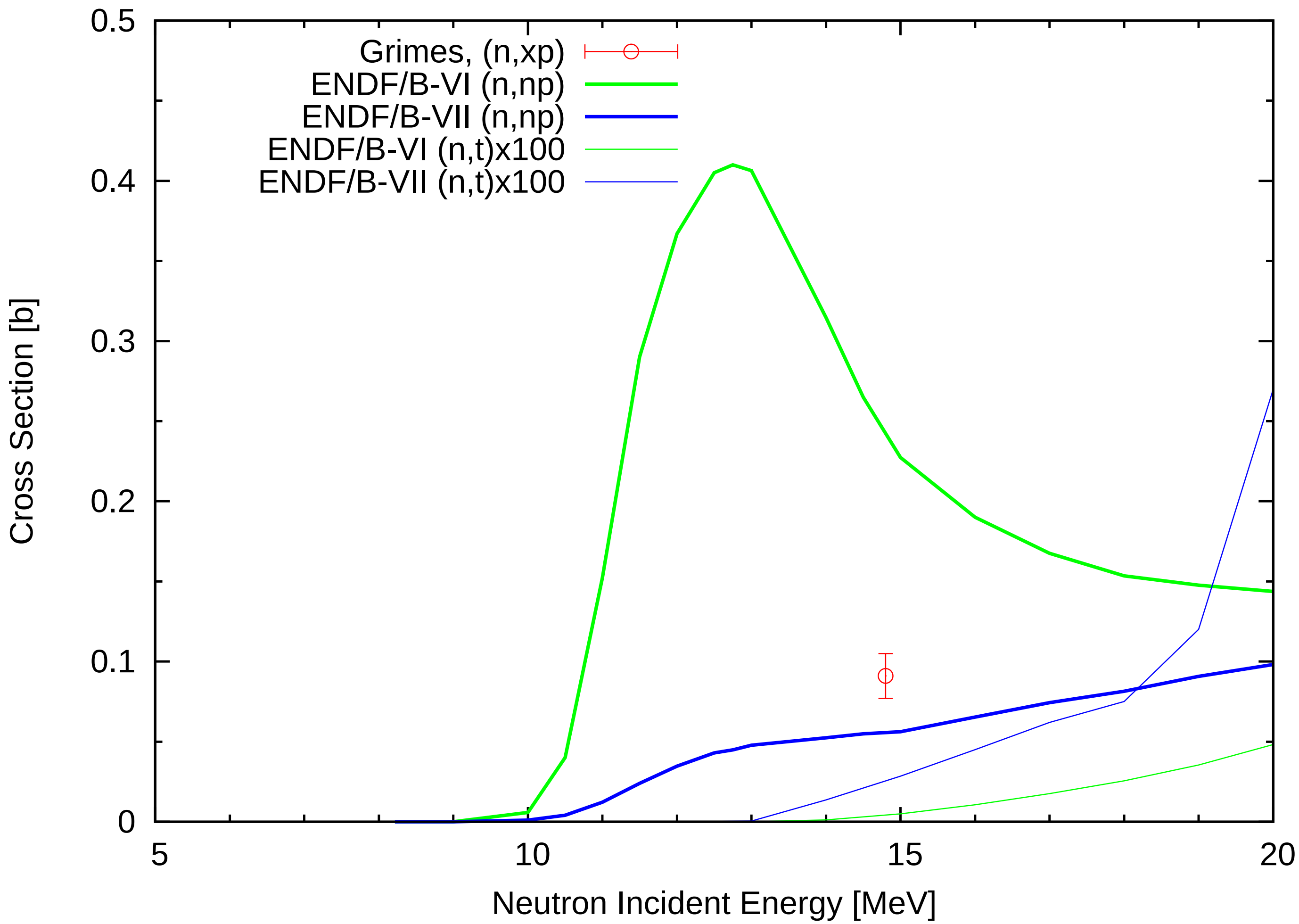
Covariance Data

Covariances are evaluated with the KALMAN method

En	Error	Correlation																
0.4	5.3	100																
0.5	5.4	100	100															
0.6	5.3	99	100	100														
0.7	5.3	98	99	100	100													
0.8	5.3	97	98	99	100	100												
1	5.3	94	96	98	99	100	100											
1	6.2	60	63	67	71	74	79	100										
2	7.5	73	75	76	77	77	78	69	100									
3	13	58	60	59	58	56	53	23	85	100								
4	26	44	45	43	40	37	32	-6	66	95	100							
6	24	32	32	30	26	23	19	-7	53	77	86	100						
8	21	29	29	25	22	19	15	-3	53	70	77	92	100					
10	19	23	23	21	19	17	15	8	50	61	65	90	96	100				
12	20	11	11	11	11	11	11	16	37	40	43	79	79	92	100			
14	18	12	13	12	12	12	13	24	49	47	46	74	83	92	93	100		
16	20	14	15	14	14	13	14	26	57	51	46	50	72	71	56	82	100	
18	29	15	15	14	13	12	12	19	51	46	39	24	50	40	16	50	90	100

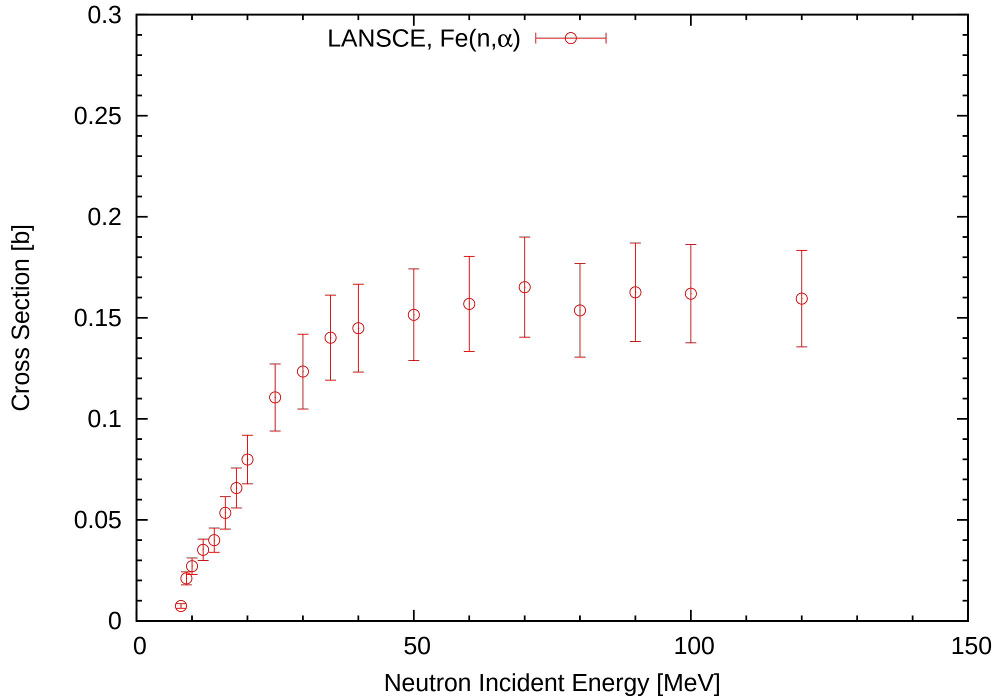
Covariance matrix for ^{48}Ti capture cross section,
including compound radiative capture and DSD processes.

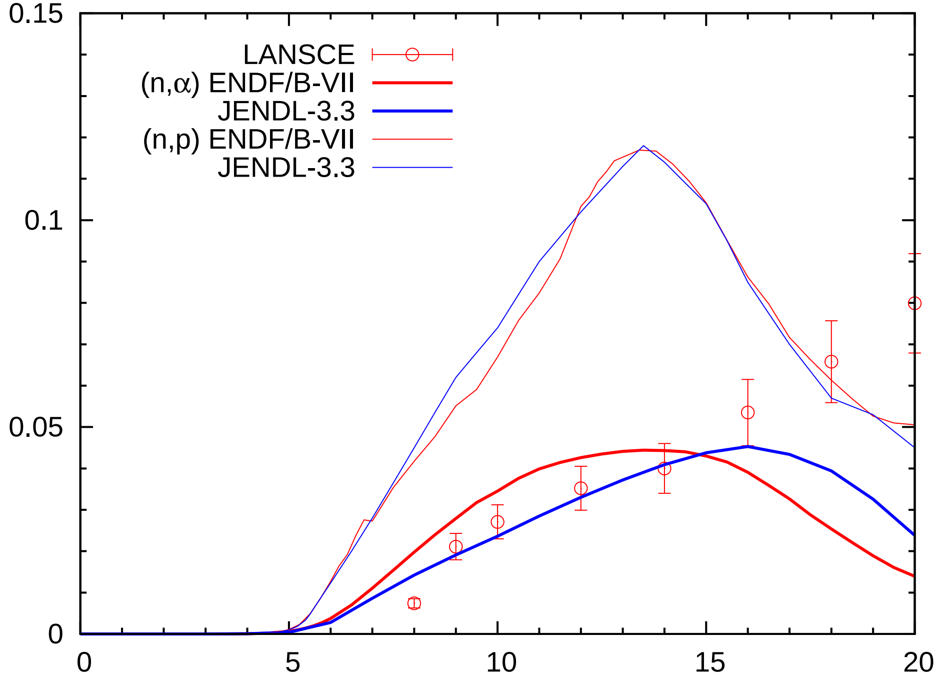
V(n,np) Data Revised by D. Rochman



Problem reported by D.L. Smith (Fusion Eng. Des. **47**, 61 (1999)). EMPIRE calculations to fit experimental data of Grimes et al. and Kokoo elt al. for proton production cross section.

High-Energy Neutron Induced Reaction Data for Fe





Data preliminary. Further analysis may give smaller incident energy steps and lower uncertainties.

New Reaction Modeling Capabilities at LANL

- Hauser-Feshbach theory for deformed nuclei
  - Transmission coefficients by Coupled-Channels model for the excited states
  - Cross section calculations on the excited states feasible
  - Width-fluctuation, need more work
- Monte Carlo technique for sequential particle emission
  - Prompt fission neutron spectrum calculation
  - Monte Carlo Hauser-Feshbach calculation
- Quantum mechanical pre-equilibrium process
  - Fully microscopic, Hartree-Fock-BCS, with RPA
- Model Codes
  - We continue developing McGNASH, though it slowed down somewhat.
  - New Hauser-Feshbach Monte Carlo code, CGM, underway.
  - CoH capable for calculating nuclear reactions on excited states.

DSD with Hartree-Fock BCS Theory

L. Bonneau, T.K., T. Watanabe, S. Chiba, Phys. Rev. C **75**, 054618 (2007)

Model Improvements

spectroscopic factor S_{ljK}

- previous studies
  - experimental data (often not available for astrophysical calculations)
- DSD/HF-BCS
  - single-particle occupation probabilities
  - no experimental data needed

single-particle wave-function, $R_{ljK}(r)$

- previous studies
  - spherical Woods-Saxon, Nilsson model, coupled-channels model to bound states
- DSD/HF-BCS
  - HF-BCS calculation and decomposition into spherical HO basis
  - consistent treatment for all nuclei from spherical to deformed nuclei

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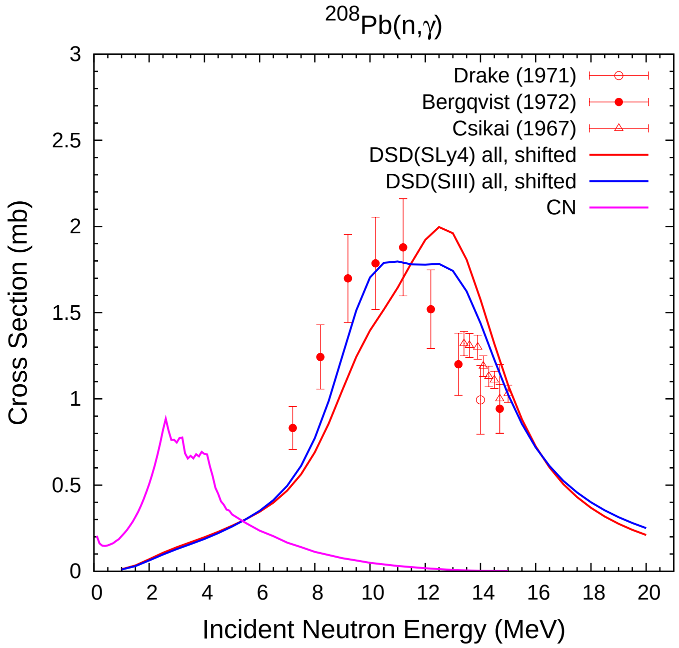
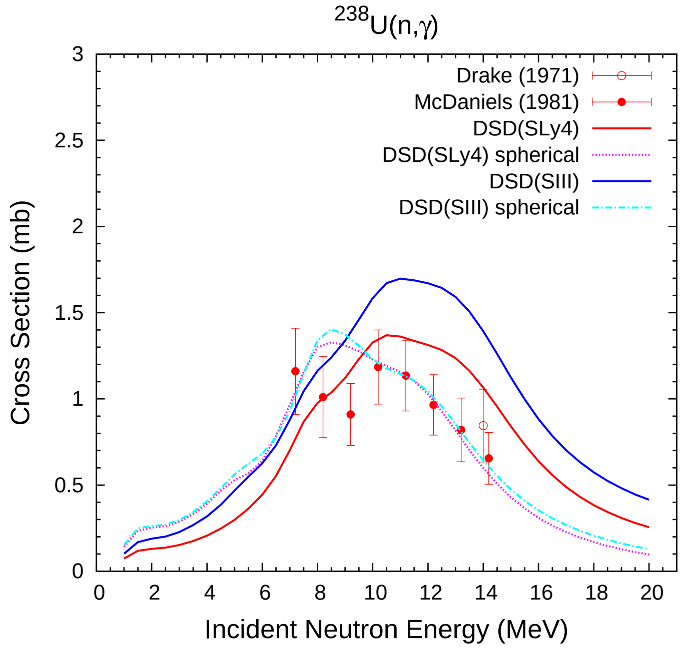
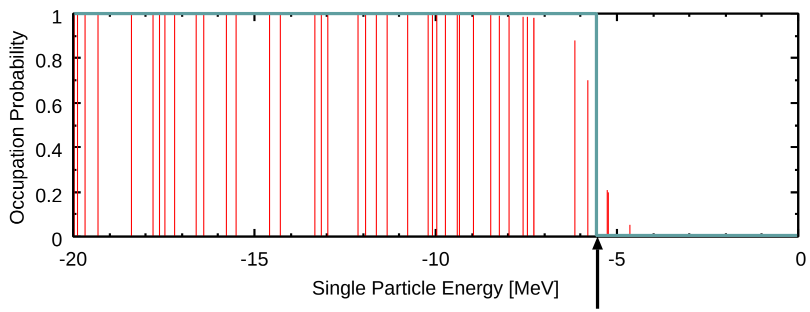
Calculated Results

DSD Cross Sections for Spherical and Deformed Cases





Occupation Probabilities for U-238



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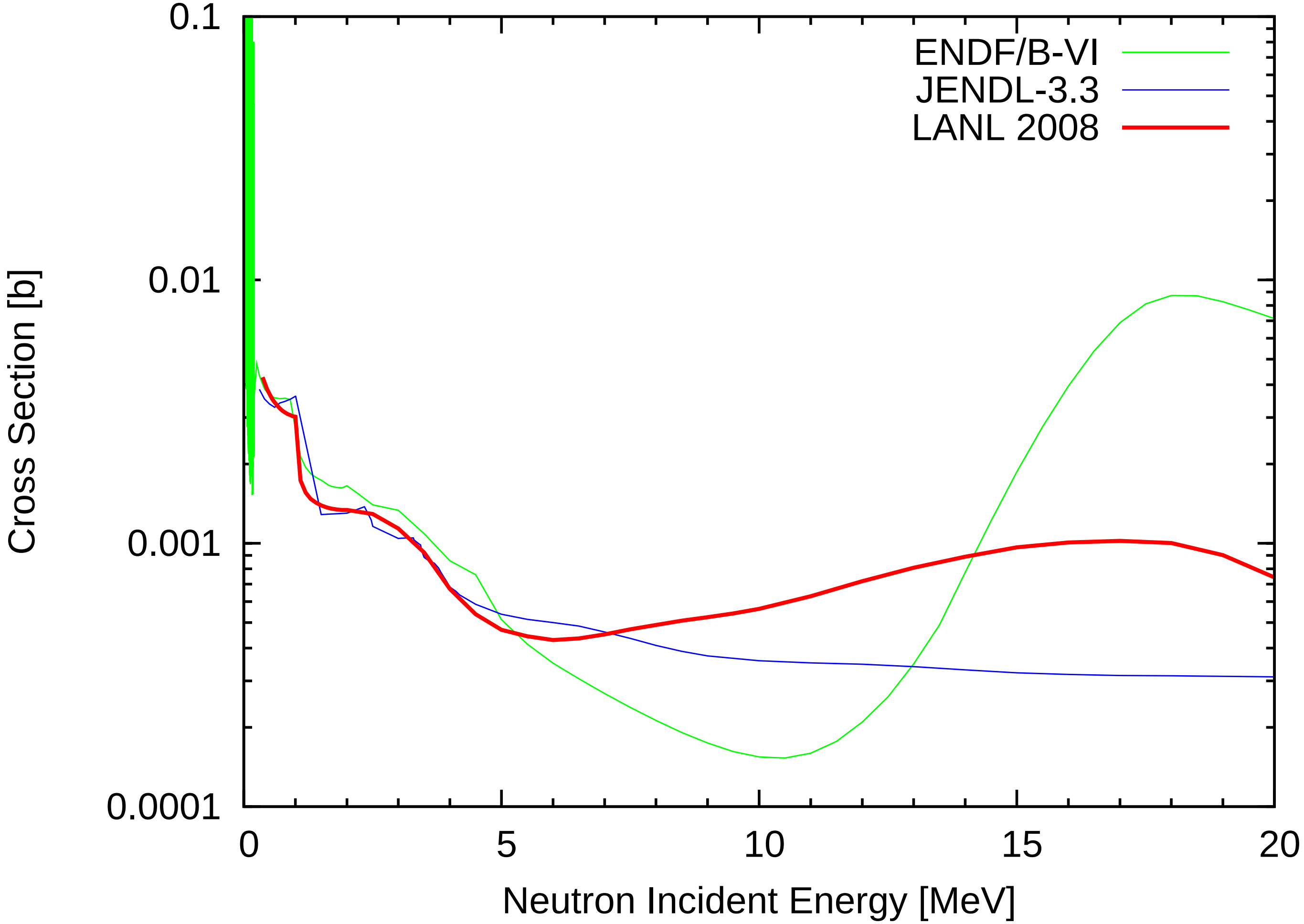
DSD, Simplified Version

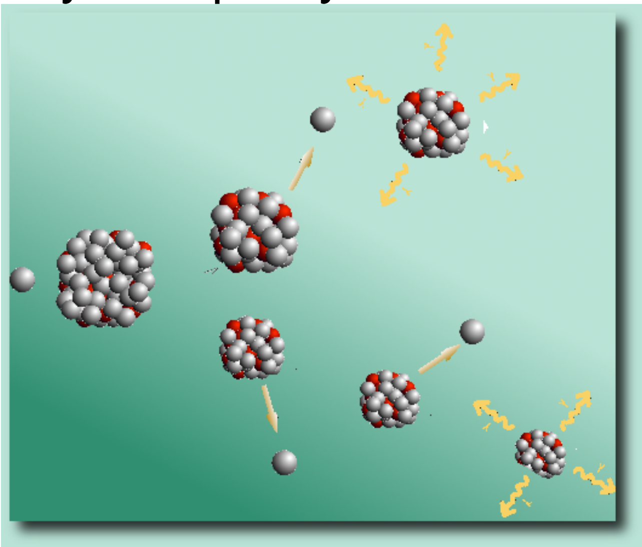


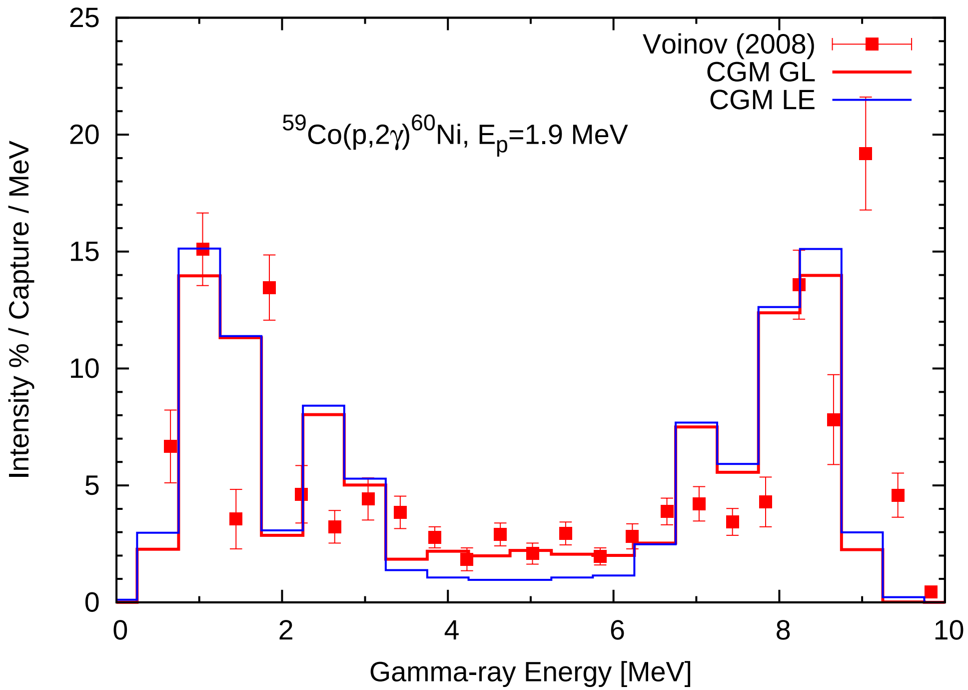
- Single particle states generated in a spherical potential.
- BCS equation solved for fixed Δ.

Monte Carlo Simulation for Particle Emission

Application of Monte Carlo to Hauser-Feshbach model at LANL

- prompt fission neutron spectra
  - correlation between n and γ
- β-delayed γ spectra
- γ-ray multiplicity distribution





- Internal MC gives all correlation between a specific reaction and observables.
- External MC gives target recoil in the laboratory frame.

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PRECO-2006, Released Spring 2007

- Exciton pre-equilibrium model
- Projectile Break-up
  - Important for composite particle induced reactions
  - Deutron breakup model, extended to He-3 and α-particle
  - The peak energy and width systematics were investigated, while angular distributions and total breakup cross sections remain to be studied.
- User's Manual available
- Impact on initial configuration in exciton model with complex particles will be examined.

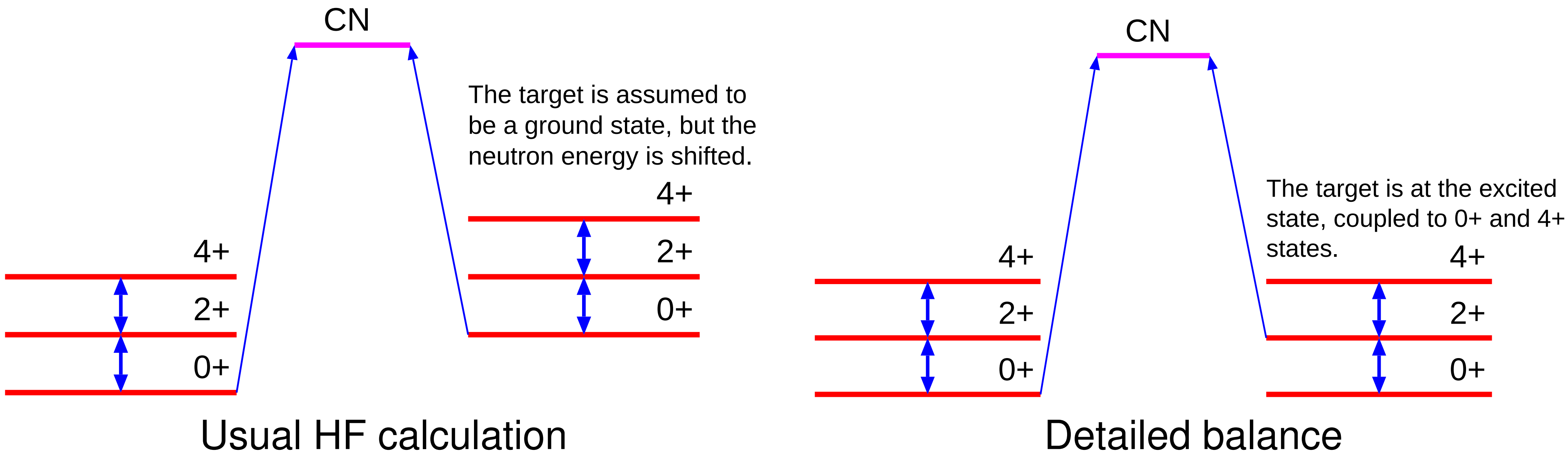
Coupled-Channels Hauser-Feshbach Method

Neutron Reaction on Deformed Nuclei at Low Energies

- Incorporate Coupled-Channels (CC) method into Hauser-Feshbach formula
  - Inverse channel problem
    - What is the appropriate transmission coefficient for the excited states ?
    - Replaced by the one for the ground state (historical)
    - Solve the CC equation for the excited state (detailed balance)
  - Width fluctuation correction when off-diagonal elements exist
    - Moldauer
    - Engelbrecht-Weidenmüller transformation
    - Kawai-Kerman-McVoy (KKM)
    - Nishioka-Weidenmüller-Yoshida, GOE for coupled-channels
- I will report :
  - Coupled-Channels Hauser-Feshbach (CCHF) method
  - Apply to calculate neutron capture cross sections for deformed nuclei (no fissile)
  - Super-elastic calculation

Detailed Balance for Compound Reaction

Neutron Emission Probabilities $\propto$ Transmission

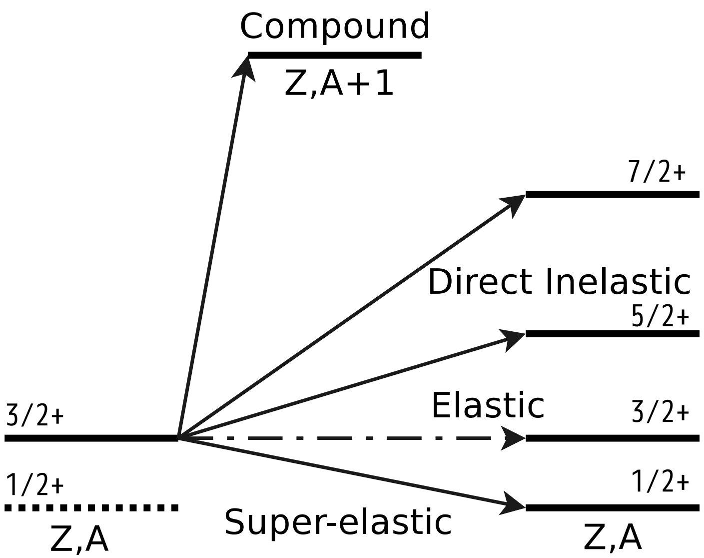


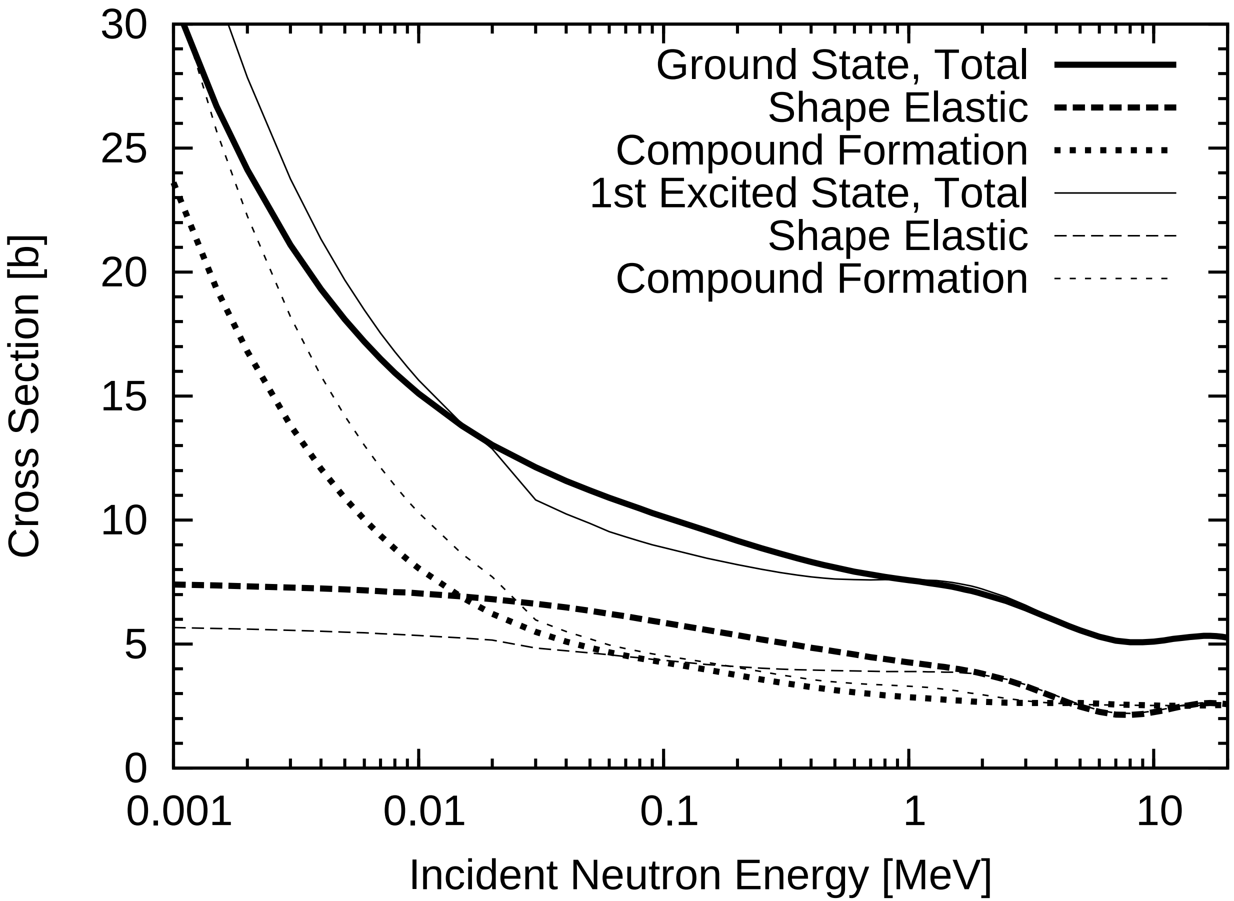
- The same transmission coefficients are used for both entrance and exit channels.
- Sometimes exit channels are corrected by a factor of $1 + \sigma_D/\sigma_R$.
- Solve the Coupled-Channels equations for the excited state, which couples to the negative energy states (super-elastic).

Direct Cross Sections

Coupled-Channels Calculations for the Excited States

Calculation for n + ^{169}Tm



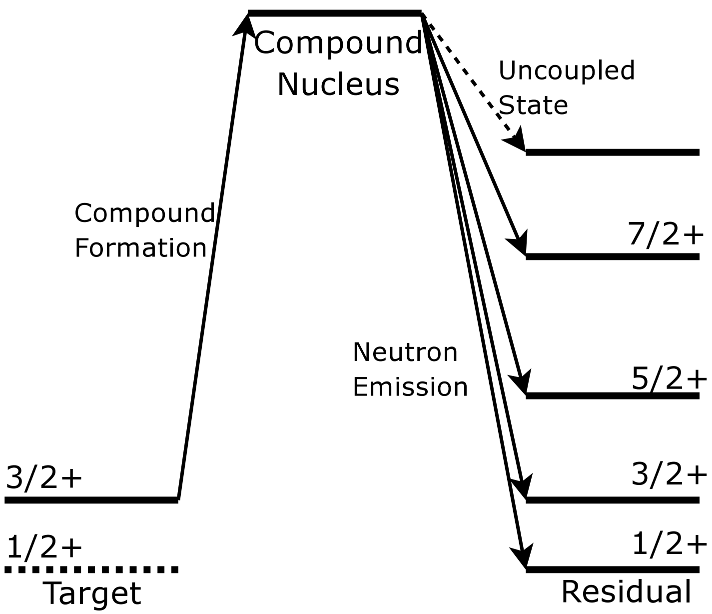


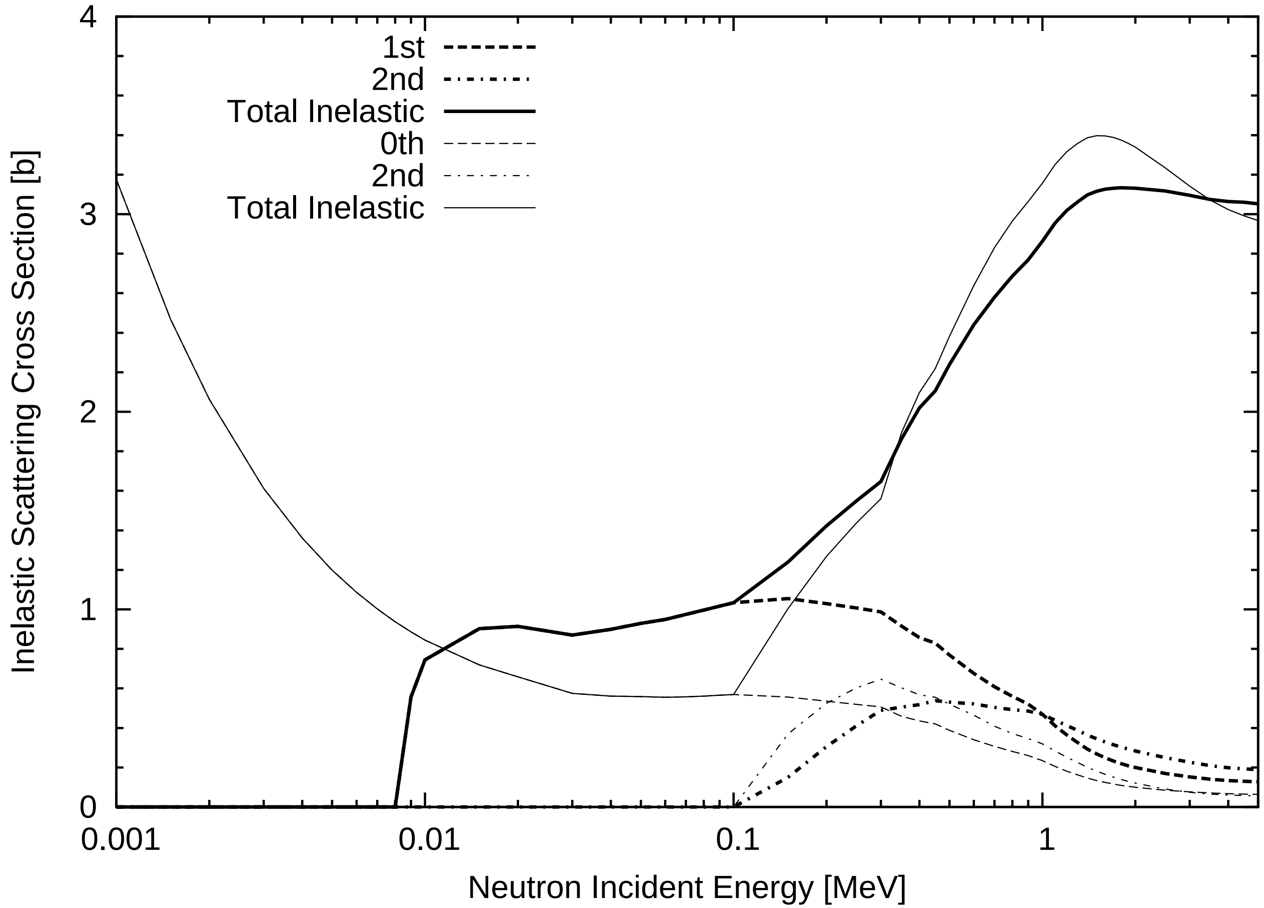
Preliminary

Inelastic Scattering Cross Sections

Hauser-Feshbach Calculations for the Excited States

Calculation for n + ^{169}Tm





Preliminary

Concluding Remarks

Nuclear Data Evaluation for Structural Materials

- New Ti evaluations including covariance data for ENDF/B-VII.1.
- V data evaluation underway.
- Upgrade of Fe and Ni high energy data planned, based on LANSCE experimental data.

Theory Developed for Nuclear Data Evaluation

- Improved Hauser-Feshbach model for capture reaction, including nuclear deformation effect.
- The Hartree-Fock BCS theory for the DSD process has a potential to predict neutron capture cross-sections near the neutron drip-line.
- Developed a simplified version for more general nuclear data evaluations.
- Beta-delayed and EC neutron emission
- Prompt fission neutron spectra
- Monte Carlo approach : correlations of particle emissions

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