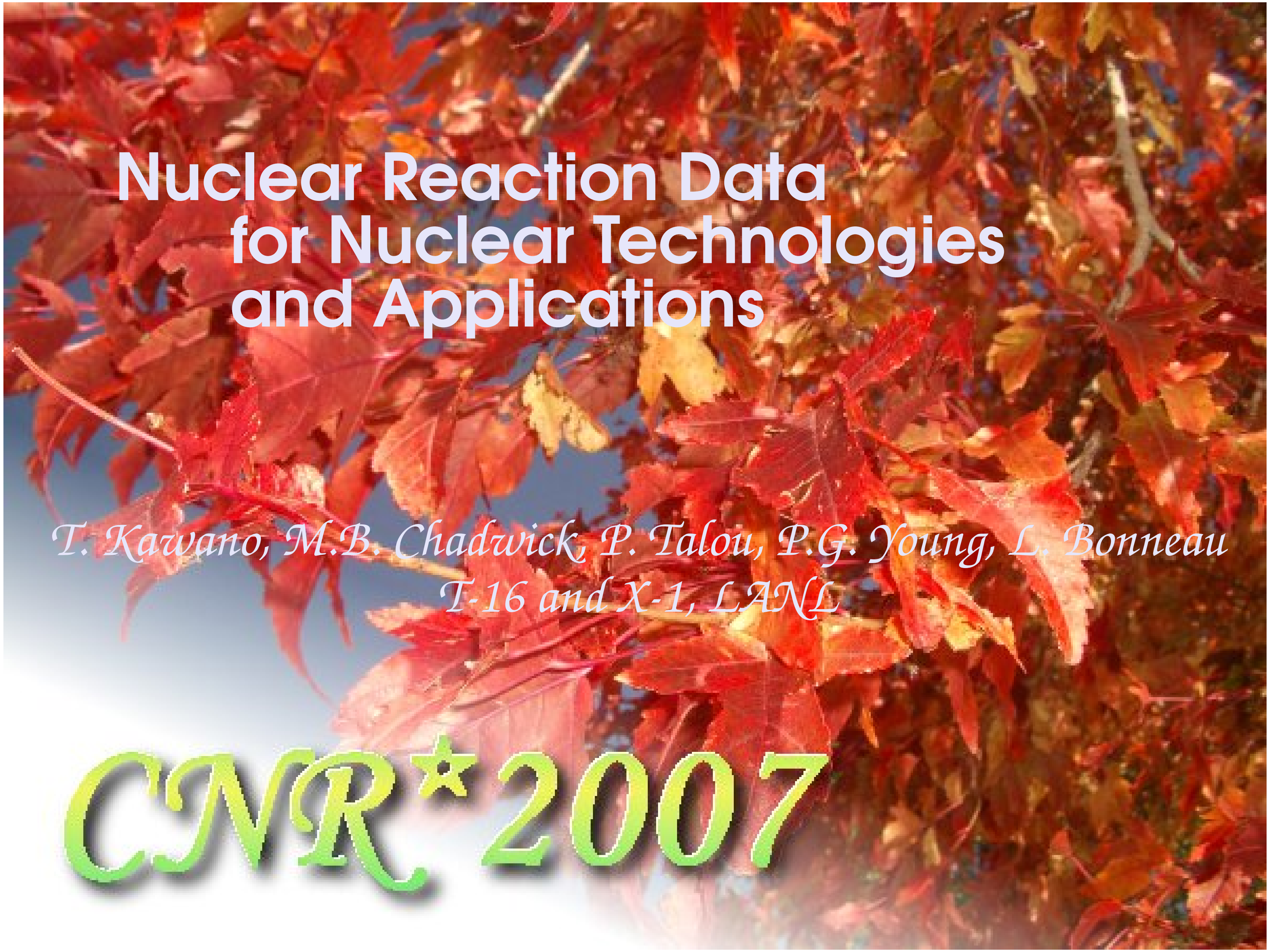

Nuclear Reaction Data for Nuclear Technologies and Applications

T. Kawano, M.B. Chadwick, P. Talou, P.G. Young, L. Bonneau
T-16 and X-1, LANL

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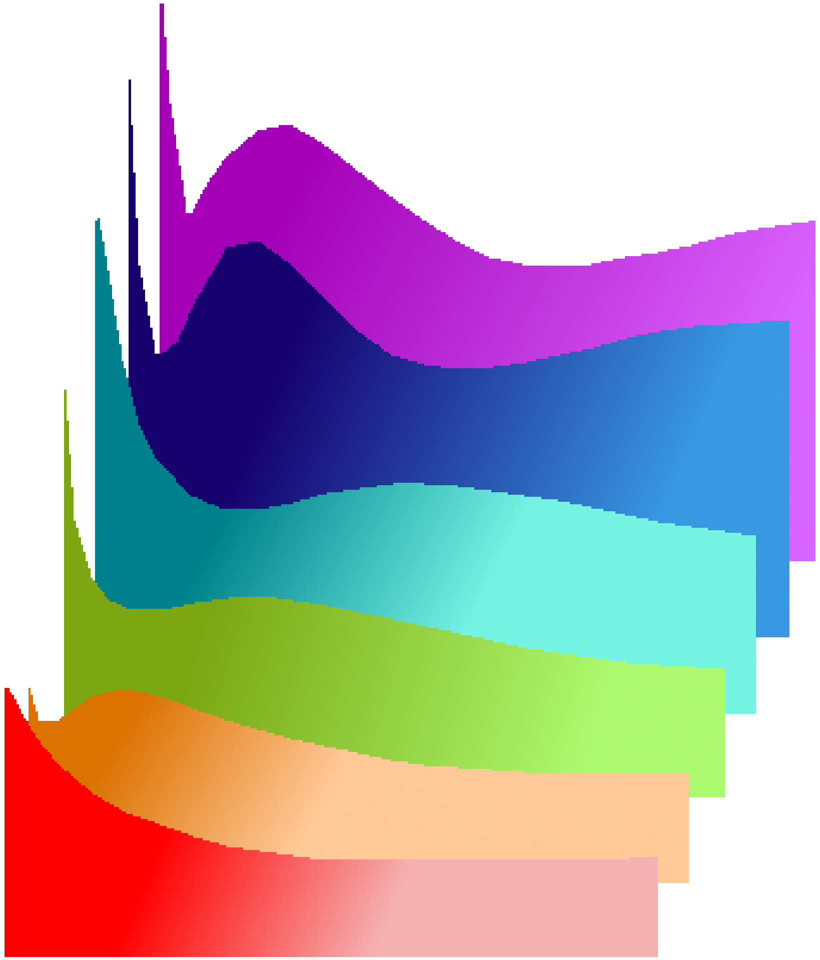
Introduction

Nuclear Data Required for:



- Energy Production
  - Fusion Reactor (DT, DD, D^{3}He)
  - Fission (thermal and fast)
- Nuclear Waste Management and Transmutation
  - Criticality Safety, ADS, AFC, GNEP
- Nuclear Astrophysics
  - s-process and r-process
- Accelerator Applications — radiation shielding
- Space Applications

  — radiation shielding, space reactor
- Semiconductor Device

  — single event upsets (Si)
- Medical Applications — charged particle

Technology areas where nuclear data play an important role are expanding, and more accurate data are demanded.

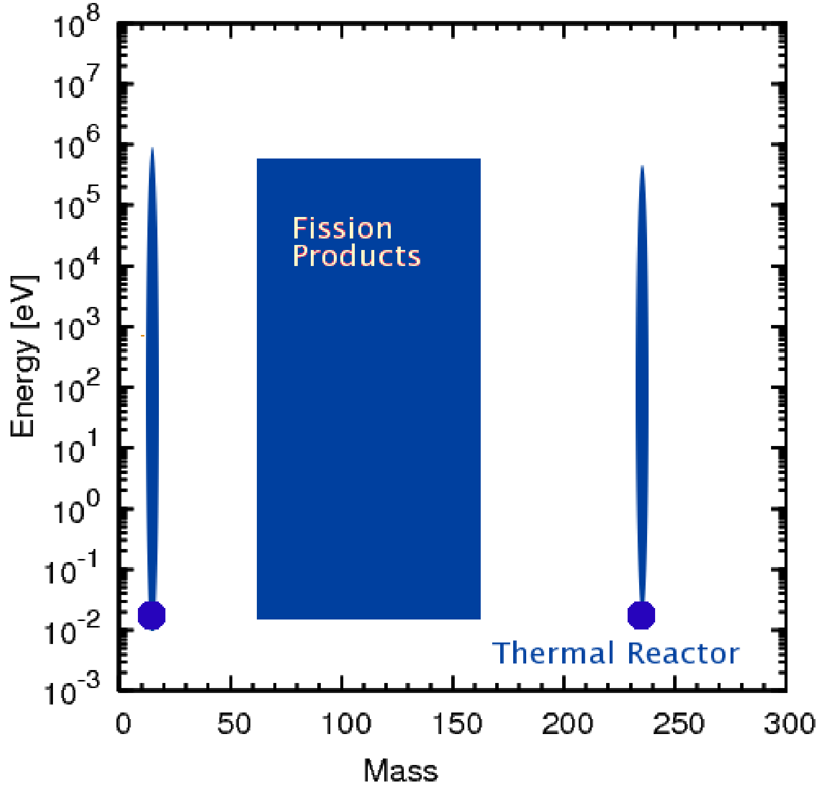
Nuclear Data Library

Database for Particle Transport Calculations

- Each application requires different types of data —
  - target mass and atomic numbers, energy range
  - quantities — cross section, scattering angular distribution, resonance parameters, secondary particle energy distribution, isomeric state production, etc.
- General purpose data libraries try to cover all the requirements.
  - ENDF/B-VII (USA), JENDL-3.3 (Japan), JEFF-3.2 (Europe), CENDL-3 (China), BROND-3 (Russia)
  - international competition / collaboration
  - mainly for energy applications
- Special purpose files are also provided
  - dosimetry, high energy, decay data, photo-reaction, etc.

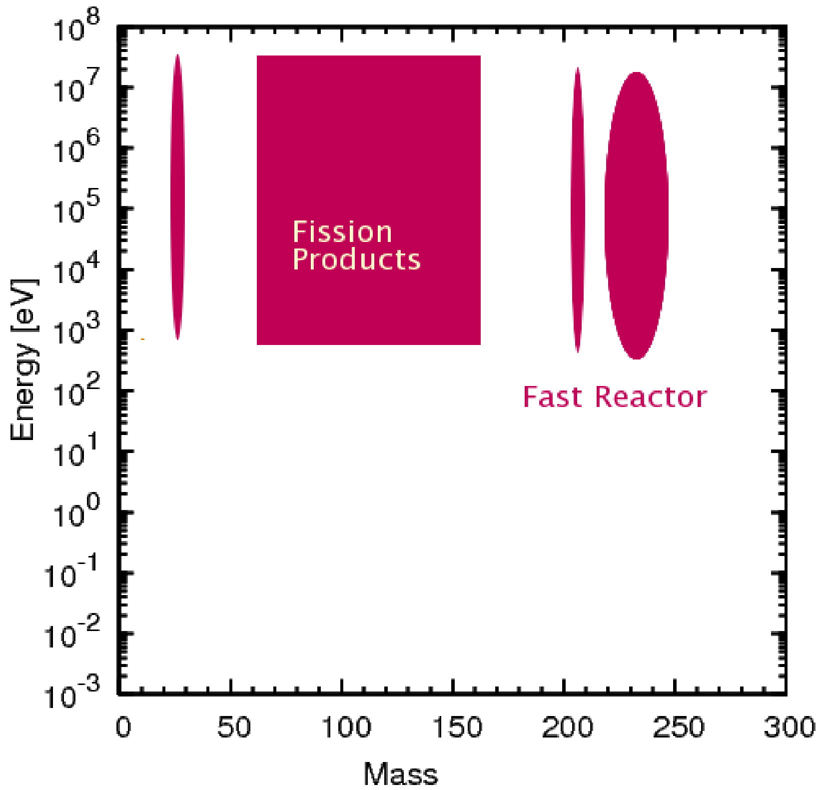
Data Needs for Thermal Nuclear Fission Reactors

- Resonance parameters of actinides (^{233}U, ^{235}U, ^{238}U), which determine the thermal cross sections
  - fission and capture cross sections at the thermal energy (0.0253 eV) have very low uncertainties ($\sim$0.5%)
  - cross sections on other components O (H_2O), Zr (zircaloy) required
- Average number of neutrons per fission $\overline{\nu}_p$
- Prompt neutron fission spectrum χ
  - fission generates high energy neutrons $\overline{E} = 2$ MeV
  - Maxwellian, Watt, Madland-Nix
- β-delayed neutron
  - delayed neutron yield $\overline{\nu}_d$, precursor distribution (fission products yield)



Data Needs for Fast Reactors

- Reaction cross sections on actinides in the keV – MeV range
  - often represented by unresolved resonance parameters
  - D, $\langle \Gamma_n \rangle$, $\langle \Gamma_f \rangle$, $\langle \Gamma_\gamma \rangle$
- Very accurate σ_f and $\overline{\nu}_p$ are required, $\delta(\sigma_f \overline{\nu}_p) \sim 1\%$ or less
- Elastic / inelastic scattering
  - angular distribution, $\overline{\mu}$
  - neutron slowing down by inelastic scattering process
- Fission cross sections of minor actinides (Am, Np, Cm) for transmutation technology



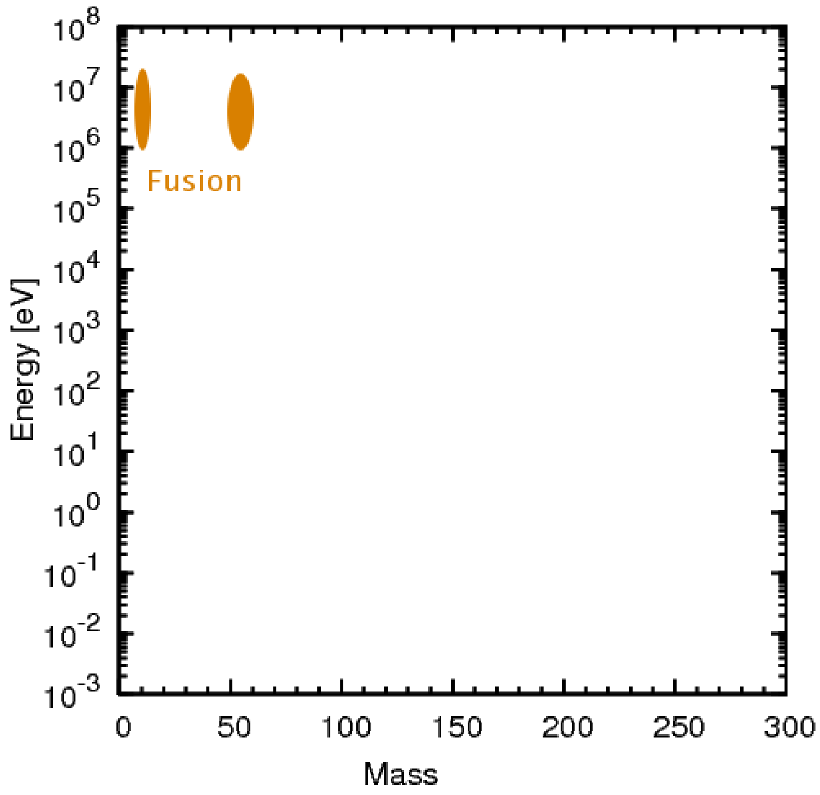
For conceptual designs of next generation reactors, uncertainty quantification and estimation of design margin are crucial. It requires the estimation of uncertainties in the nuclear data.

Data Needs for Fusion Energy

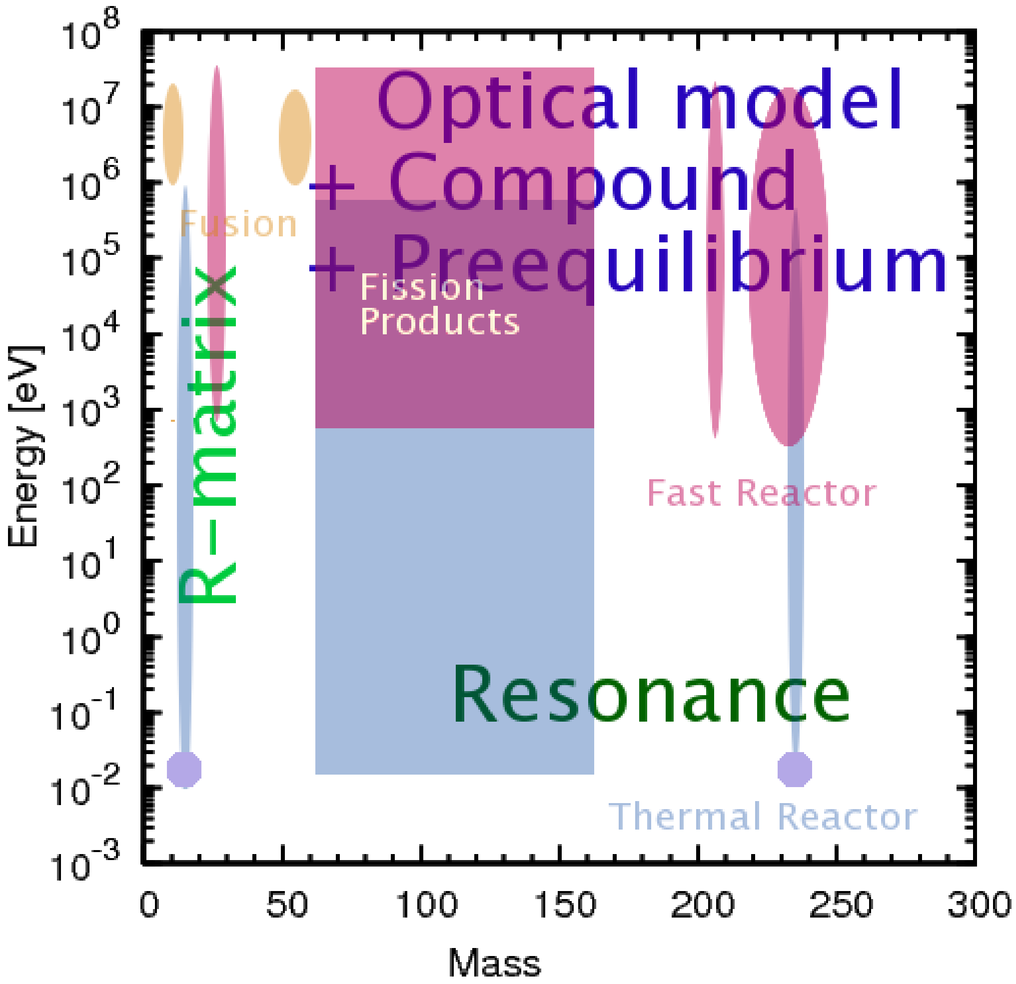
- Fusion cross sections
- Tritium breeding reaction on ^{6,7}Li
- 14-MeV neutron interactions

  on structural materials, Fe, Cr, Ni, V, C, B, ...
  - radiation shielding, γ heating, gas-production
  - life-time of structural materials, swelling, blistering, embrittlement
  - neutron scattering process

    $\longrightarrow$ pre-equilibrium becomes important
  - general purpose files contain data upto 20 MeV
- IFMIF
  - Fusion Material Irradiation Facility
  - 40-MeV deuteron on Li target
  - High energy neutron data



Nuclear Reaction Modeling

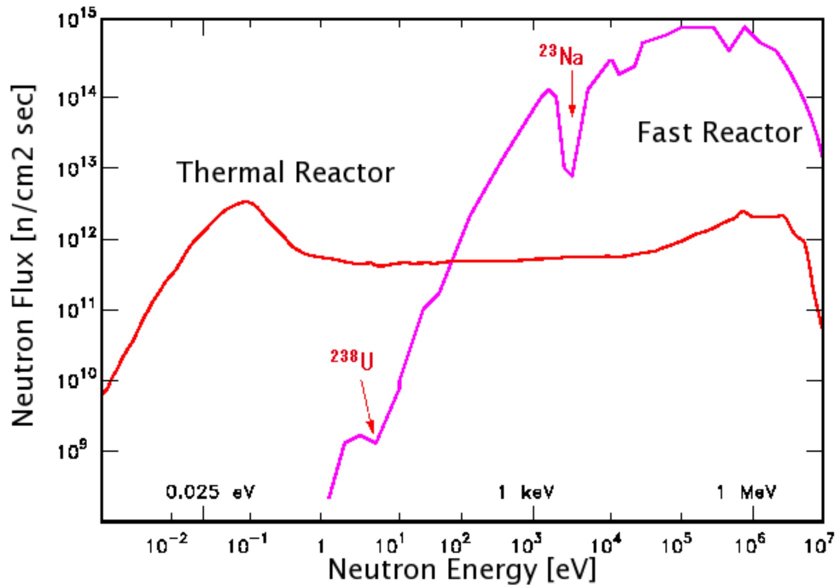


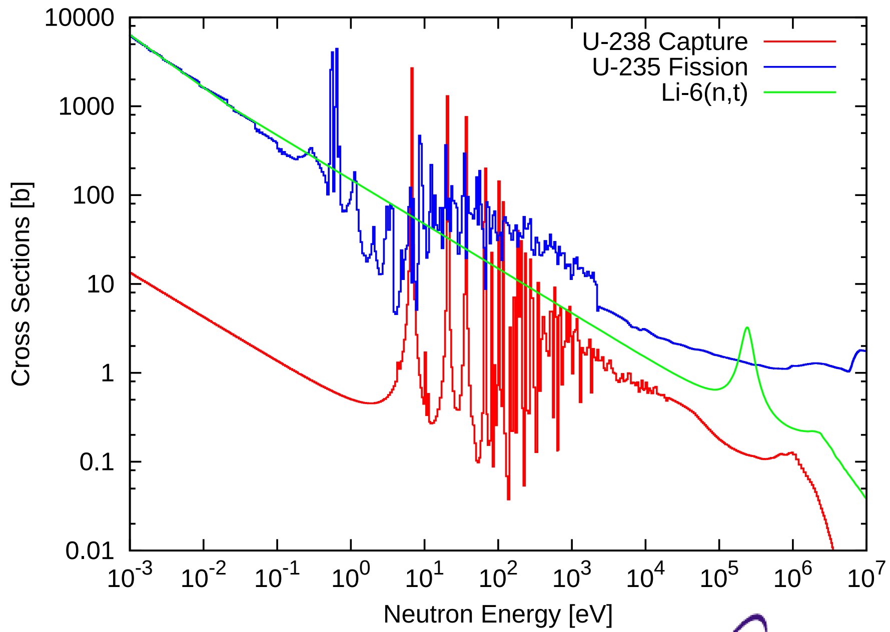
- R-matrix
  - Rigorous, but can be applied to light elements only
- Resonance
  - single or multi-level Breit-Wigner
  - Reich-Moore R-matrix
- Optical model
  - spherical optical model
  - coupled-channels model for deformed nuclei
  - DWBA for inelastic process
- Compound Reaction (continuum)
  - Hauser-Feshbach theory
  - width fluctuation correction
- Pre-Compound Reaction
  - Exciton model
  - quantum mechanical models — FKK, TUL, NWY

Important Reactions for Fission Engineering

Cross sections on major actinides (^{235,238}U and ^{239}Pu) have been studied extensively in the past.
Fission and capture processes are particularly important for fission energy applications.

- fission and $\overline{\nu}_p$: $k_{\rm eff} \geq 1.0$ to sustain a chain reaction
- capture : nuclear transmutation
  - fuel breeding
    ^{238}U+n $\rightarrow$ ^{239}U $\rightarrow$ ^{239}Np $\rightarrow$ ^{239}Pu
  - production of minor actinides
    ^{239}Pu+2n $\rightarrow$ ^{241}Pu $\rightarrow$ ^{241}Am
- (n,2n) reaction : nuclear transmutation
  - ^{239}Pu(n,2n)^{238}Pu
  - ^{241}Am(n,2n)^{240}Am $\rightarrow$ ^{240}Pu





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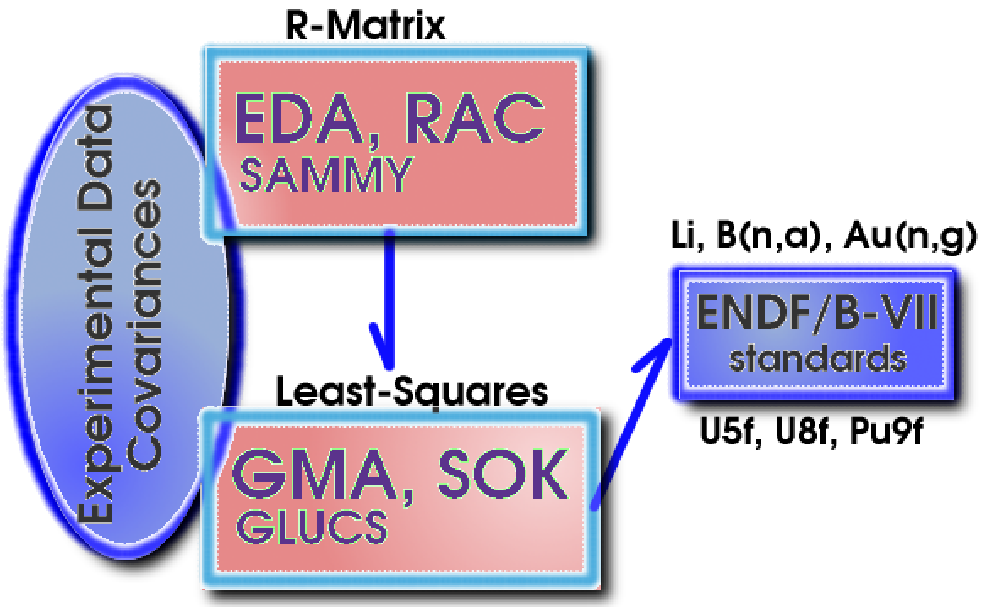
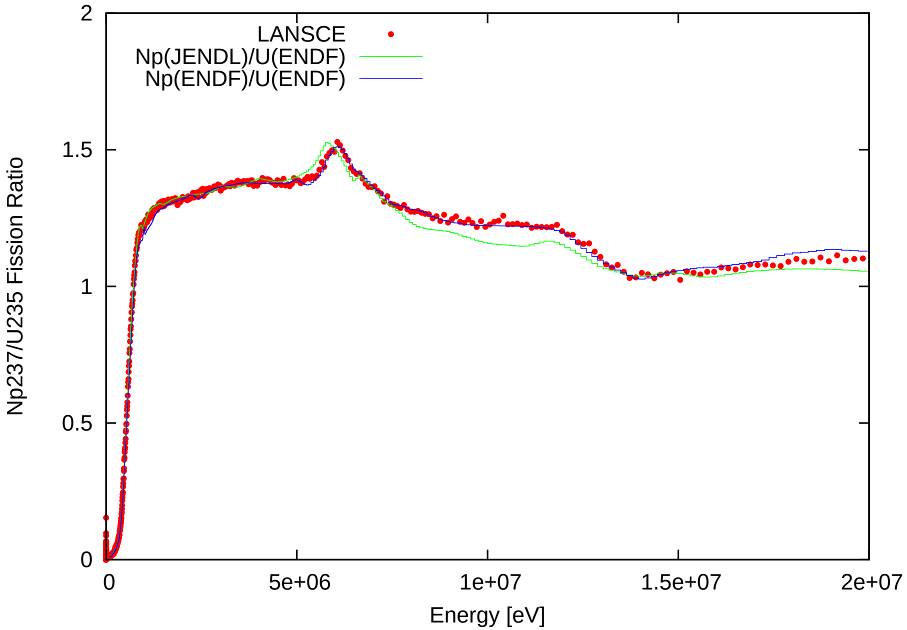
Standards, IAEA Coordinated Research

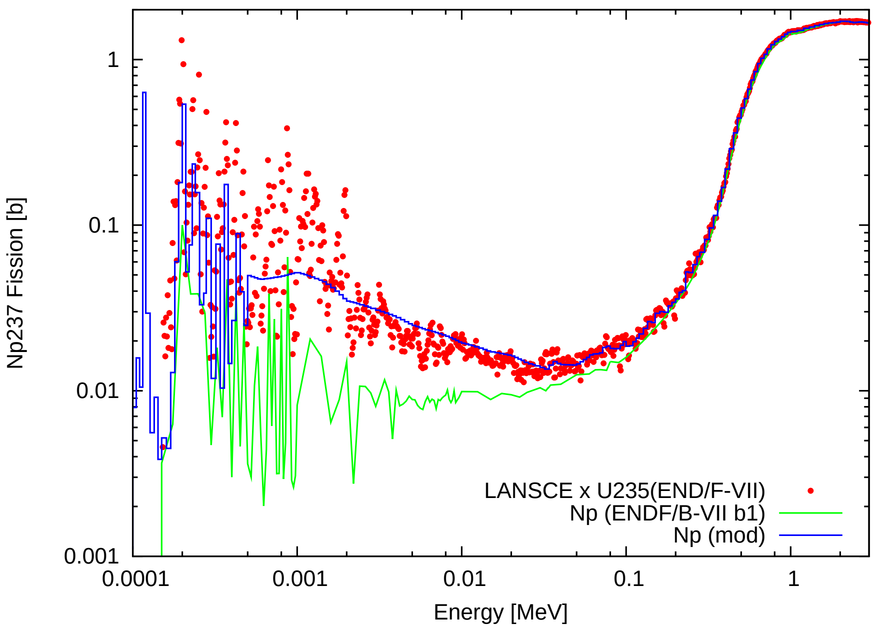


- Coordinated by A. Carlson (NIST) and V. Pronyaev (IAEA)
- Re-evaluation / re-normalization of experimental data
- EDA R-matrix analysis for hydrogen
- R-matrix analysis for light elements
- Least-squares fitting for fission c.s.
- Combining two results

- The fission cross sections for major actinides are in $0.5 \sim 2\%$ acuracy now.
- Ratio measurements (ratio to hydrogen or ^{235}U fission) are converted into the absolute values by using the new standards.

Np-237 Fission in the Fast Energy Region





Experimental Data at LANSCE

- The data were taken as ratios to ^{235}U fission c.s.
- They were re-normalized by using the standards.

Evaluation

- We adopted the JENDL-3.3 resonance parameter evaluated by Nakagawa.
- Unresolved parameters were modified to match the LANSCE data.
- The Hauser-Feshbach model calculation is feasible, but still problematics.
- Direct use of experimental data gives a very precise evaluation in this case.

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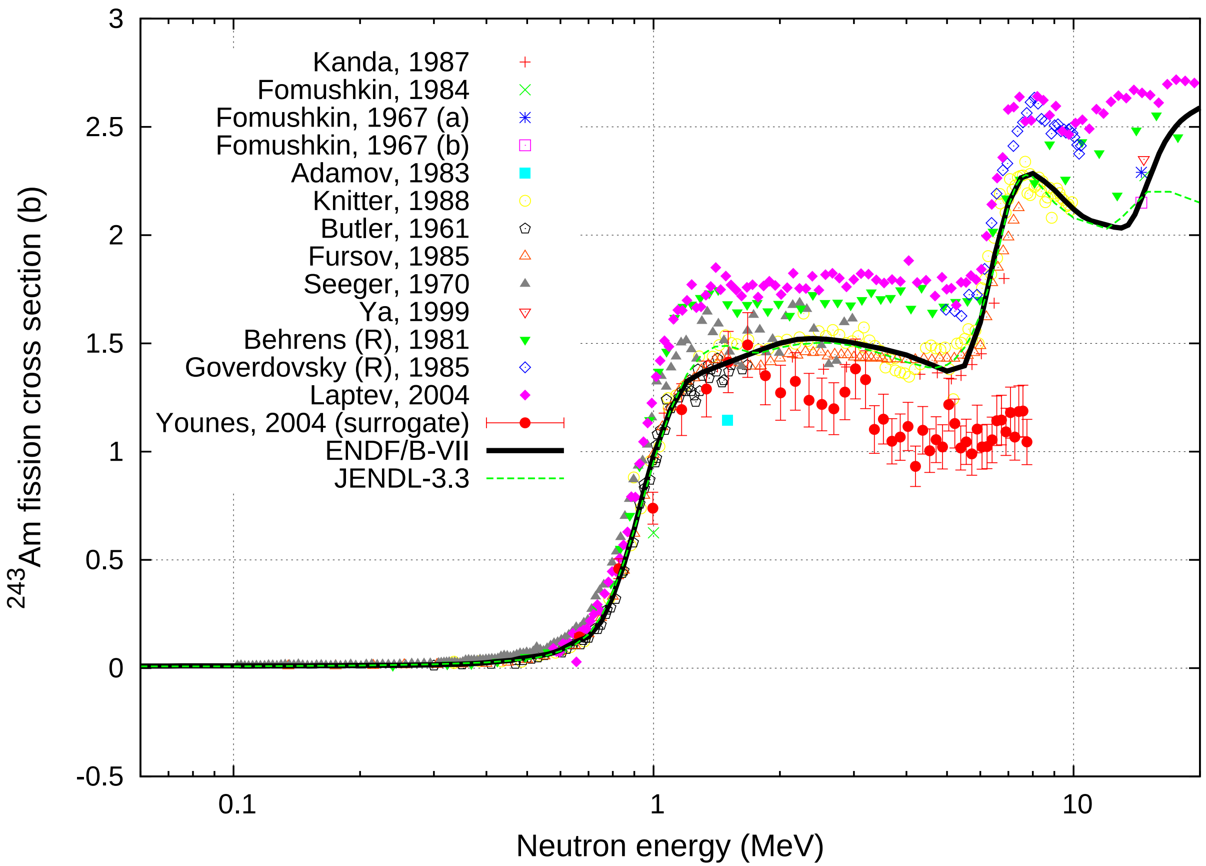
Fission Cross Section - Am-243



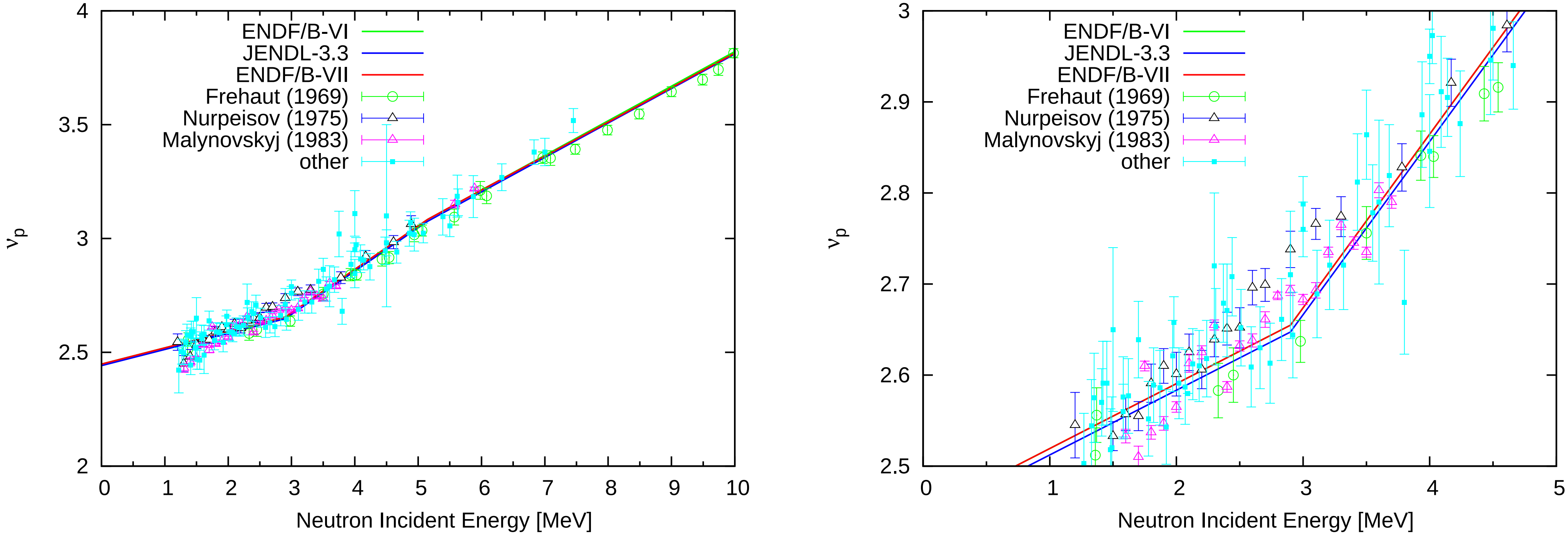
GNASH calculation agreed fairly well with experimental data.

There are two (inconsistent) groups of experimental fission cross section data.

It seems integral experiments with the ZEBRA reactor support lower group — other information, such as the integral data, may help to resolve the discrepancy.

Number of Prompt Neutrons Per Fission

ν_p for ^{238}U Fission

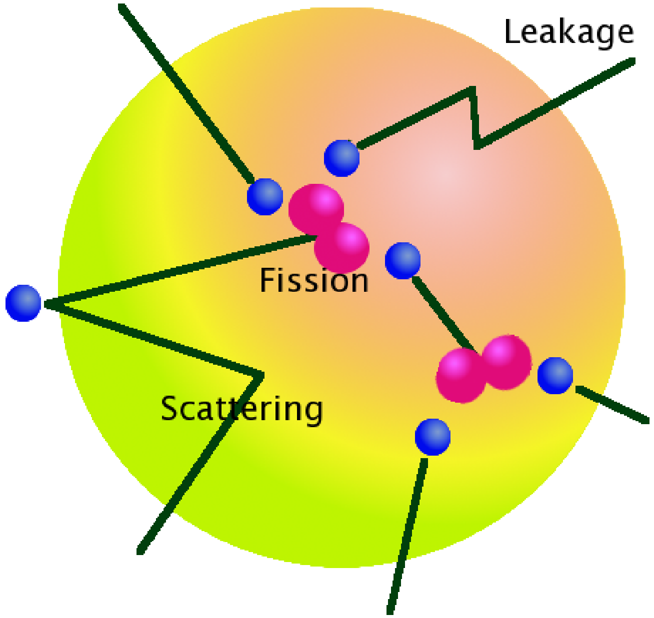


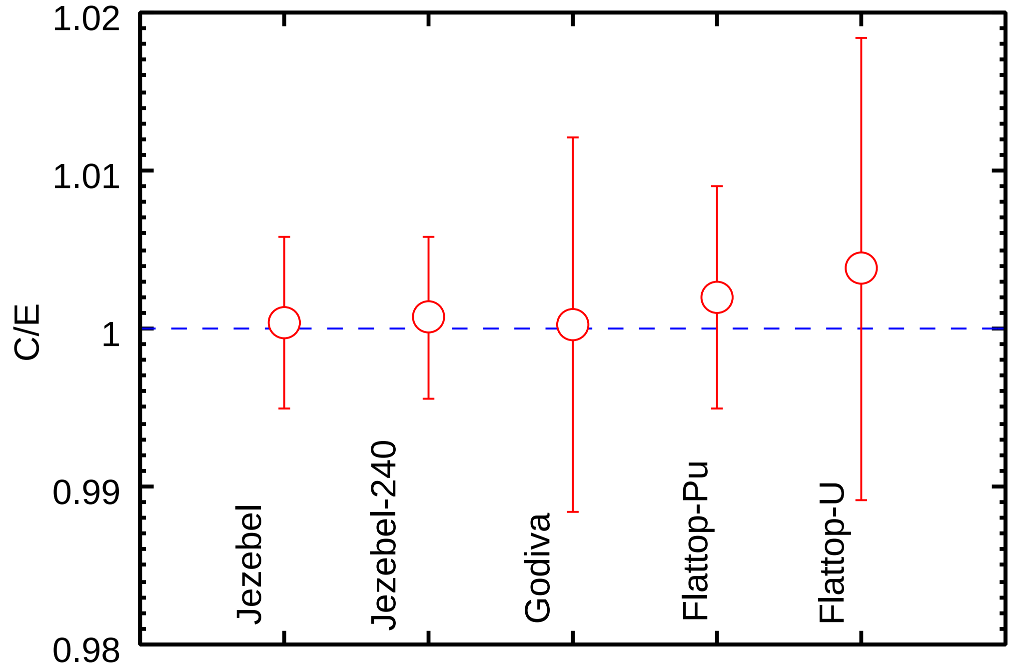
A simple linear function is used to represent ν_p, which ensures the uncertainties of less than 1%.

More microscopic descriptions of the fission process, such as the Monte Carlo approach would be a breakthrough to improve the accuracy, when experimental data are inaccessible.

Fission Cross Section in the Fast Energy Range

Neutron Multiplicity, $k_{\rm eff}$





Uncertainty Calculation for LANL Critical Assemblies

Uncertainties taken into account for the calculated $k_{\rm eff}$ are, the nuclear data (covariance), experimental uncertainty in the integral data, and statistical error in the Monte Carlo method.

G. Chiba (JAEA)

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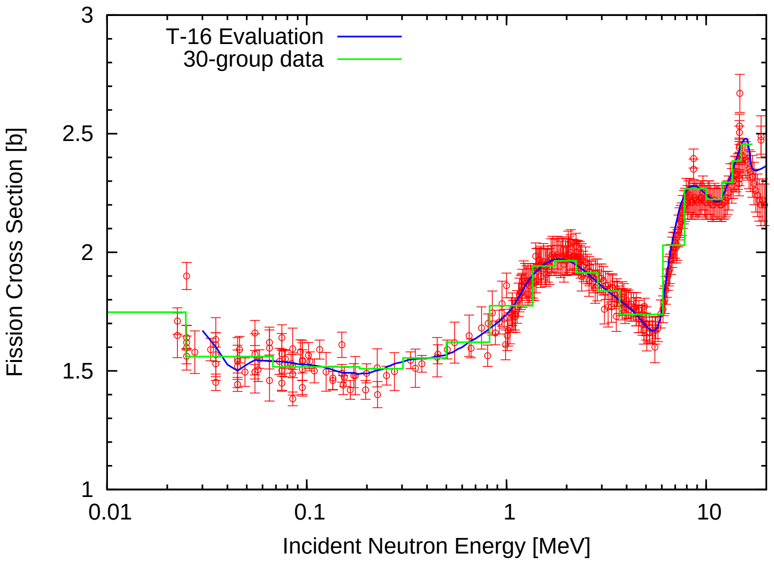
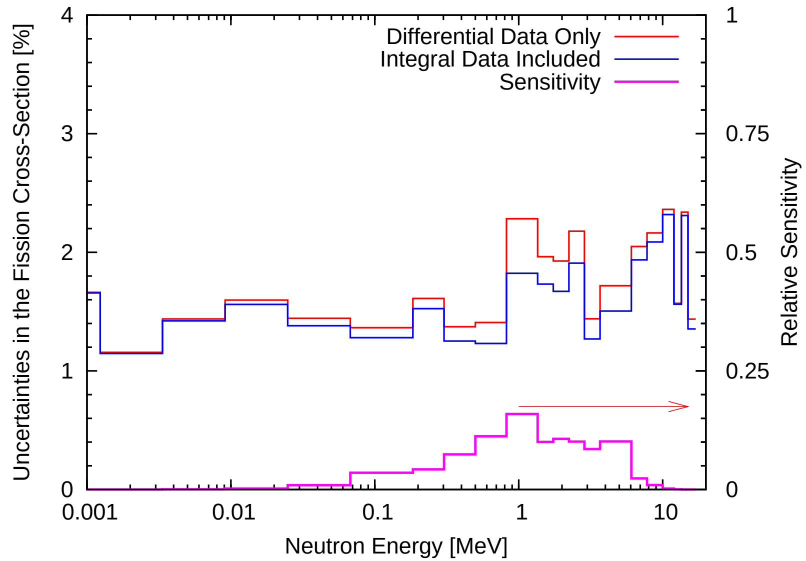
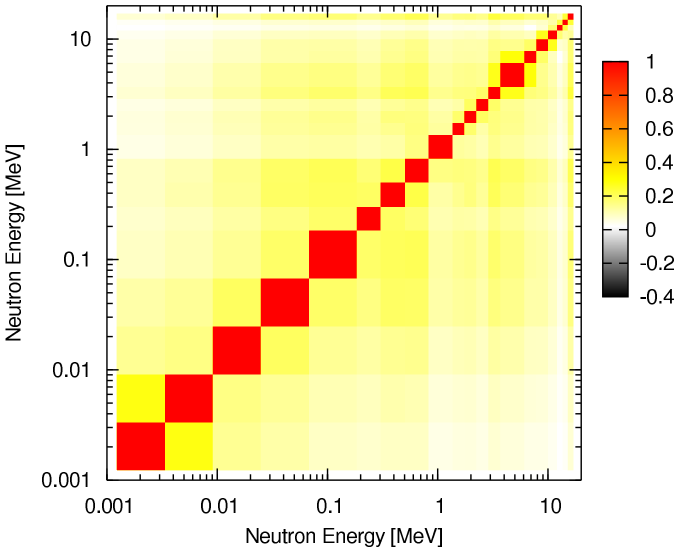
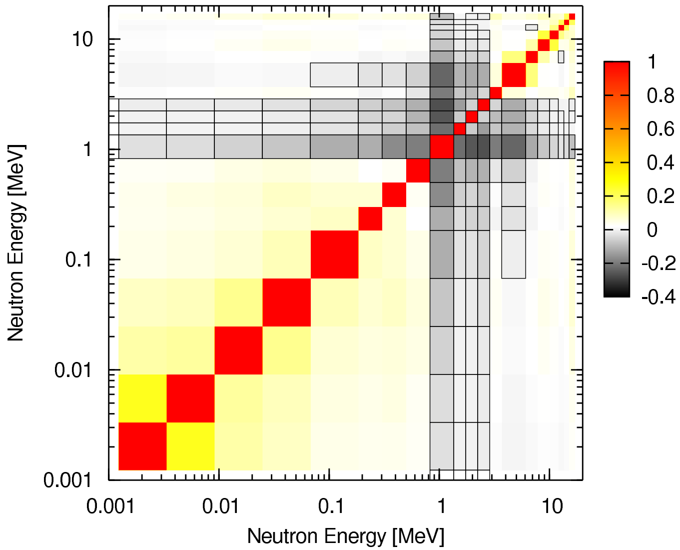
Reduce Uncertainties in the Fission Cross Sections









The neutron multiplicity of Jezebel is proportional to $\sigma_f \overline{\nu}_p$

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Nucleon Capture Process

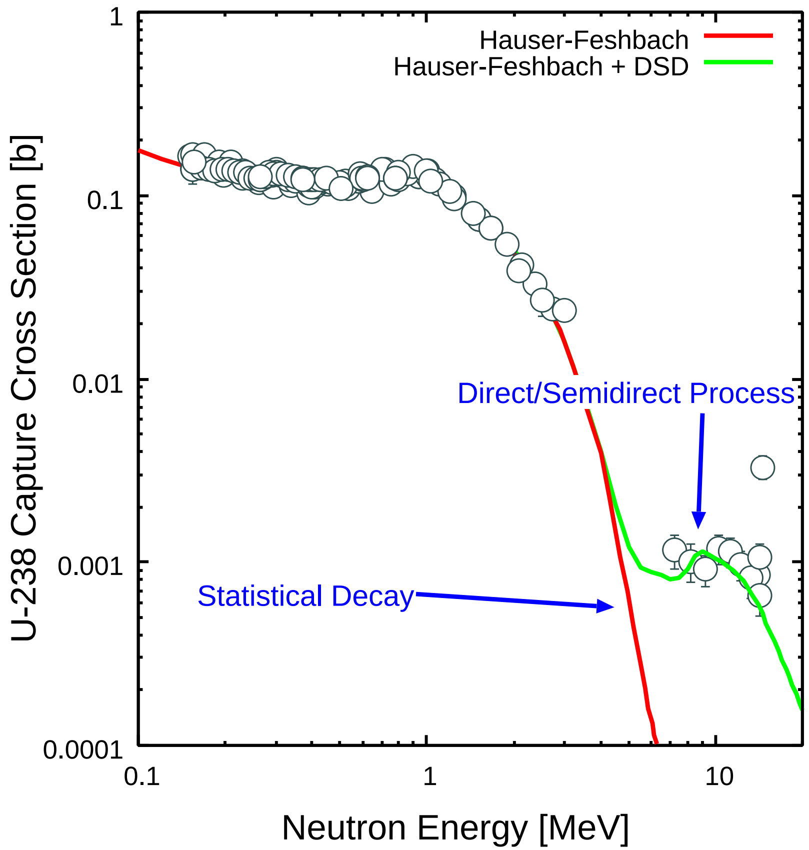
CN and DSD Processes

Compound Reaction

- An incident neutron and a target form a compound nucleus, and it decays.
- Hauser-Feshbach statistical theory, with width fluctuation.
- Cross section decreases rapidly when neutron inelastic channels open.

Direct/Semidirect Capture

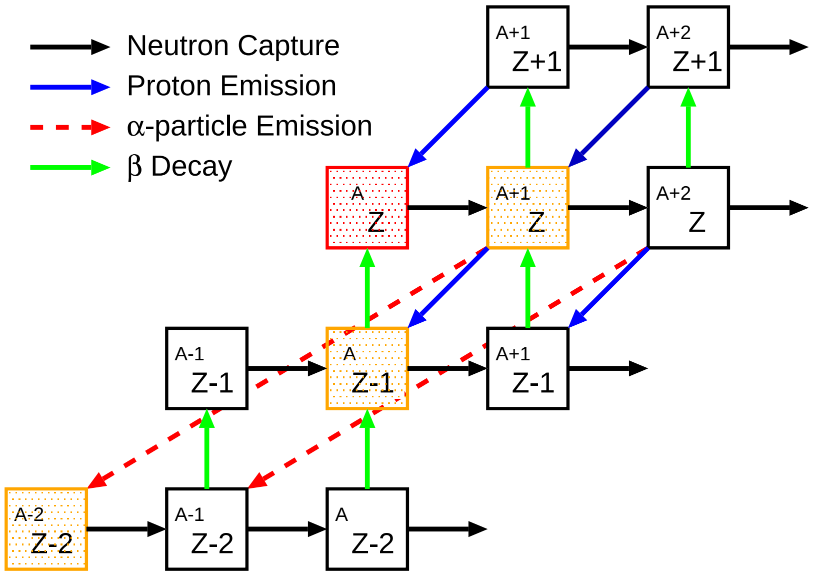
- Direct transition to one of the unoccupied single-particle state.
- Giant Dipole Resonance (GDR)



DSD becomes important when (1) incident particle energy is high, or (2) compound capture cross section is small (few resonance, neutron-rich, doubly-closed shell nuclei.)

Nuclear Reaction Rate in Astrophysics

Nuclear Reaction Chain



- Nuclear reactions in astrophysical environments
  — s and r-processes
  - targets are often neutron-rich and unstable
  - neutron capture process is mostly important
  - β-delayed neutron emission and fission
- Model prediction is crucial for
  - reaction cross section
    — Hauser-Feshbach theory
  - nuclear structure
    — marco/microscopic model, Hartree-Fock

Reaction rate calculations based on microscipic theories are favorable for unstable tagets. We have developed a direct/semi-direct nucleon capture process based on the Hartree-Fock BCS model.

DSD Theory for Deformed Nuclei

DSD Amplitudes

$$T_d \propto \sqrt{S_{ljK}}\langle R_{ljK}(r)|r|R_{LJ}(r)\rangle$$

$$T_s \propto \sqrt{S_{ljK}}\langle R_{ljK}(r)|h(r)|R_{LJ}(r)\rangle$$

DSD with Hartree-Fock BCS Theory

spectroscopic factor S_{ljK}

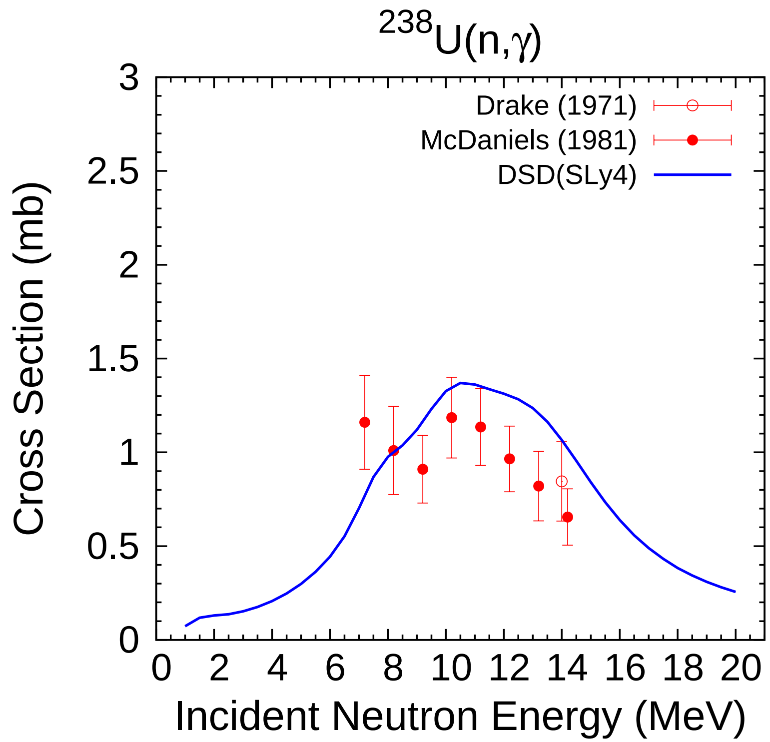
- single-particle occupation probabilities, $v^2 = 1 - u^2$
- no experimental data needed

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

- HF-BCS calculation and decomposition into spherical HO basis
- consistent treatment for all nuclei from spherical to deformed nuclei

U-238 Calculated Result

We have validated our model against the existing experimental data.



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Hauser-Feshbach-Moldauer Calculation

Program CoH

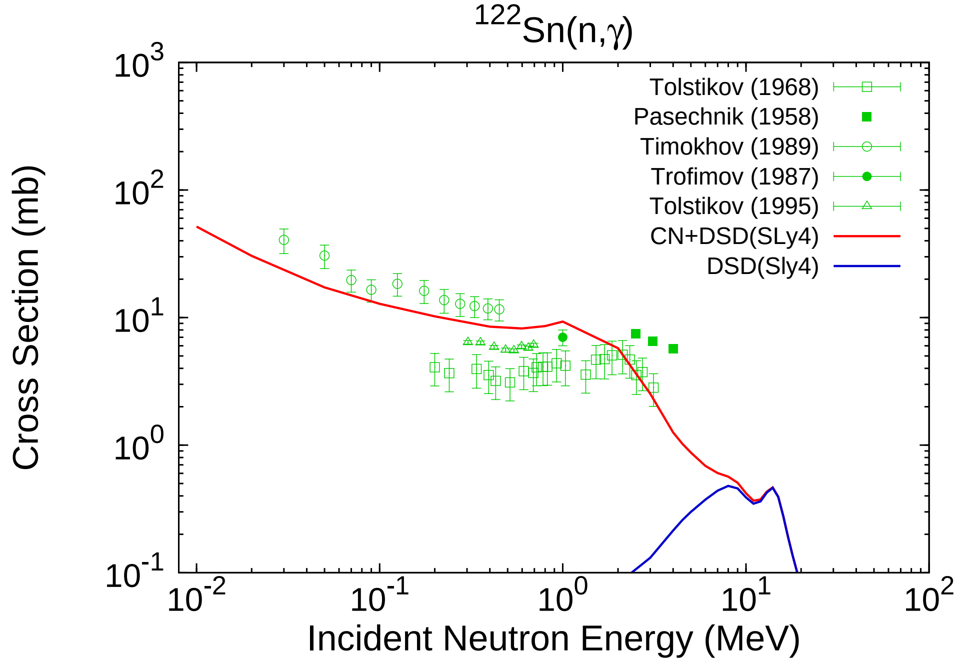
- Spherical optical model, and coupled-channels model
  - The global parametrization is adequate for cross section calculation of unstable nuclides.
  - Koning-Delaroche Global Potential for n and p
  - CoH also contains some potentials for α, d, t, and ^{3}He.
- Hauser-Feshbach model, width fluctuation by Moldauer
- Particle induced process, (n, pX), (α, nX), *etc.*
- Neutron capture, E_1, E_2, and M_1 transitions

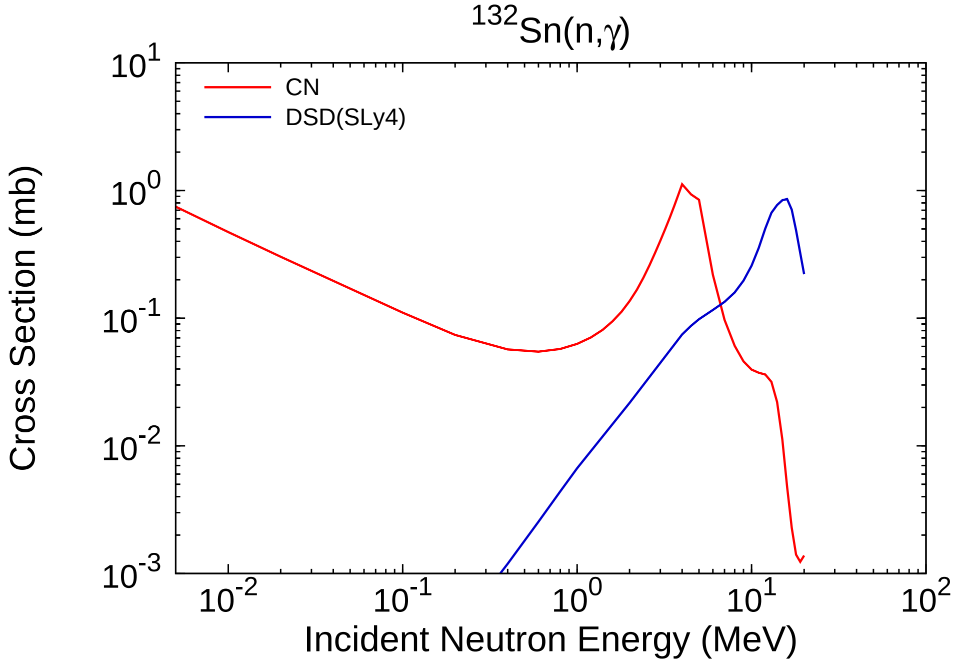
Supplemental Programs and Database

- Interface mini-programs to retrieve input parameters.
- Mass excess data (KUTY00, KTUY03), and ground state $J\pi$

Neutron Capture Off-Stability — Sn-122,132

DSD + Hauser-Feshbach Calculations for Tin





stable target

unstable, but important for r-process

Since global Hartree-Fock-BCS calculations for all nuclides are feasible, this technique will be a powerful tool to estimate the neutron capture rates in the r-process.

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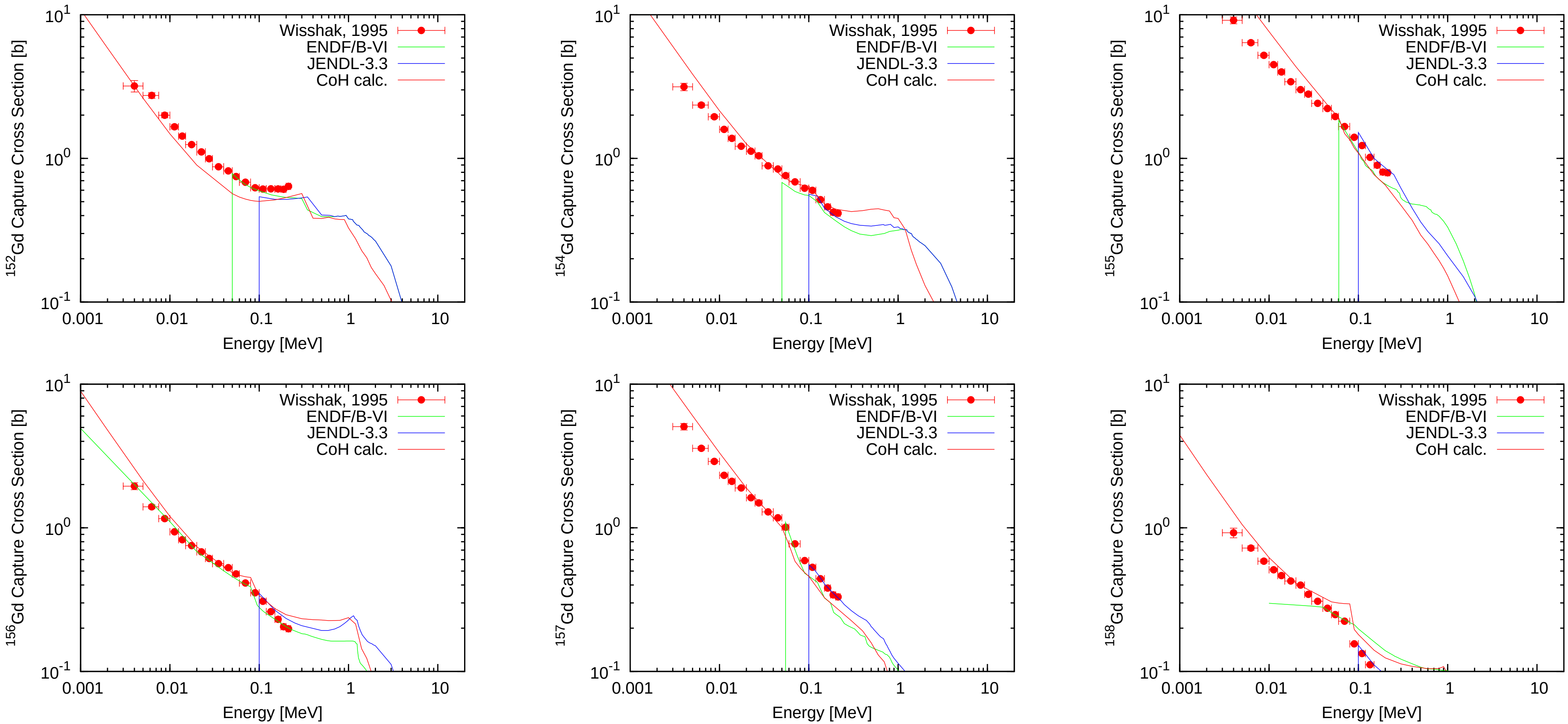
Default Calc. to Test Predictive Capability

Gd Isotopes, Comparison with FZK Data



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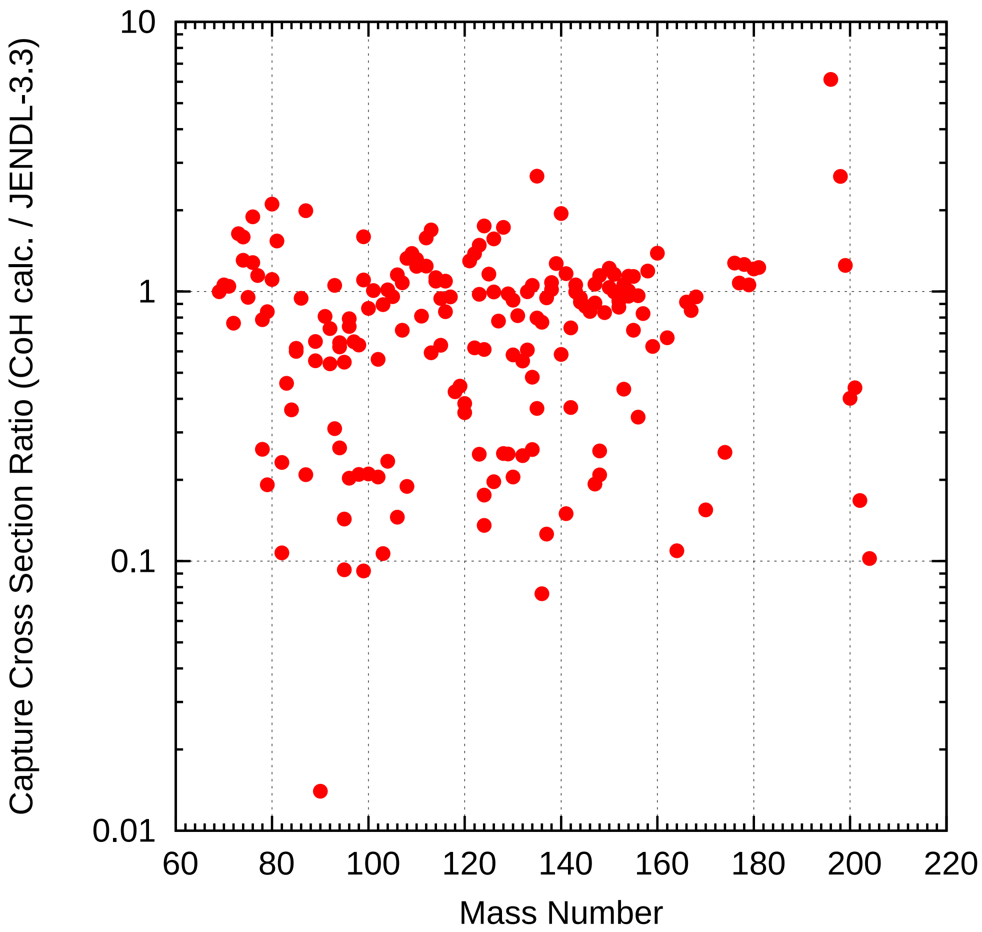
Blind Calc. Using Global Parameters

Comparison with JENDL-3.3/Fission Products Region

- Capture cross sections at 100 keV were calculated with this system.
- from ^{69}Ga to ^{204}Hg (195 nuclides)
- Blind calculation, no adjustment.

Result

- Many of calculated σ_γ 's were from $0.1\times$(JENDL) to $2\times$(JENDL).
- CoH calc. tends to underestimate.
- Possible reasons —
  Level densities used, especially for nuclides with no available discrete level info. We need to improve the level density systematics for unstable targets.
- Cross section prediction can be improved by tuning parameters to measured data.



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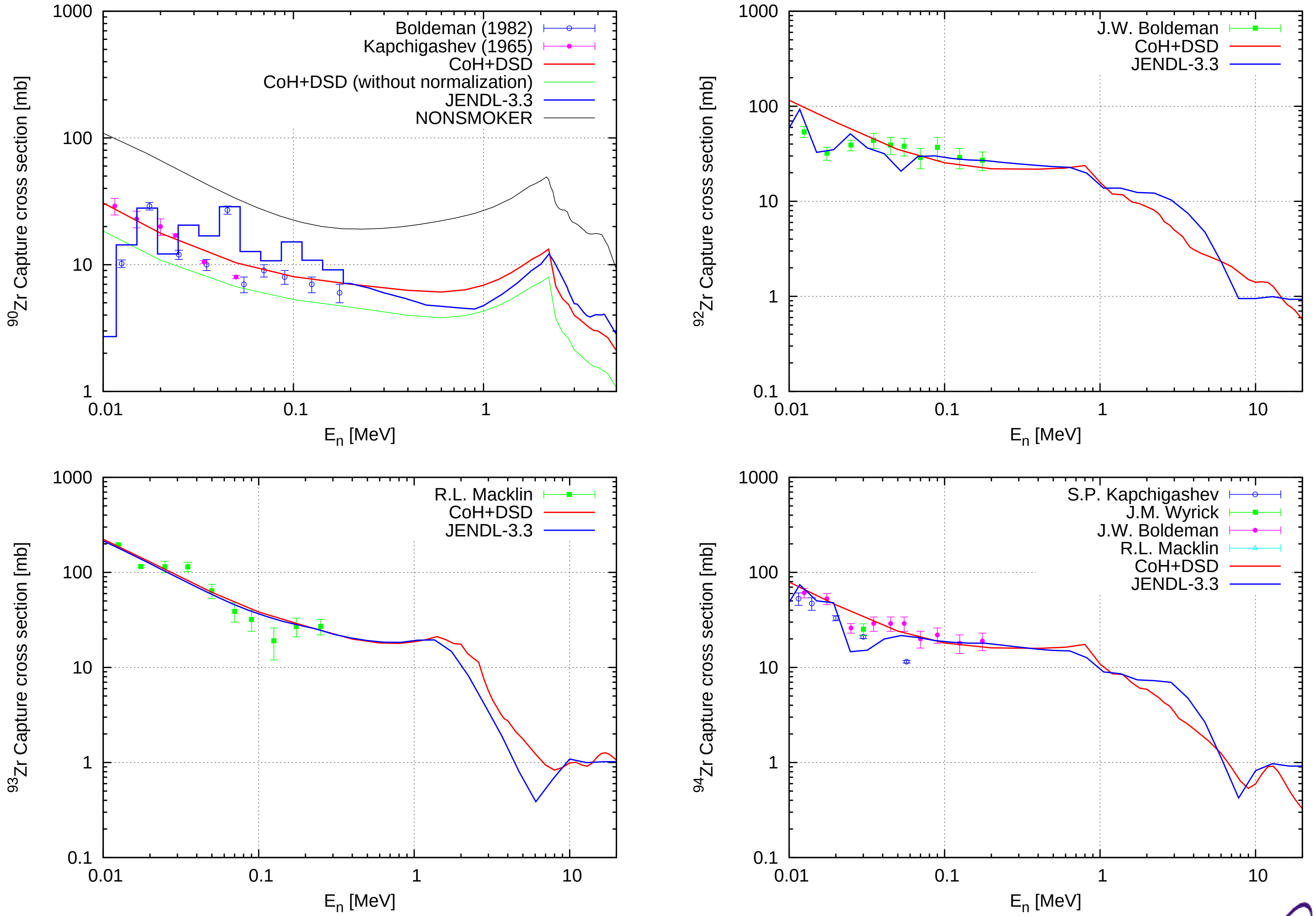
Capture Cross Sections on Zr Isotopes

Zr Isotopes, Parameters Adjusted to Experimental Data



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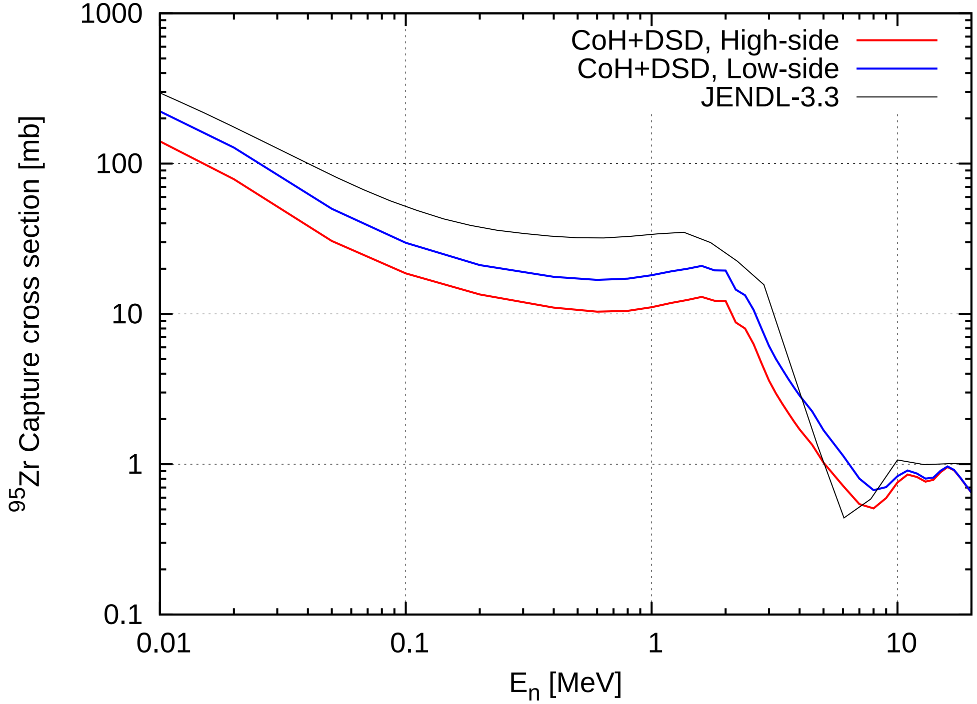
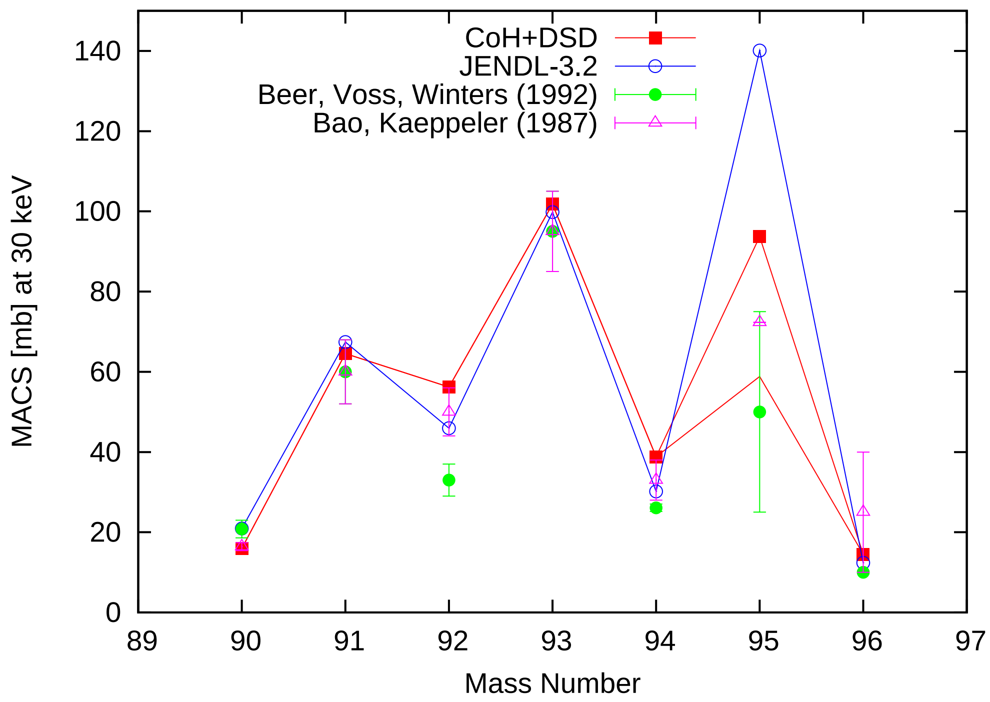
MACS for Zr-95 Capture, 30 keV

Zr-95 Capture Rate for s-process



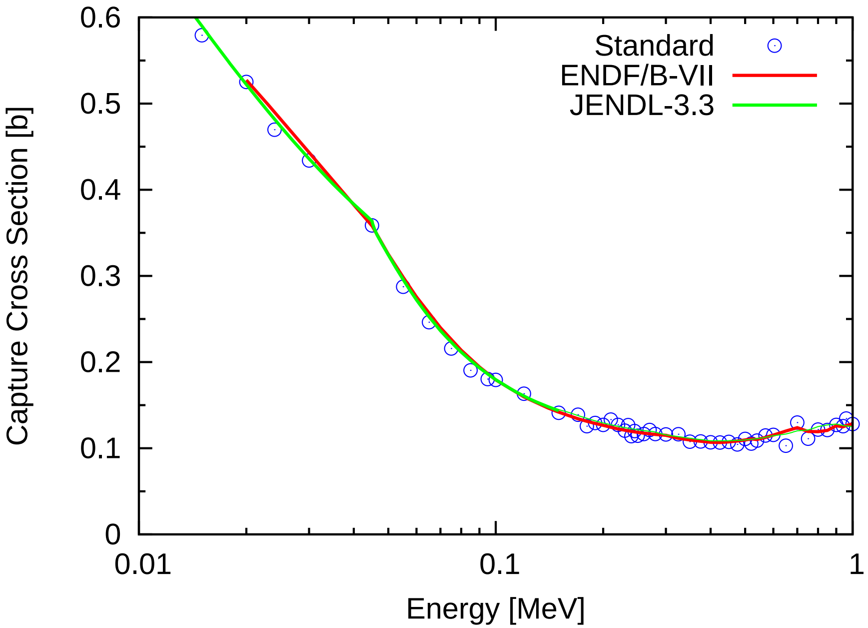


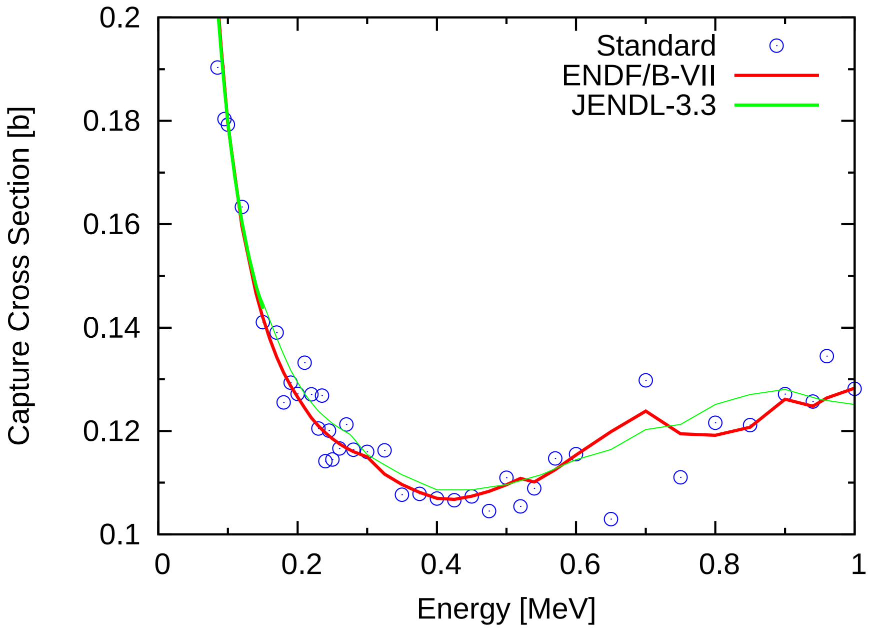
Zr-95 β-decays to Nb-95 with the half-life of 64 days.

U-238 Capture Cross Section in ENDF/B-VII

IAEA Standards Evaluation

The ^{238}U capture cross was evaluated at the IAEA standards projects, the results were not included in the standards data library. We re-fitted the HF model calculation to the standards results for ENDF/B-VII.





The HF model calculation enables us to discriminate numerical wiggles.

This reaction is particularly important for ^{239}Pu breeding. The accuracy of this capture cross section is “uncommonly” good (3% or so).

Code System Utilized in the Cross Section Calculations

- Several Hauser-Feshbach model codes with the pre-equilibrium emission are available / under development.
  - GNASH/McGNASH (LANL), TALYS (NRG Petten, CEA), EMPIRE (BNL,IAEA), STAPRE (Vienna and more), CCONE (JAEA), UNF (CIAE) etc.
- Capablility
  - particle-induced particle-emission cross sections, discrete level excitation, isomer production, energy spectra (angle-integrated)
  - incident energy from 1 keV up to 200 MeV
  - mass range above $A = 20$
- Model Parameters
  - optical potentials (particle transmission coefficients)
  - discrete states J^π and level densities in the coninuum
  - fission parameters (barrier height and width)
  - γ-ray strength functions, GDR parameters
  - pre-equilibrium parameters (depends on the model employed, $|M|^2$ for example)

Reference Input Parameter Library

A library which contains nuclear model parameters, mainly for the statistical Hauser-Feshbach model calculation.

Masses	Experimental nuclear masses by Audi and Wapstra Mass excess calculated with several mass formulae
Levels	Energy, spin, parity, and γ-ray decay probabilities of excited states. (ENSDF-II)
Resonances	Average resonance parameters for s and p-waves.
Optical	Optical potentials for both spherical and deformed nuclei.
Densities	Level density parameters with several level density formulae, and numerical data calculated with a microscopic model.
Gamma	GDR parameters, and expressions of γ-ray strength functions.
Fission	Experimental / calculated fission barriers.

http://www-nds.iaea.org/RIPL-2/

McGNASH

What's New Since GNASH

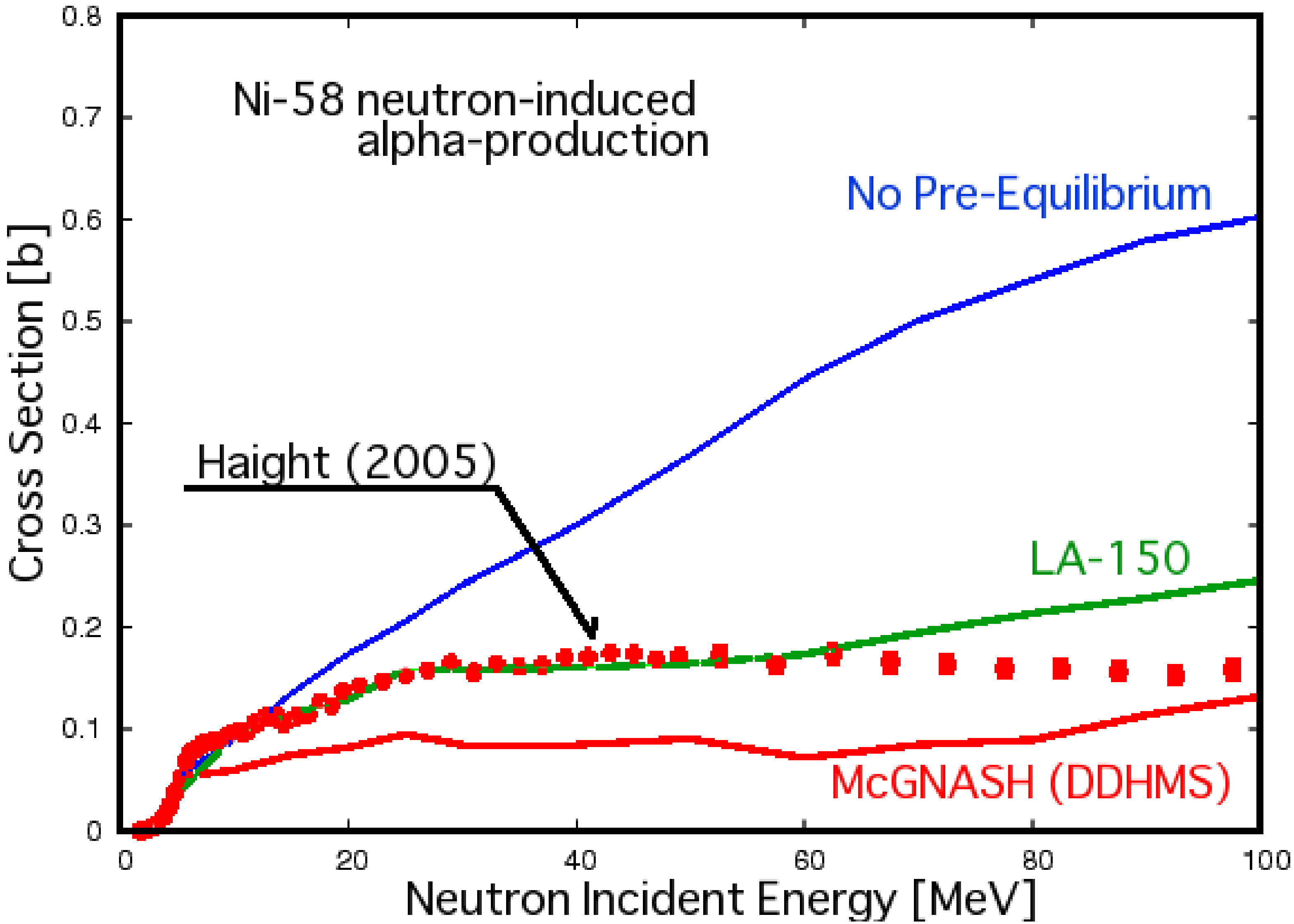
- Written in modern Fortran95 vs. FORTRAN77
- New physics — width fluctuation and pre-equilibrium

Physics Models in McGNASH

- Default GNASH capabilities
  - Hauser-Feshbach theory of the compound nucleus evaporation
  - Ignatyuk-Gilbert-Cameron level densities formalism
  - Kopecky-Uhl γ-ray strength-function formalism
  - pre-equilibrium exciton model + FKK theory (optional)
  - fission physics: two uncoupled inverted parabolas (Hill-Wheeler)
- Additional capabilities
  - automatic retrieval of optical potential parameters from RIPL database
  - direct reactions and coupled-channels calculations (ECIS03 included)
  - width-fluctuation corrections (Moldauer, HRTW, GOE)
  - pre-equilibrium Hybrid Monte Carlo Simulation model (HMS)
  - two-component exciton model (GNASH: one-component exciton model)
  - new fission model under development

Comparisons of McGNASH and GNASH

Helium Production on Ni, Compared with Experimental Data

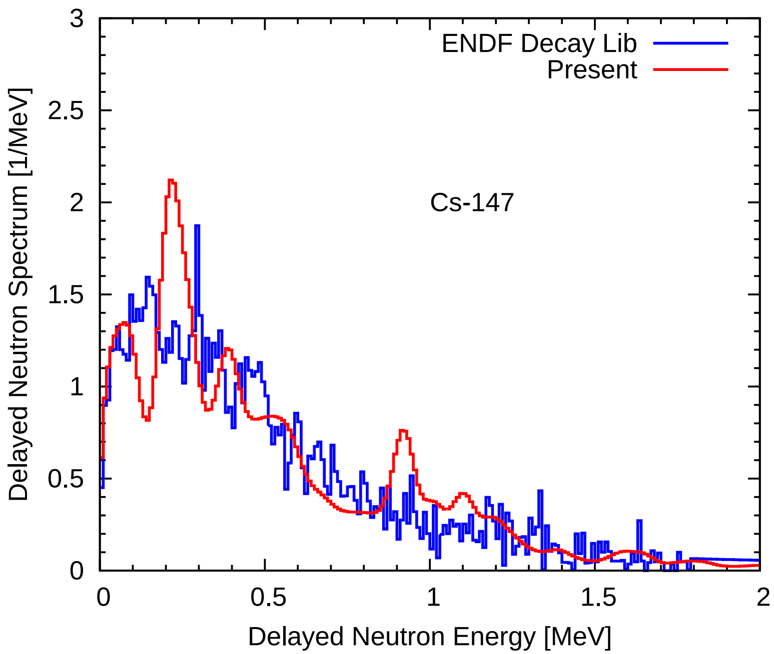


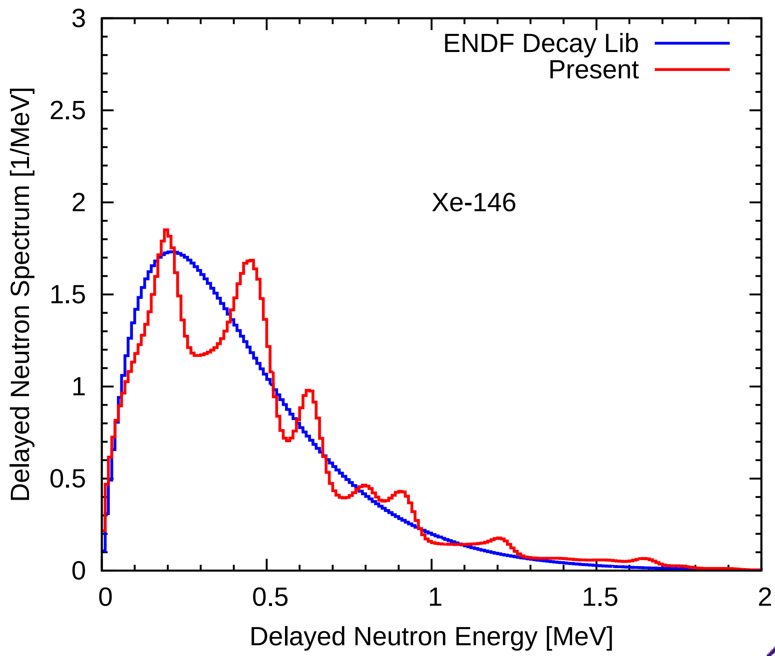
Application of HF to Delayed Neutron Emission

Neutron Emission from the Daughter Nucleus

- We assume that the excited state after β-decay is a compound state, having a fixed J value, $|I-1| \leq J \leq I+1$, where I is the spin of precursor.
- Neutron and γ-ray emissions are calculated with the statistical Hauser-Feshbach theory (modified CoH code).
- The γ-ray emission competition is included, except for the $(n, \gamma n)$ process.

Delayed Neutron Spectra





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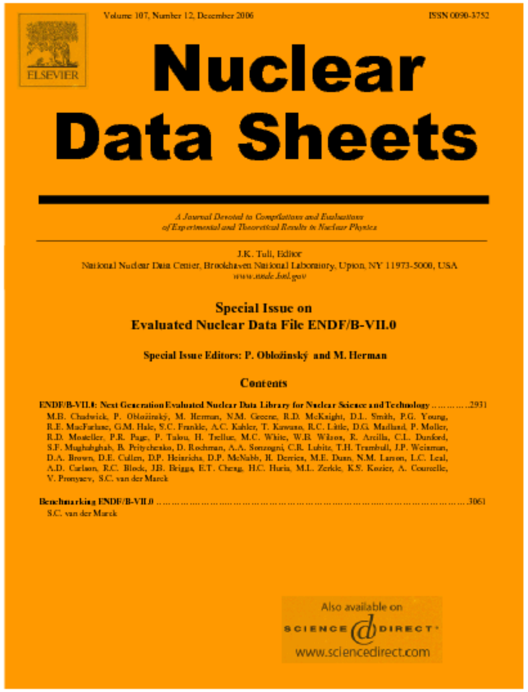
Evaluation Summary


Volume 107, Number 12, December 2006 ISSN 0090-3752

ELSEVIER

Nuclear Data Sheets

A Journal Devoted to Compilations and Evaluations of Experimental and Theoretical Results in Nuclear Physics

J.K. Tuli, Editor
National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY 11973-5000, USA
www.nndc.bnl.gov

Special Issue on Evaluated Nuclear Data File ENDF/B-VII.0

Special Issue Editors: P. Obložinský and M. Herman

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  - LANL, BNL, ORNL, NIST, LLNL, KAPL, Bettis, ANL

The report was published in Nuclear Data Sheets, special issue, **107**, (2006).

year	68	70	72	74	77	78	82	89	90	94	02	06
ENDF/B	I	II	III	IV		V			VI			VII
JENDL					1		2	3	3.1	3.2	3.3	

ENDF/B-V was not available for other countries.

Highlights, Improvement

Advances Over the Previous ENDF/B-VI Library

- New cross sections for U, Pu, Th, Np and Am actinide isotopes, with improved performance in integral validation criticality and neutron transmission benchmark tests
- More precise standard cross sections for neutron reactions on H, ^{6}Li, ^{10}B, Au and for ^{235,238}U fission, developed by a collaboration with the IAEA and the OECD/NEA Working Party on Evaluation Cooperation (WPEC)
- Improved thermal neutron scattering
- An extensive set of neutron cross sections on fission products developed through a WPEC collaboration
- A large suite of photonuclear reactions
- Extension of many neutronand proton-induced evaluations up to 150 MeV
- Many new light nucleus neutron and proton reactions
- Post-fission β-delayed photon decay spectra
- New radioactive decay data
- New methods for uncertainties and covariances, together with covariance evaluations for some sample cases
- New actinide fission energy deposition

Validation of Data Library

From Cross-Sections to Effective Neutron Multiplicity, k_{eff}

Nuclear Data Library

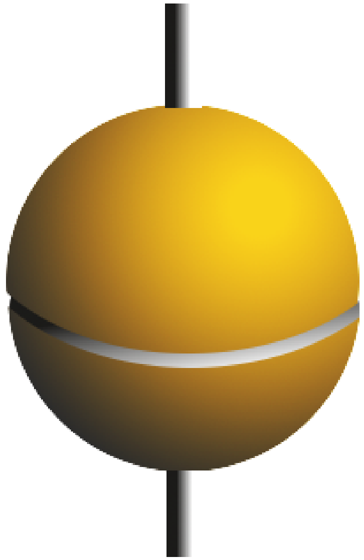
Resonance Parameter
Point-wise Cross Section
etc.

NJOY

Reconstruction of point-wise c.s. from resonance parameters
Doppler broadening
Group cross section
Convert into appl. data format

MCNP

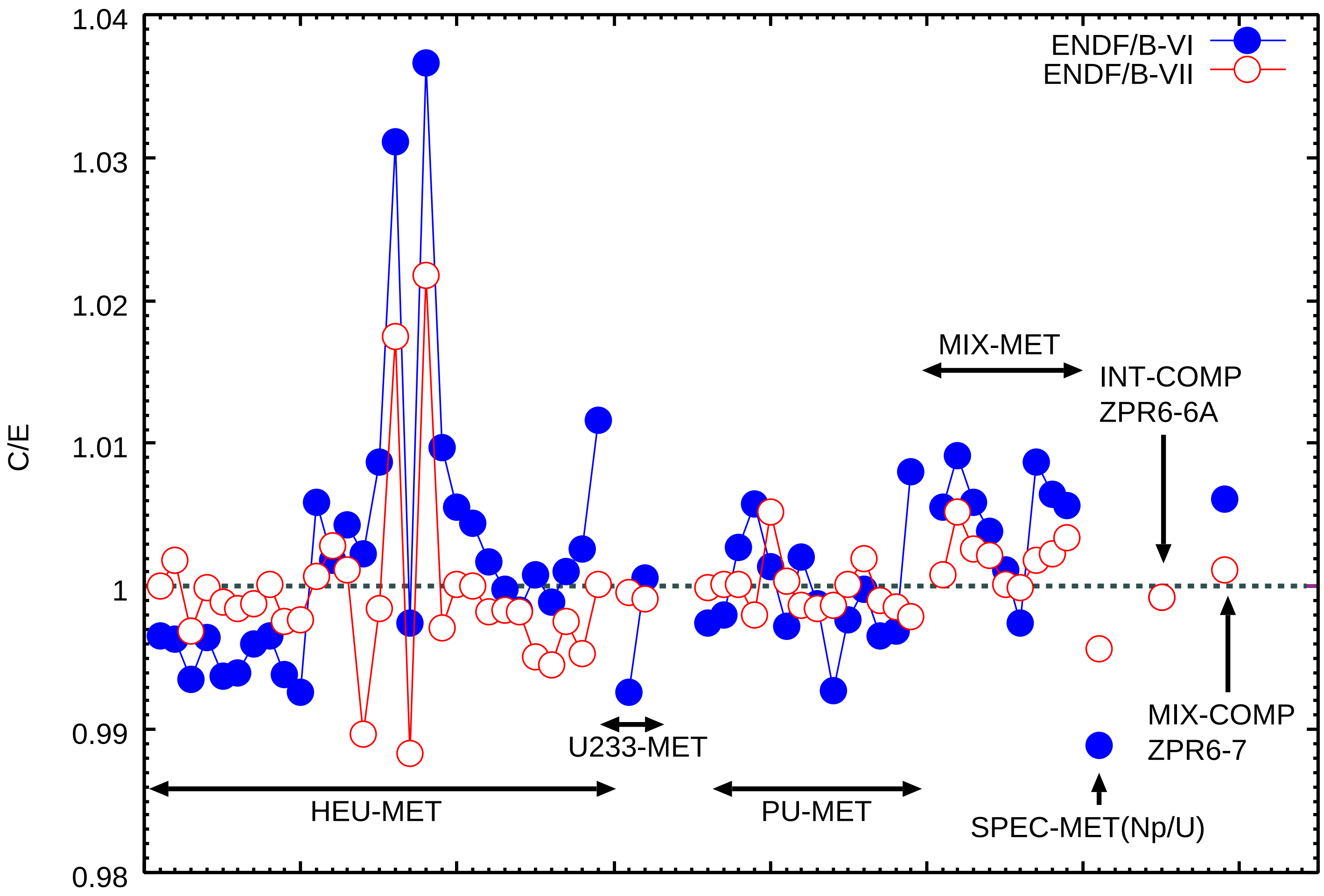
Neutron transport calculation
Neutron multiplicity



Calc / Exp = 1.0

Benchmark Testing

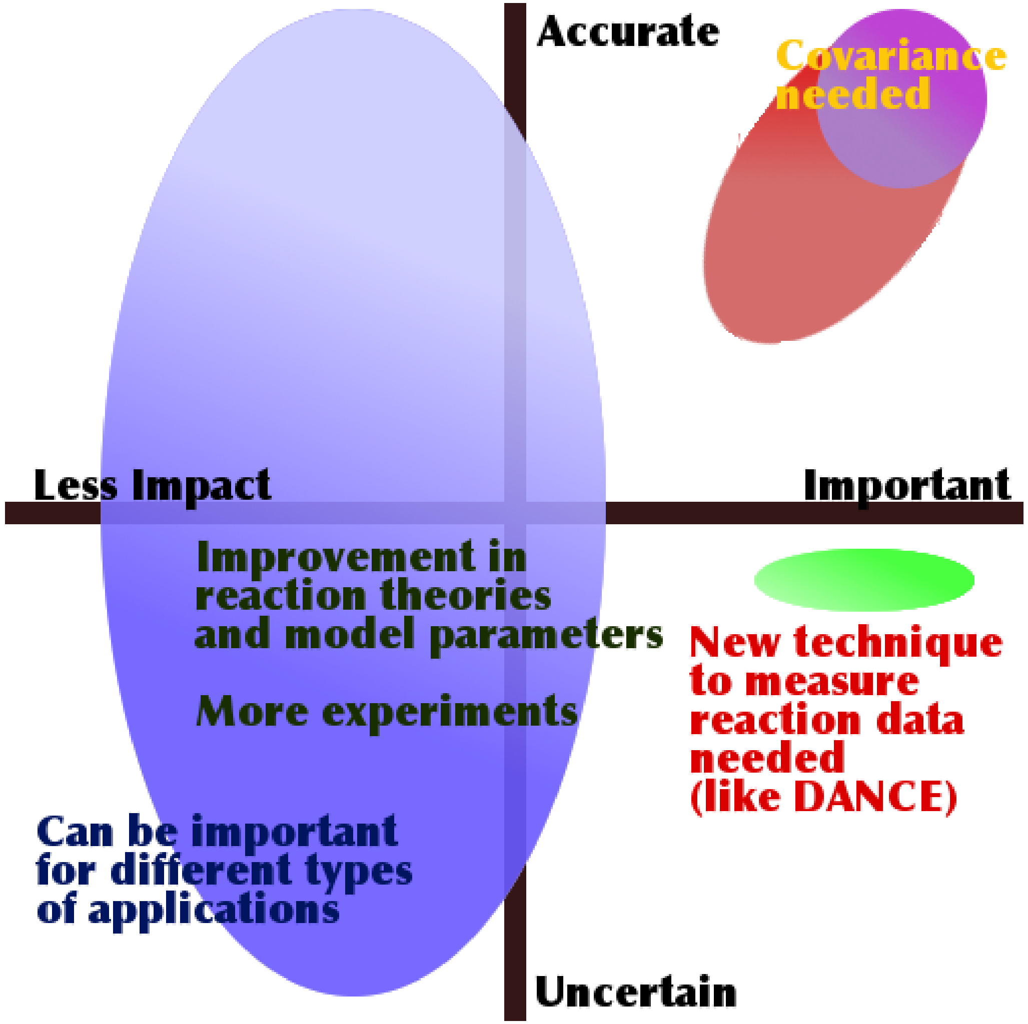
The data libraries are tested against various critical systems, including fast, medium, and thermal neutron spectra, different compositions / forms of materials.



Concluding Remarks

Reaction Data Needs

- We summarized nuclear reaction data needs for applications (energy production, astrophysics), and described how the evaluated nuclear data libraries are used for the particle transport calculations, and how they are validated.
- Nuclear reaction data on actinides are especially important for fission energy applications.
- We have shown some important reaction data for applications, which are the fission and radiative capture processes.
- Compound nuclear reactions play an extremely important role in many applications, and the prediction of accurate cross sections will become crucial.



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