# The “Voodoo Magic” of Providing Nuclear Data Libraries for Radiation Transport Calculations

**Mike Dunn**

**July 24, 2008**


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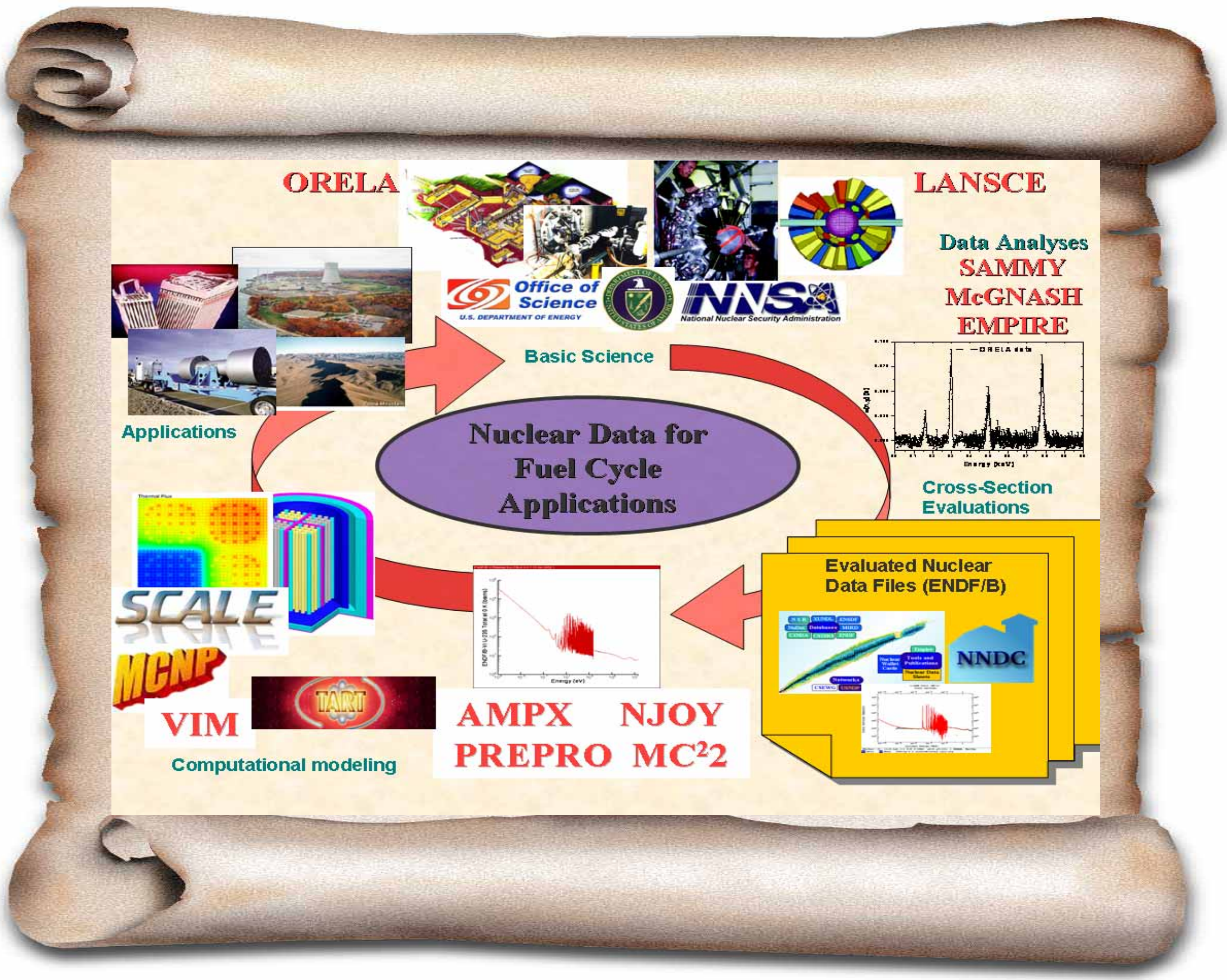
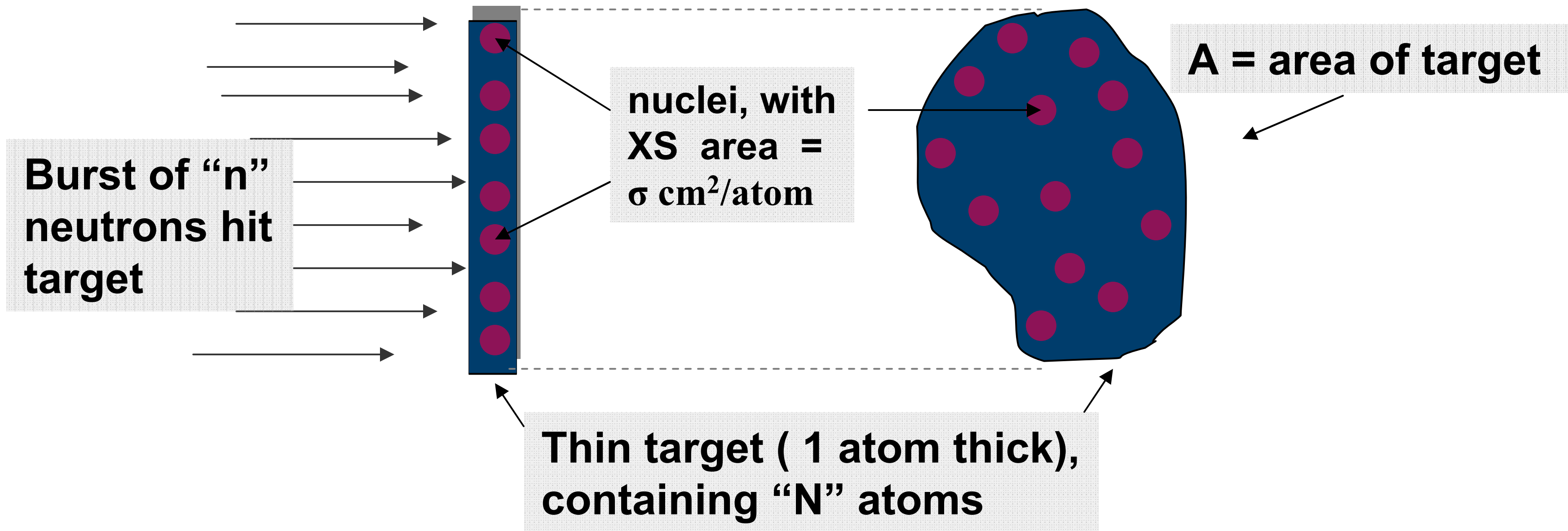
- **Nuclear data basics**
- **Where does nuclear data come from?**
- **Better yet—how does nuclear data get into SCALE?**
- **Library production nuances**
- **What’s new for SCALE 6**


ORELA
LANSCE
Office of Science
U.S. DEPARTMENT OF ENERGY
NNSA
National Nuclear Security Administration
Data Analyses
SAMMY
McGNASH
EMPIRE
Basic Science
Applications
Nuclear Data for
Fuel Cycle
Applications
Cross-Section
Evaluations
Evaluated Nuclear
Data Files (ENDF/B)
NNDC
SCALE
MCNP
VIM
TART
AMPX NJOY
PREPRO MC²2
Computational modeling

# Geometric Interpretation of Microscopic XS's




area occupied by nuclei

expected number of hits

$$R = \left(\frac{N\sigma}{A}\right) n$$

number of incident neutrons

total target area

# Reaction Interpretation of Microscopic XS's

- ***RECALL:*** **Geometric Interpretation:** $\mathbf{R} = \left(\frac{\mathbf{N\sigma}}{\mathbf{A}}\right)\mathbf{n}$
  - **$\sigma$ = target area ($cm^2$ per nucleus)**
  - **1 barn =$10^{-24}$ $cm^2$ ~ $\pi R^2$ => R~ $5.6*10^{-13}$ cm nuclear radius**

- **Reaction Interpretation:**
  - **generalization to account for energy-dependence of reaction rate**
  - **$\sigma$ = reactions (R) per unit fluence (n/$cm^2$) per atom (N)**

$$\sigma(E) = \frac{R(E)}{\left(\frac{n(E)}{A}\right) N}$$

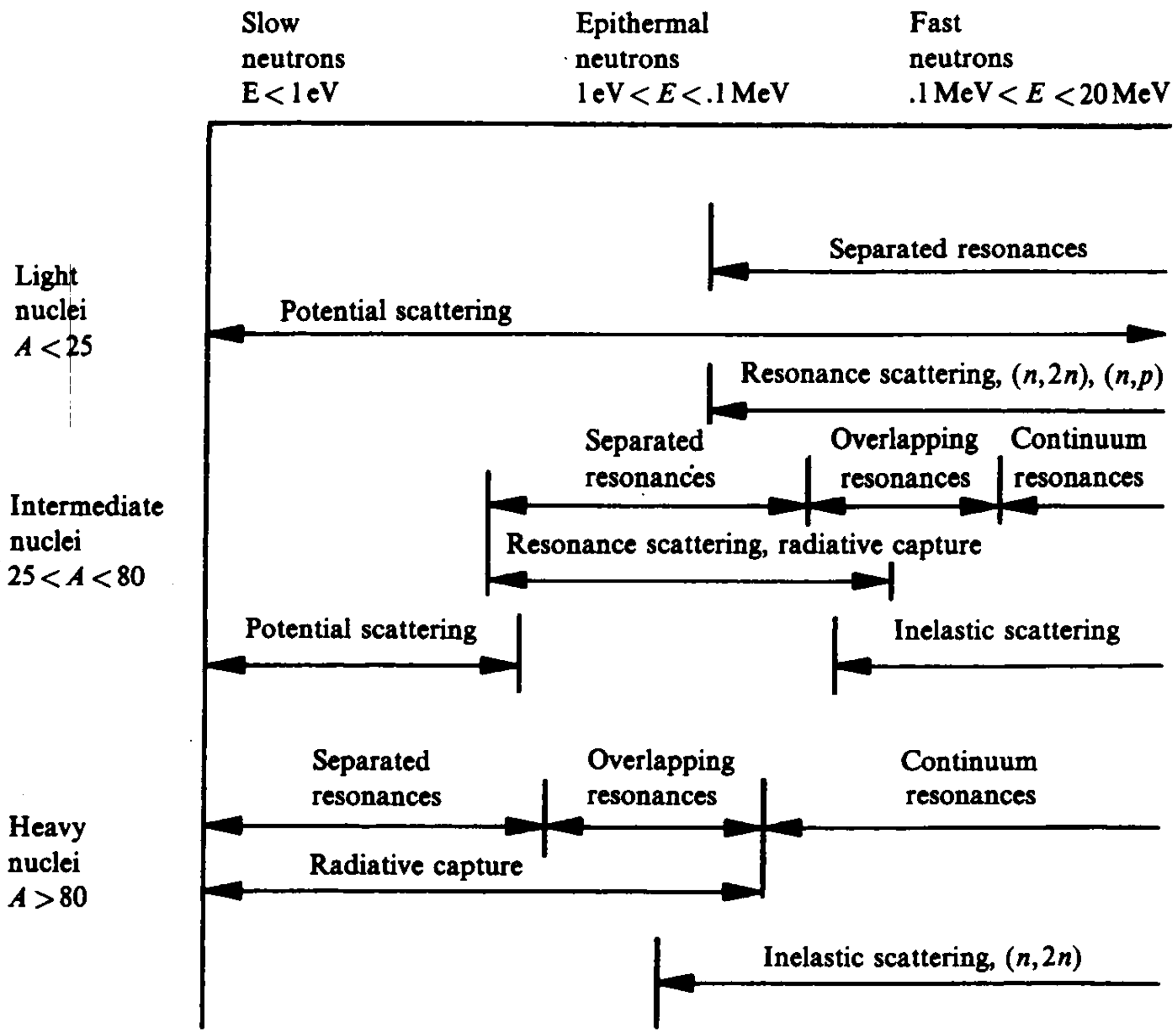
reactions in target

atoms in target

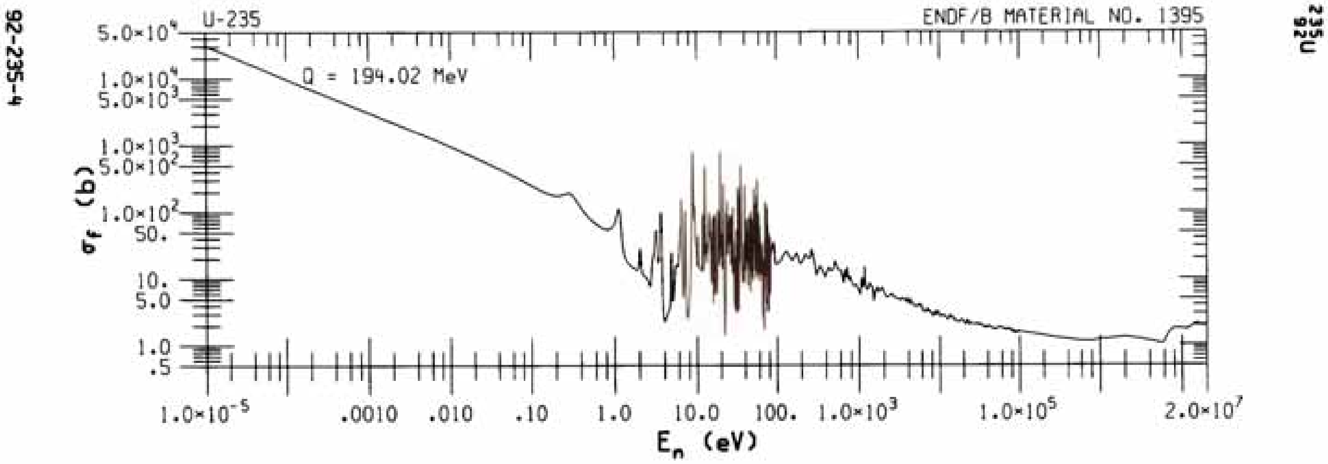
incident neutron fluence with energy E

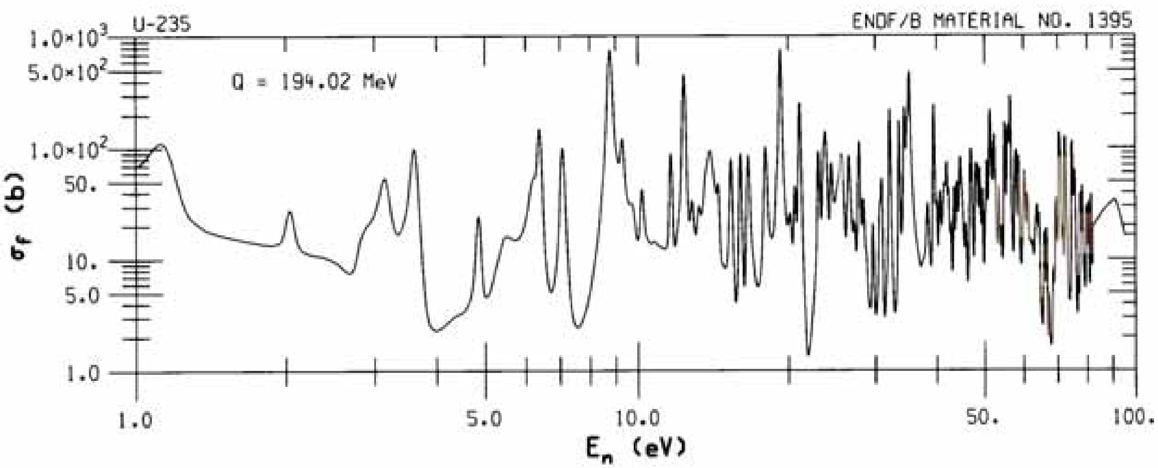
# Typical Energy Variation of XS's

(Taken from J.J. Duderstadt and L.J. Hamiliton, *Nuclear Reactor Analysis*)




# U-235 XS


92-235-4
U-235
ENDF/B MATERIAL NO. 1395
Q = 194.02 MeV
σf (b)
En (eV)
235 92U


U-235
ENDF/B MATERIAL NO. 1395
Q = 194.02 MeV
σf (b)
En (eV)

# Nuclear Physics Theory for Describing Resonance Reactions

- **General expression for $\sigma$ vs. E can be derived from quantum mechanics: "*R-Matrix Theory*"**
- **"Resonance formalisms" are simpler approximations derived from general R-matrix theory**
  - Single Level Breit Wigner (SLBW)

$$\sigma(E) = \sum_r \sigma_r(E) = \left(\frac{\pi \hbar^2}{2m_n}\right)\left(\frac{1}{E}\right)\sum_r \frac{g\,\Gamma_{n,r}\,\Gamma_{\gamma,r}}{(E - E_r)^2 - (\Gamma_r/2)^2}$$

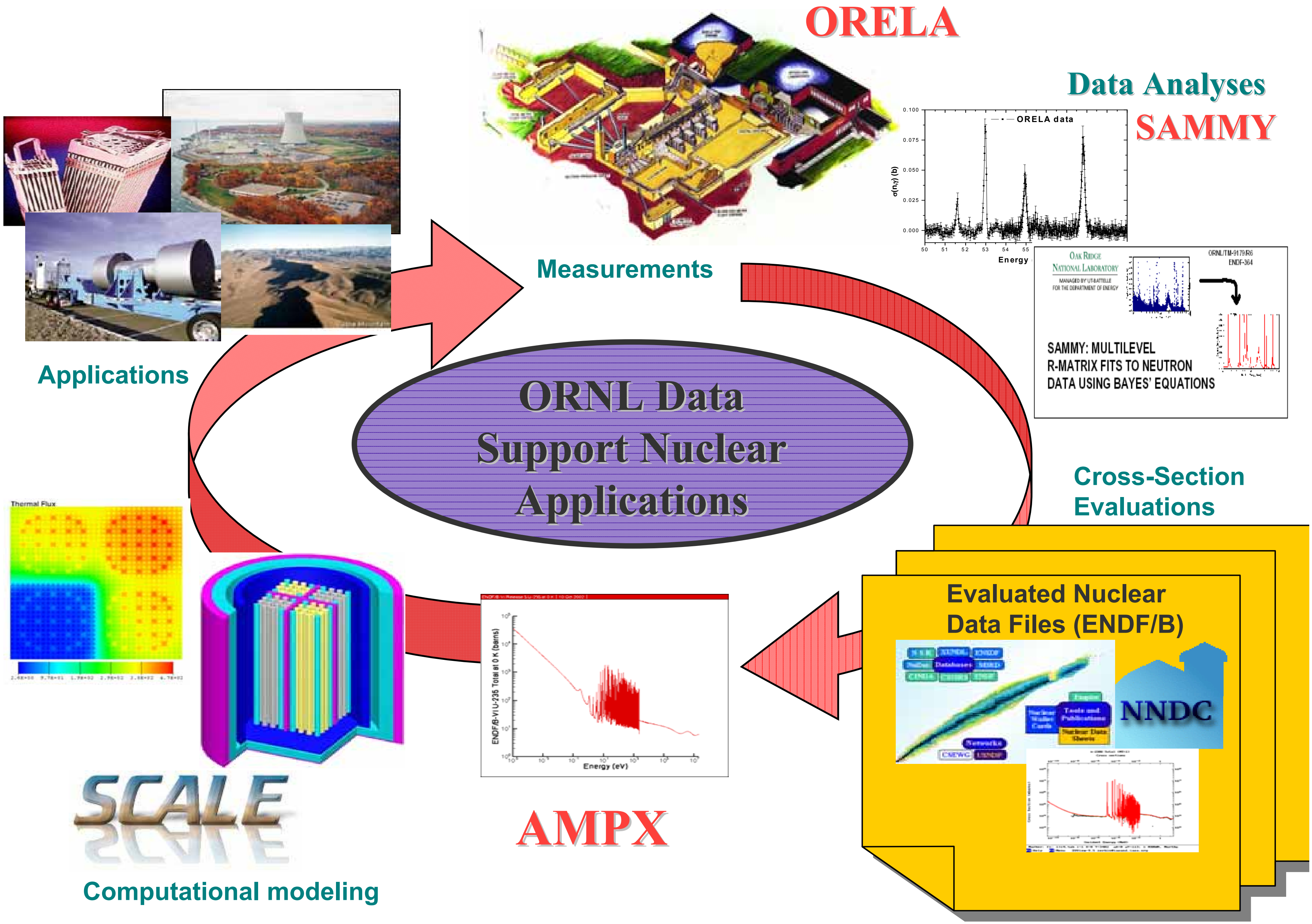
  - Multilevel Breit Wigner (MLBW)
  - Reich-Moore (RM)

- **Resonance parameters appearing in the expressions must be obtained from cross-section measurements:**

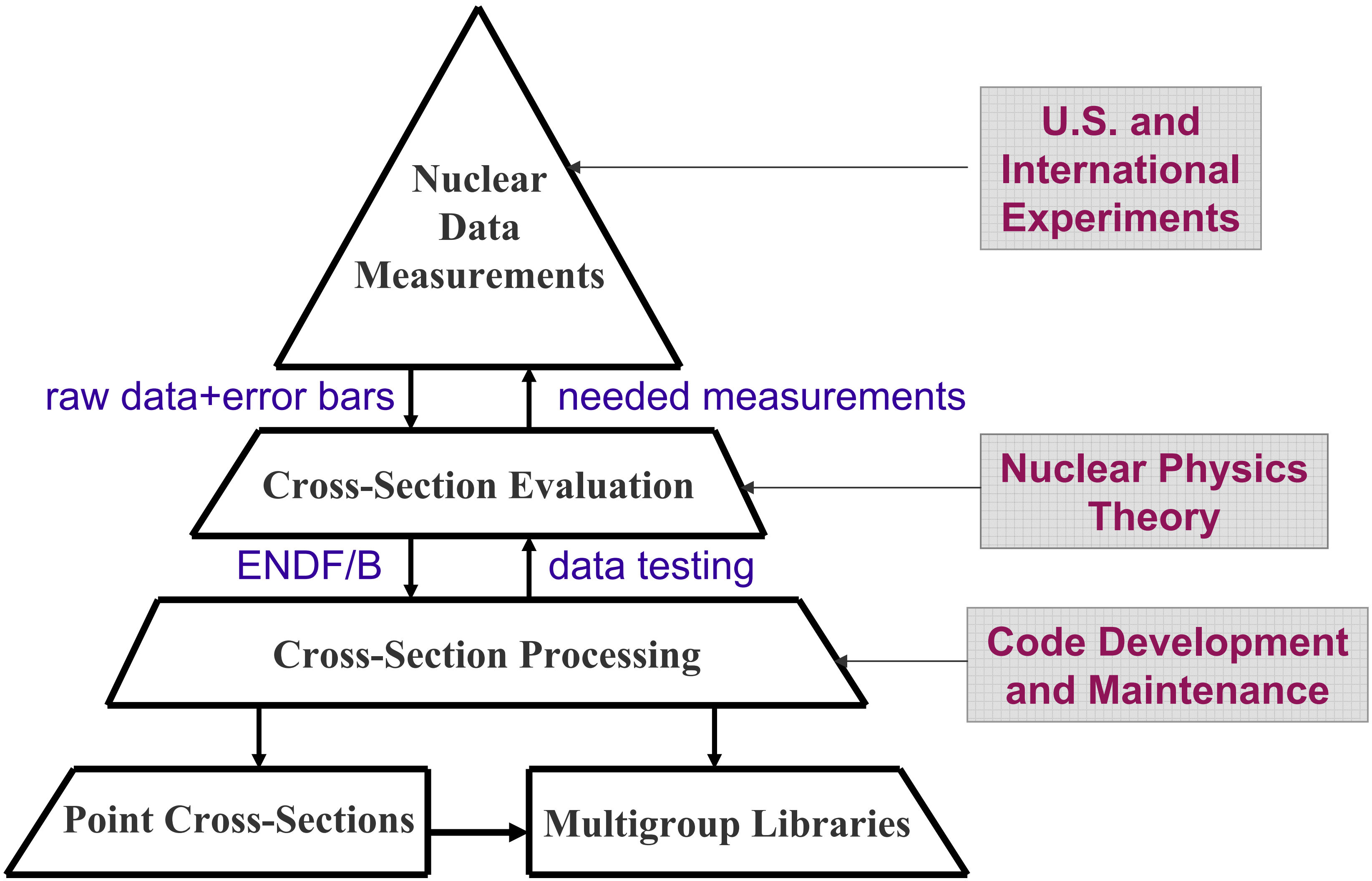
**$E_r$, $\Gamma_\gamma$ , $\Gamma_n$ , etc..**

## Description of Scattering in Thermal Energy Range (E< ~1eV)

- **Neutron energy is comparable to molecular thermal energy**
  - **Thermal neutrons can gain energy in collision**
- **Molecular bonding may be ≥ neutron energy**
  - **neutrons interact with molecules instead of individual atoms**
  - **neutron energy is transferred to vibration and rotation energy of molecules**
  - **coherent scatter caused by interference between scatter neutron waves in atomic lattice**
- **S(α,β) describes thermal interactions with bound moderator molecules**

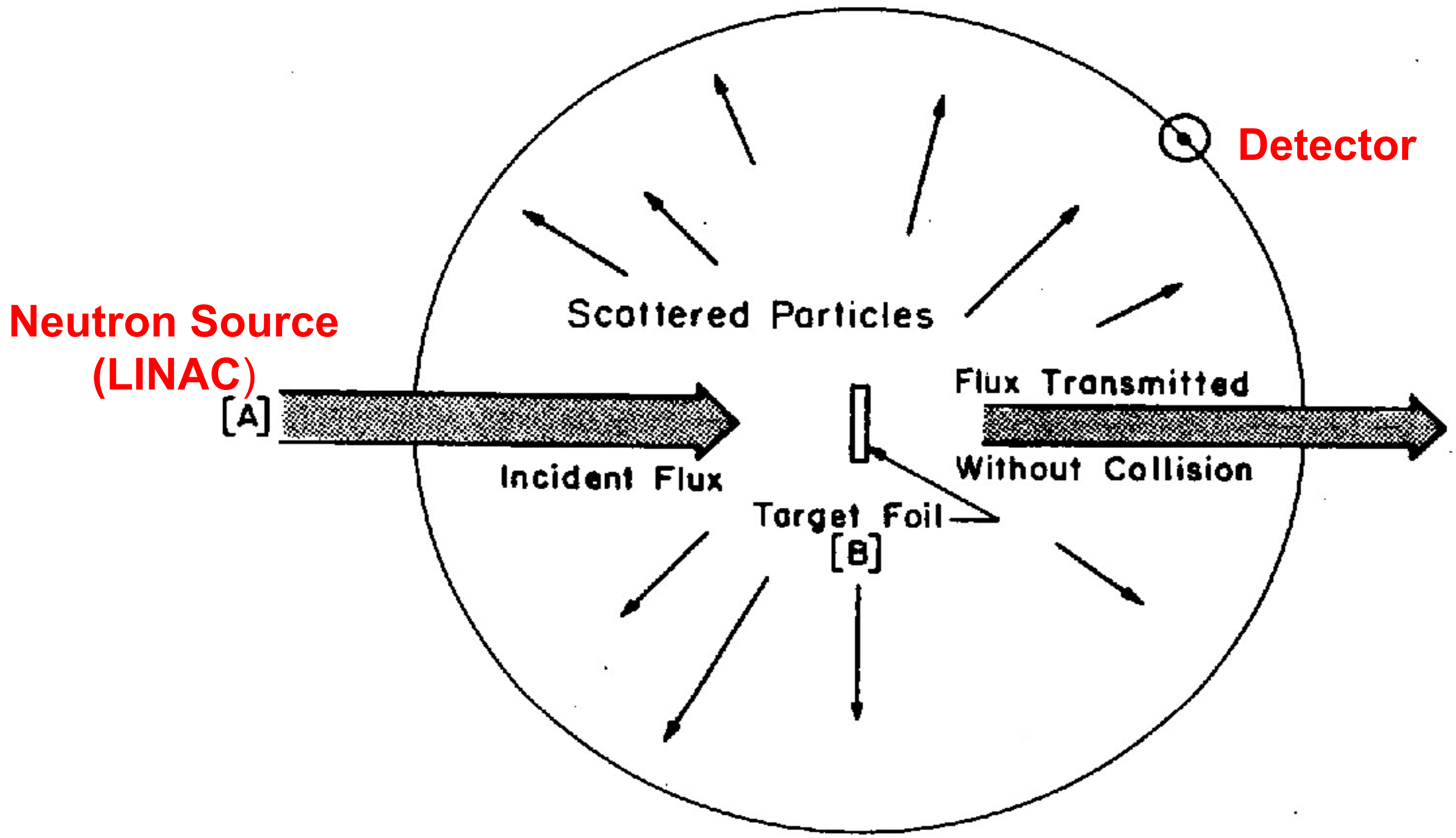


ORELA
Data Analyses
SAMMY
ORELA data
Energy
Measurements
OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY
ORNL/TM-9179/R6
ENDF-364
SAMMY: MULTILEVEL R-MATRIX FITS TO NEUTRON DATA USING BAYES' EQUATIONS
Applications
ORNL Data Support Nuclear Applications
Cross-Section Evaluations
Thermal Flux
Evaluated Nuclear Data Files (ENDF/B)
NNDC
Energy (eV)
SCALE
AMPX
Computational modeling

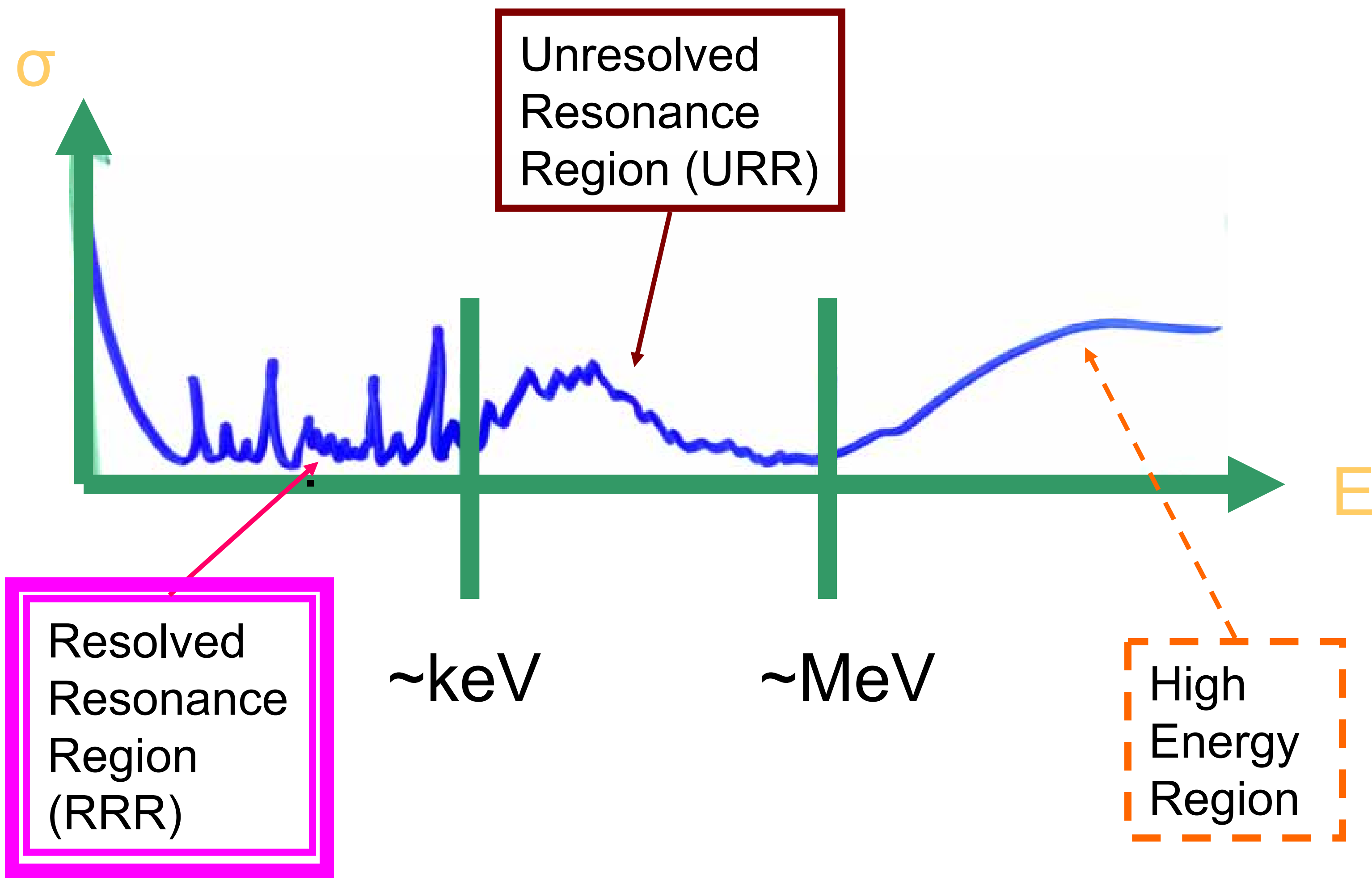


Nuclear Data Measurements
U.S. and International Experiments
raw data+error bars
needed measurements
Cross-Section Evaluation
Nuclear Physics Theory
ENDF/B
data testing
Cross-Section Processing
Code Development and Maintenance
Point Cross-Sections
Multigroup Libraries

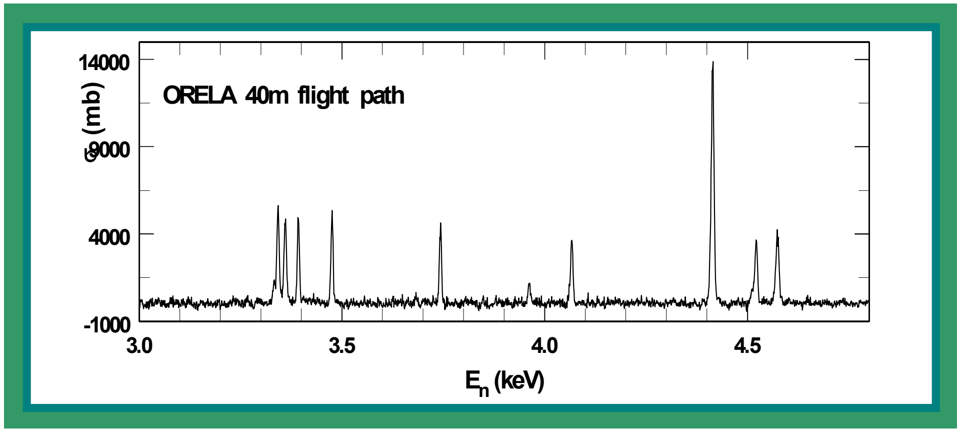
# Experimental Measurements are Performed to Obtain XS Parameters

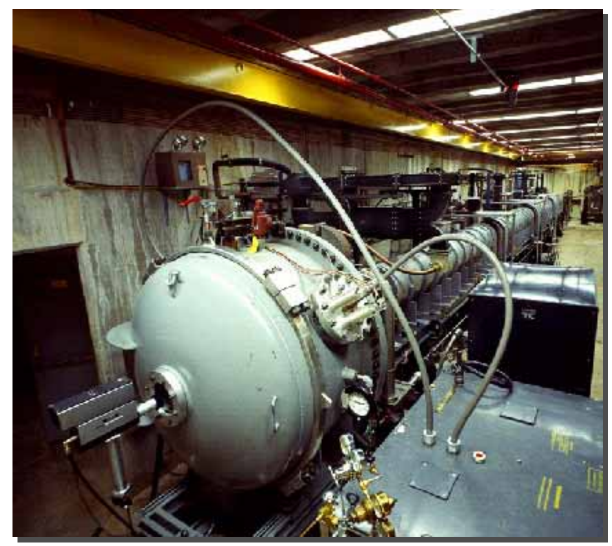


# Energy regions for nuclear data

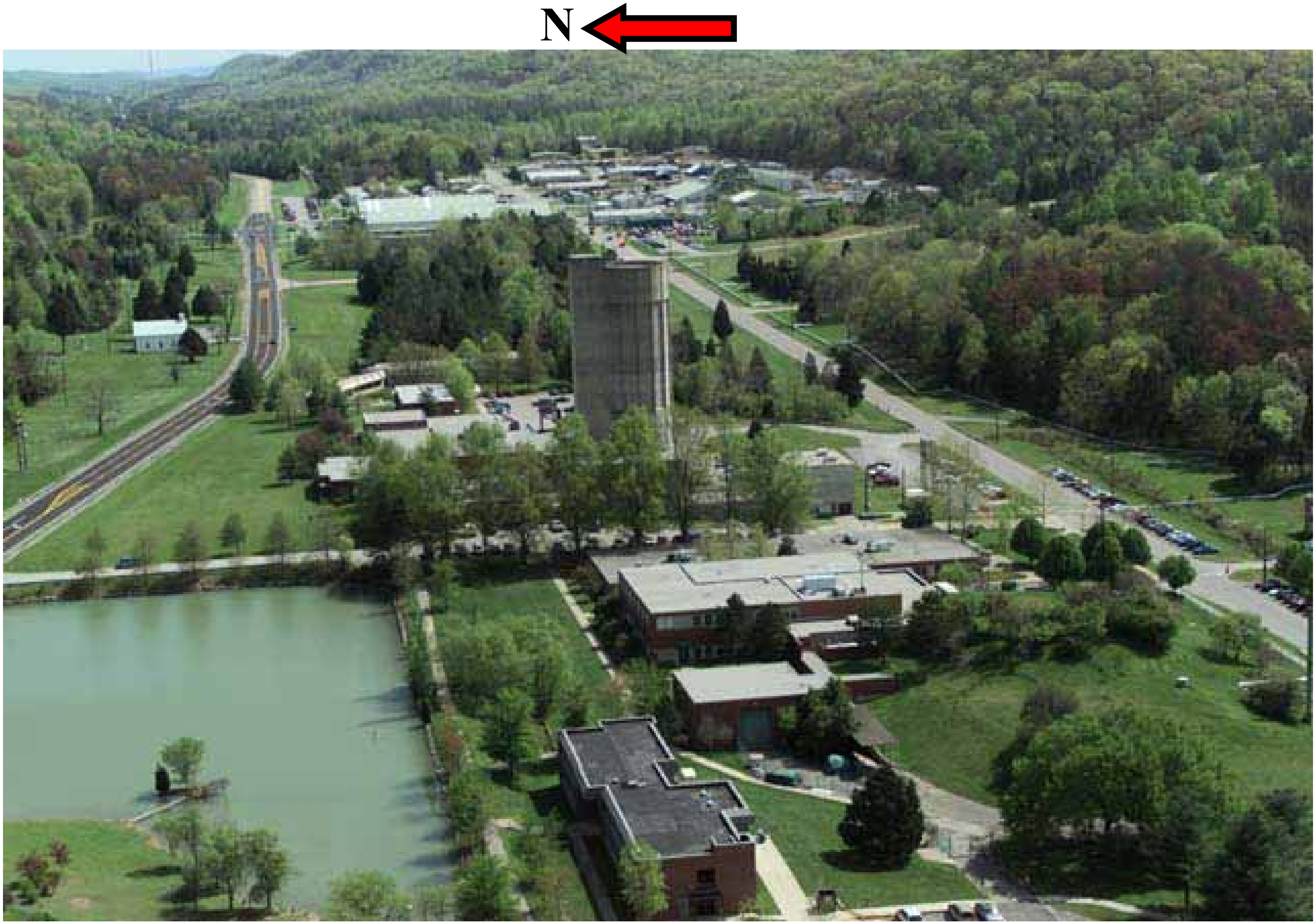


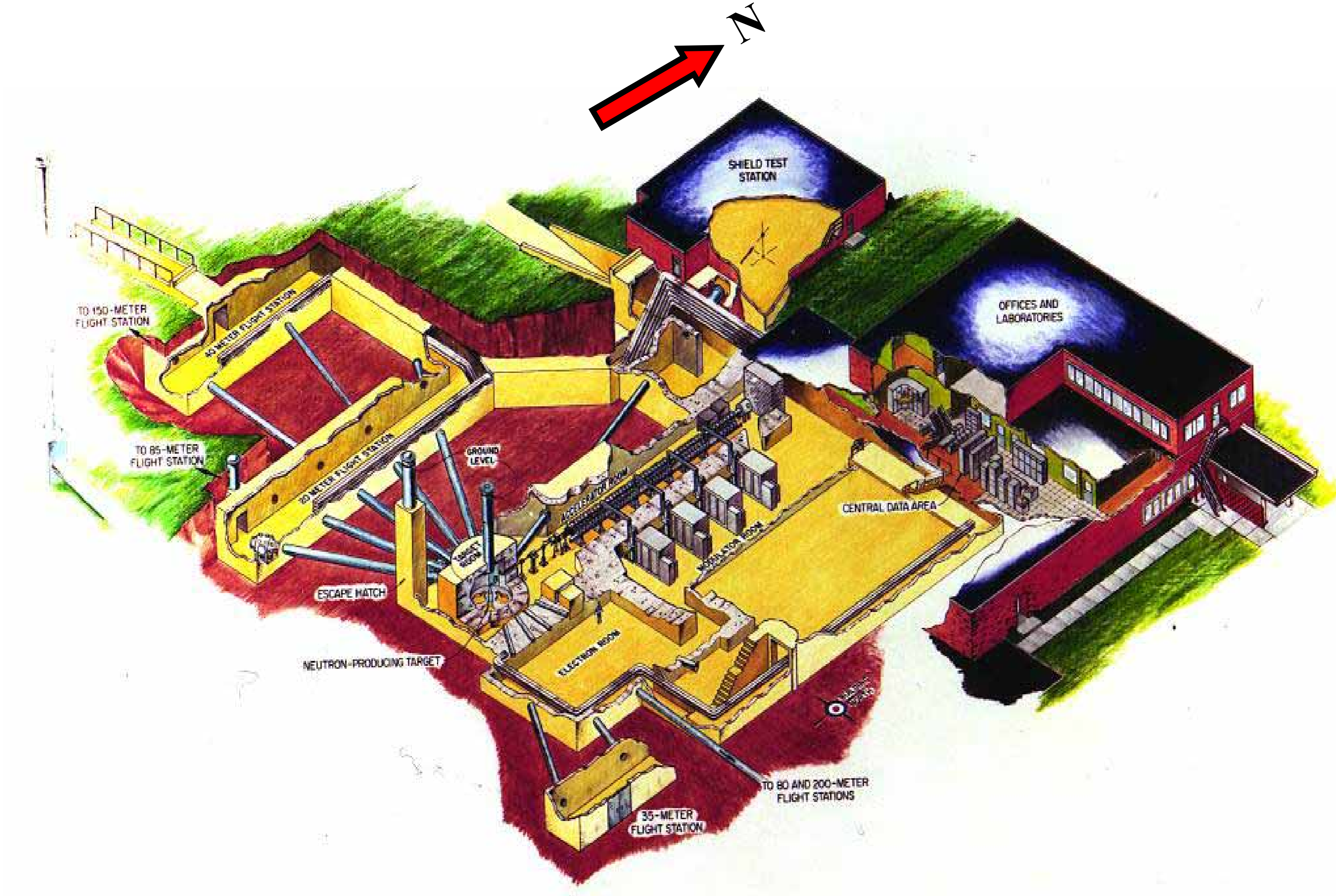
# ORELA (Oak Ridge Electron Linear Accelerator) Provides High-Resolution Cross Section Measurements For Neutron Energies Up to 2 MeV



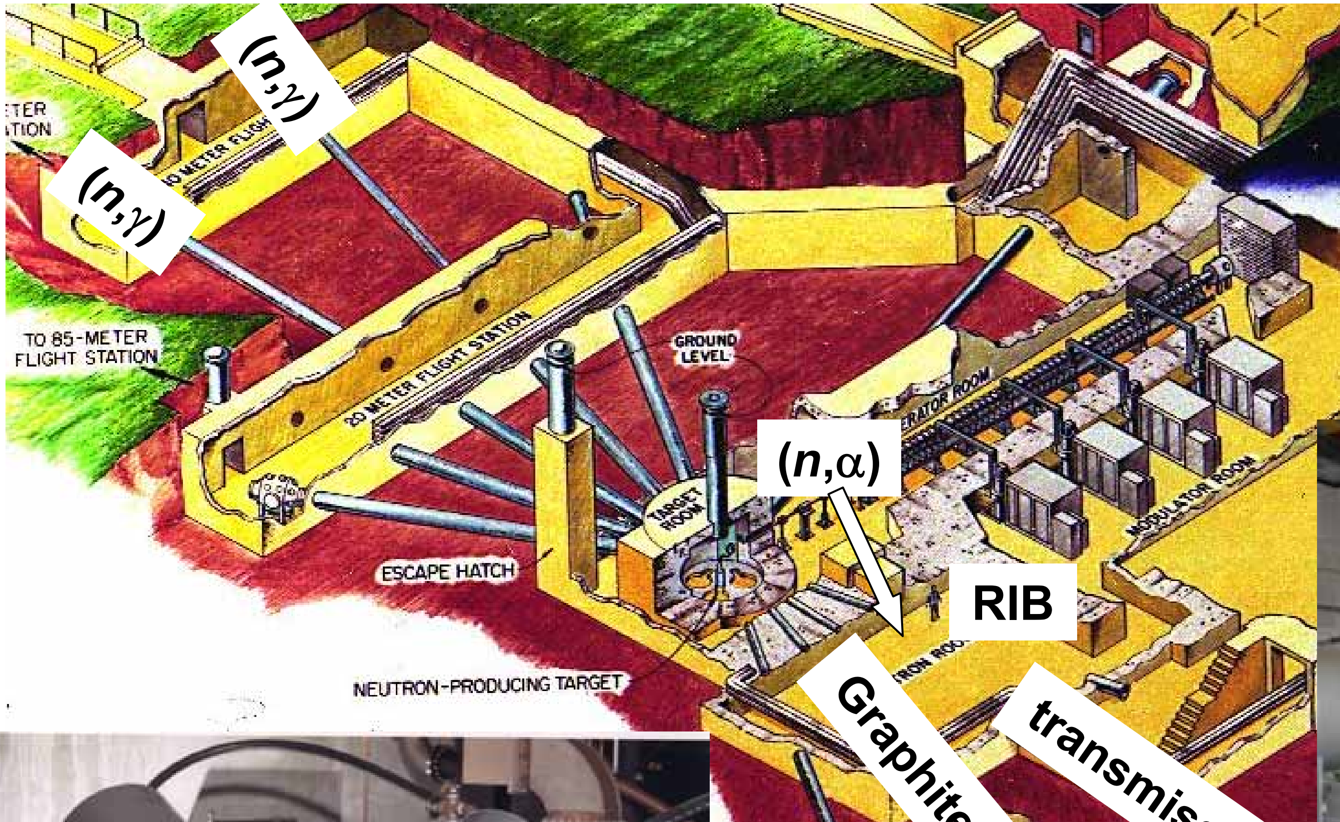
- **Facility description**
  - **180 MeV electron accelerator-based neutron source**
  - **4 – 30 ns bursts (12 – 1000 pulses / s)**
  - **Neutrons via bremsstrahlung radiation from tantalum target**
  - **$10^3$ – $10^8$ ev un-moderated and water/Be moderated neutrons**
  - **10 flight paths, 18 flight stations**
  - **9 – 200 m evacuated flight tubes**
  - **Instrumentation and data acquisition**
- **Key measurement capabilities**
  - **Neutron reaction cross sections (total, capture, fission, elastic scattering, gamma and neutron production)**
  - **Materials irradiation damage and activation data**


N


N
SHIELD TEST STATION
OFFICES AND LABORATORIES
TO 150-METER FLIGHT STATION
40 METER FLIGHT STATION
TO 85-METER FLIGHT STATION
20 METER FLIGHT STATION
GROUND LEVEL
ACCELERATOR ROOM
TARGET ROOM
MODULATOR ROOM
CENTRAL DATA AREA
ESCAPE HATCH
NEUTRON-PRODUCING TARGET
ELECTRON ROOM
TO 80 AND 200-METER FLIGHT STATIONS
35-METER FLIGHT STATION

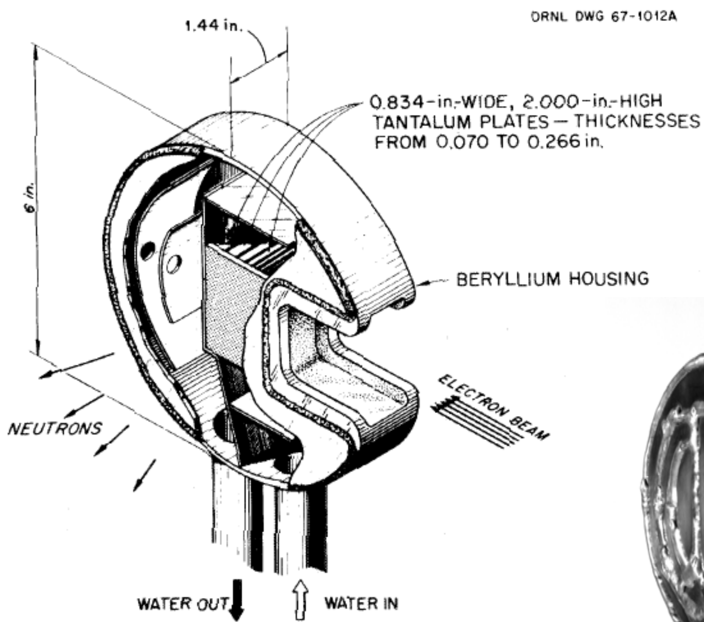
# Existing Experiments at ORELA

- 11 Flight paths
- Flight Stations:
  - 8-18, 20, 35, 40, 85, 150, and 200 m



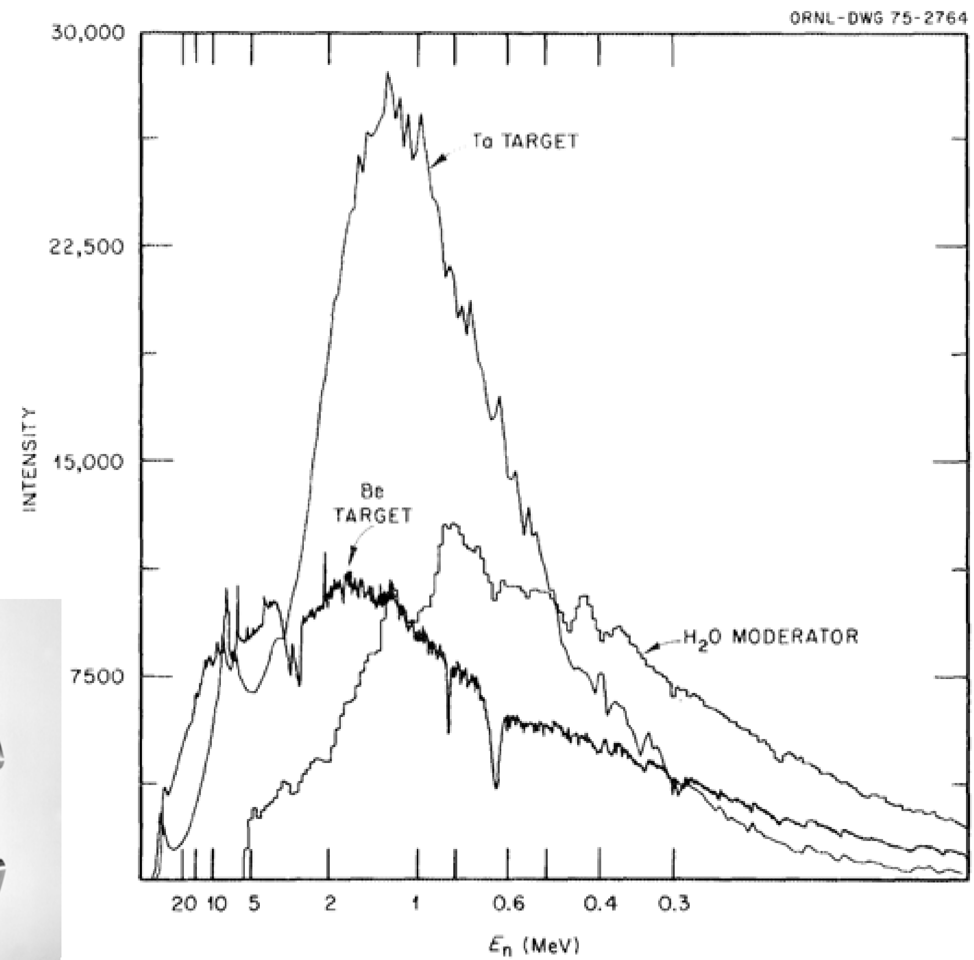

# ORELA Neutron Source

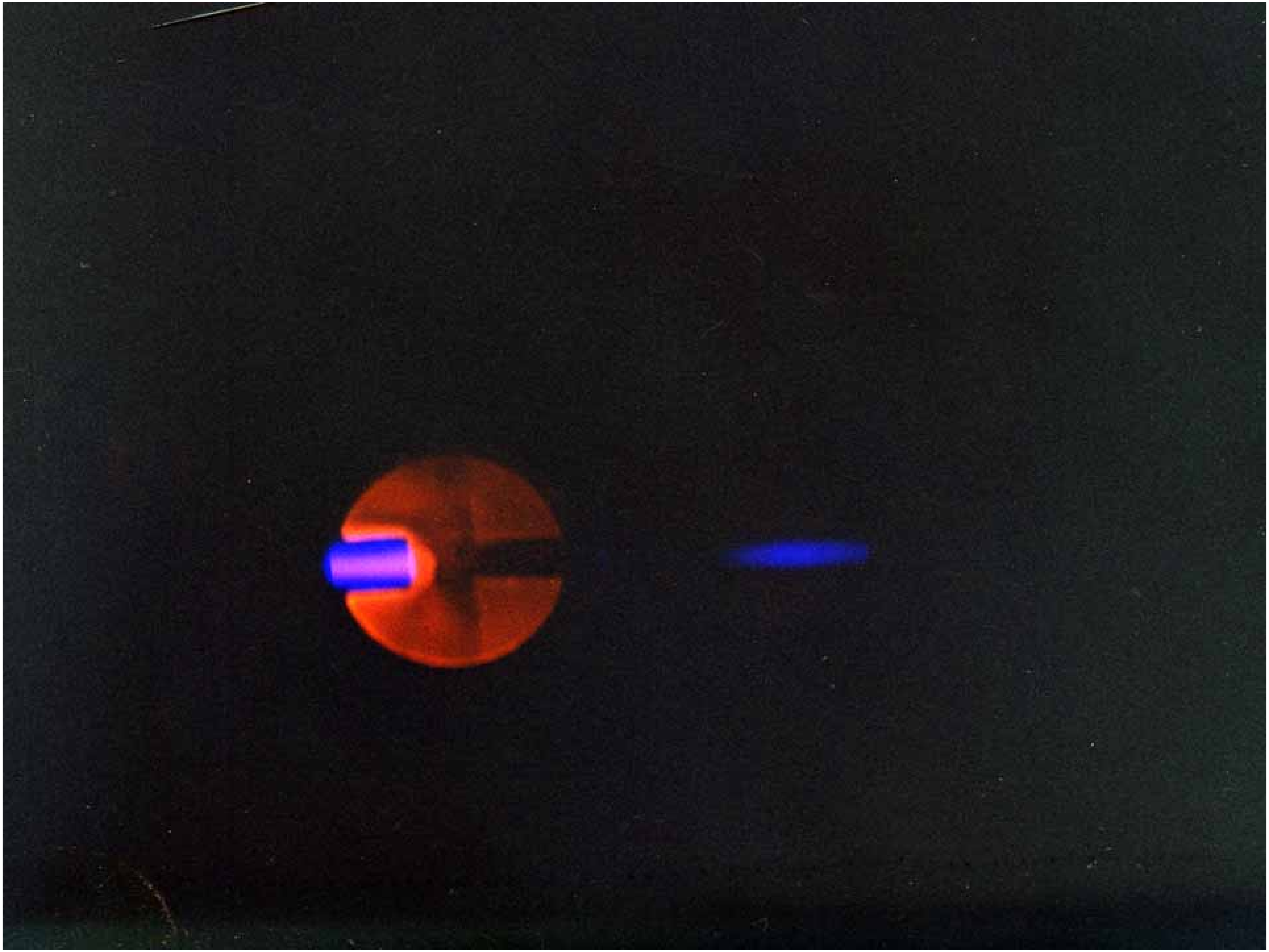
- “Ta target” spectrum produced by using collimator to only view Ta plates of the target
- “$H_2O$ moderator” spectrum produced by using collimator to only view neutron emanating from water moderator above the Ta plates



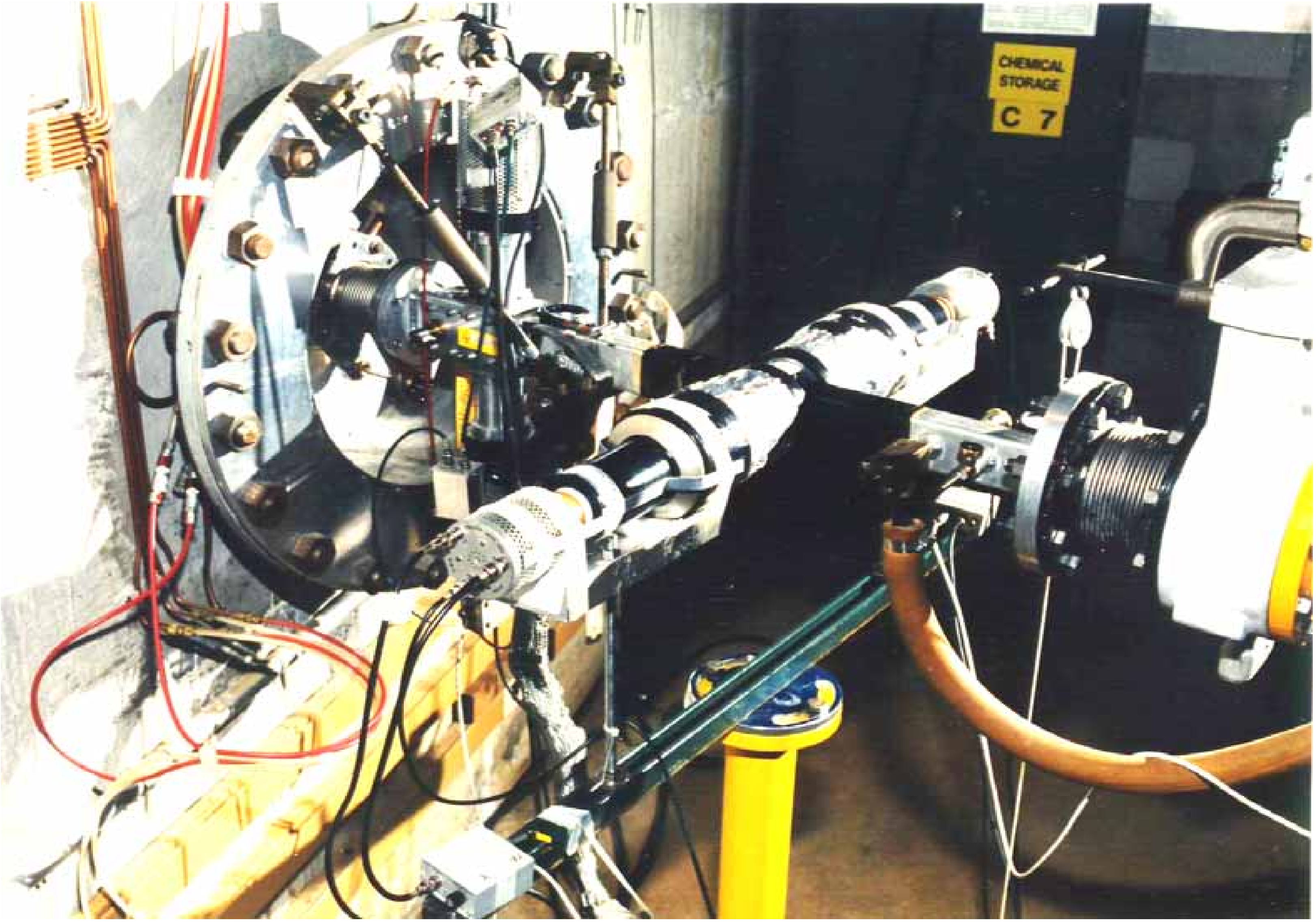

ORELA *Be* CLAD TANTALUM TARGET ASSEMBLY

Measured flux at 200 m flight path from either Ta or Be target





# Capture Measurement Setup

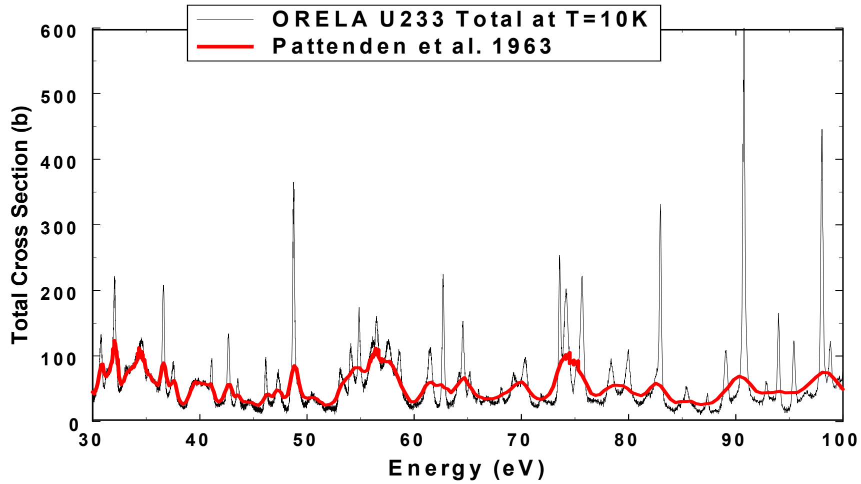


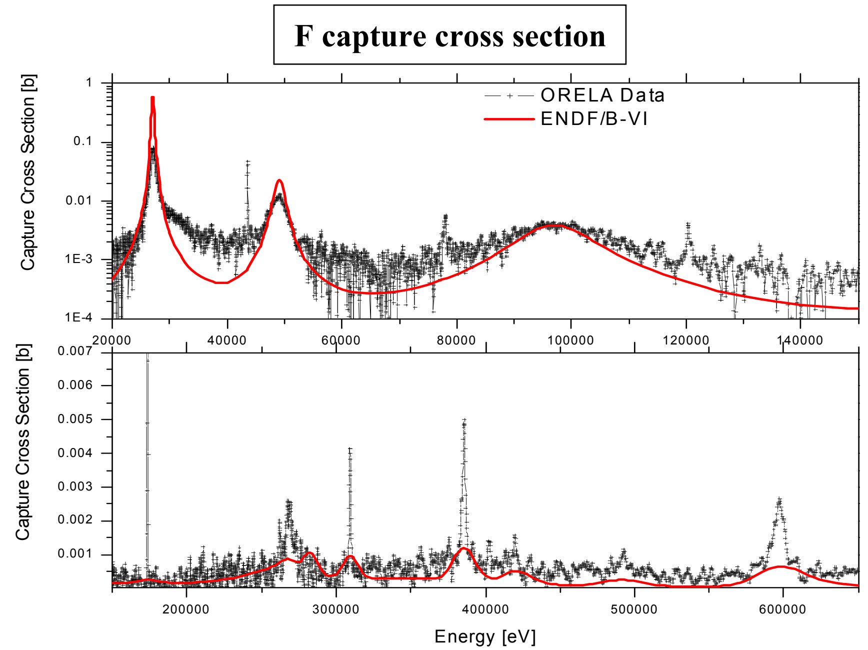
# Data Improvements from ORELA Measurements

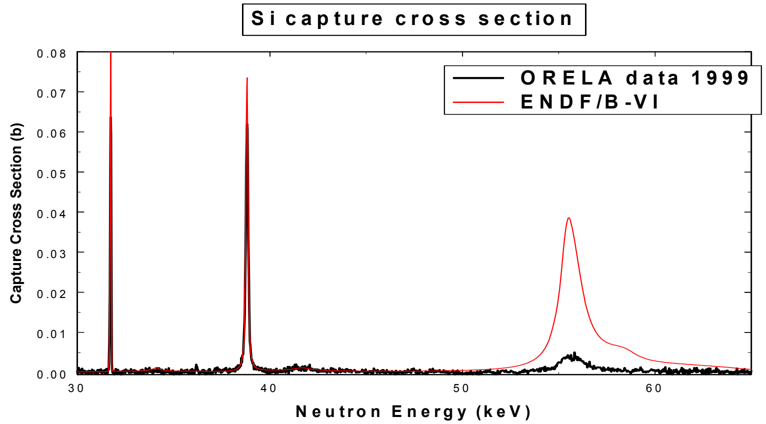
- Improvements in nuclear data capabilities are needed to keep pace with advances in computational methods development—translates to optimized nuclear applications

- Unique measurement capabilities are essential for providing accurate and improved cross section data for nuclear applications

- Recent ORELA measurements have removed large neutron sensitivity found in older cross-section measurements and identified missing resonances

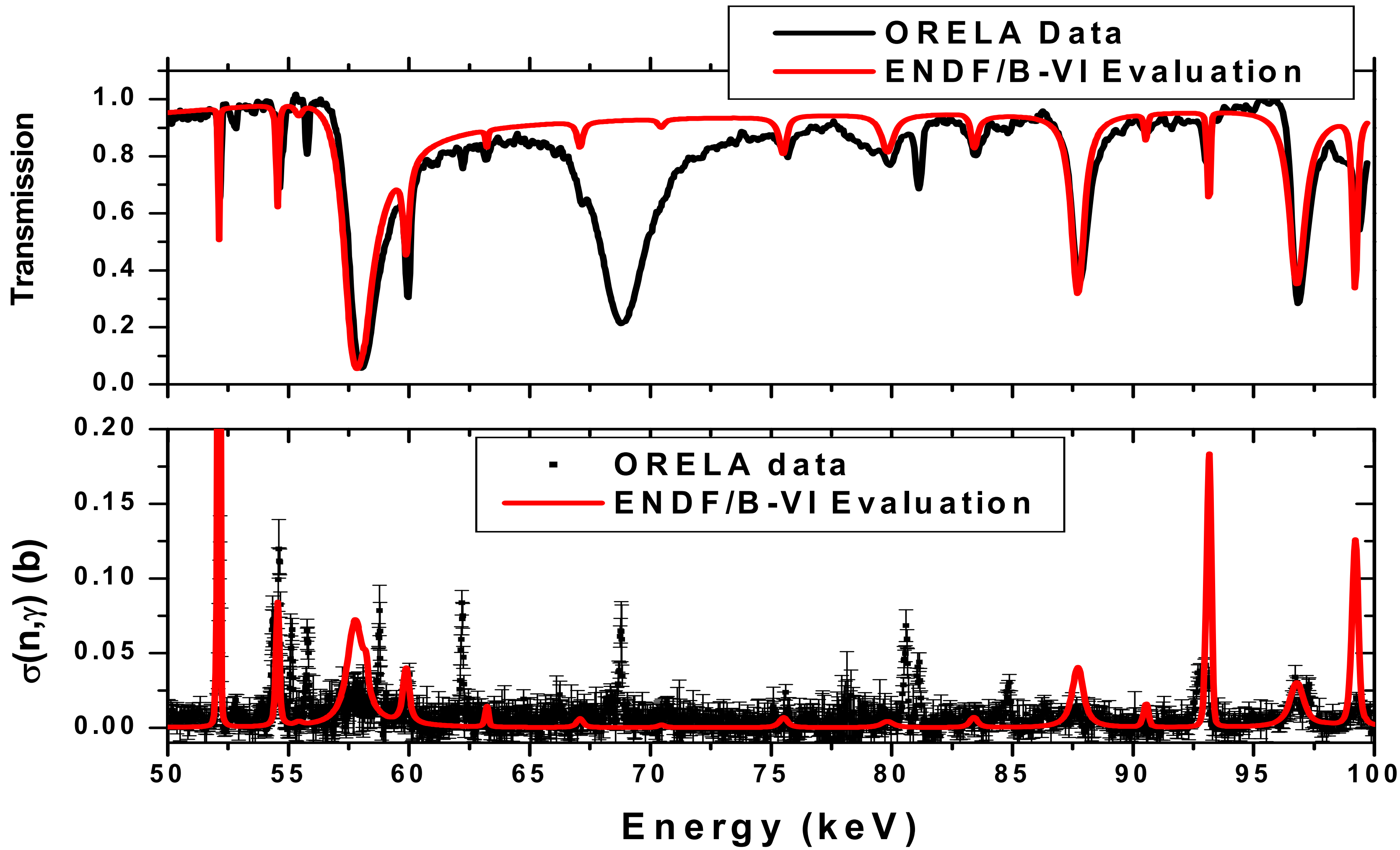


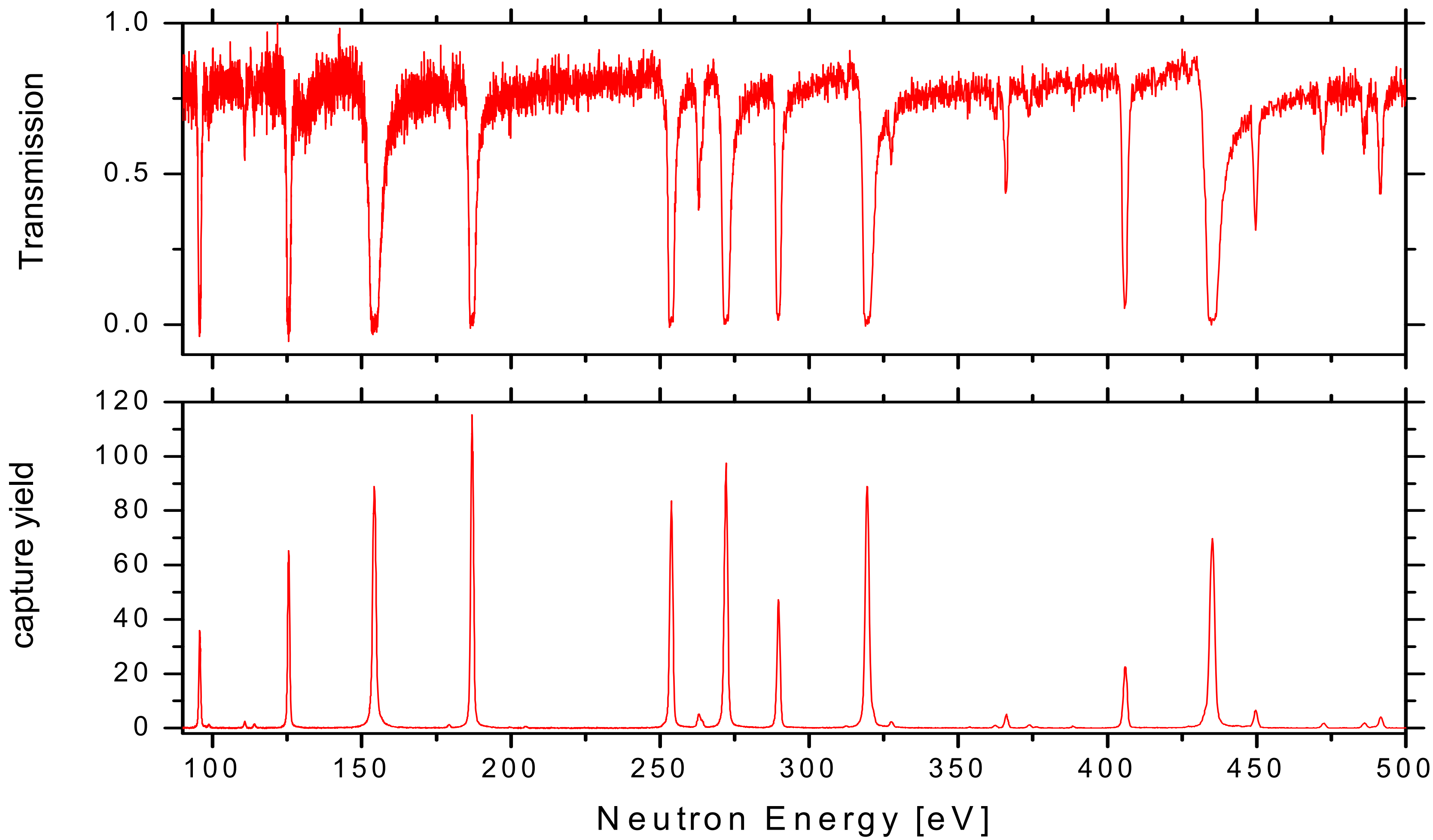



# Recent ORELA capture and Transmission Data for K compared to ENDF/B VI:

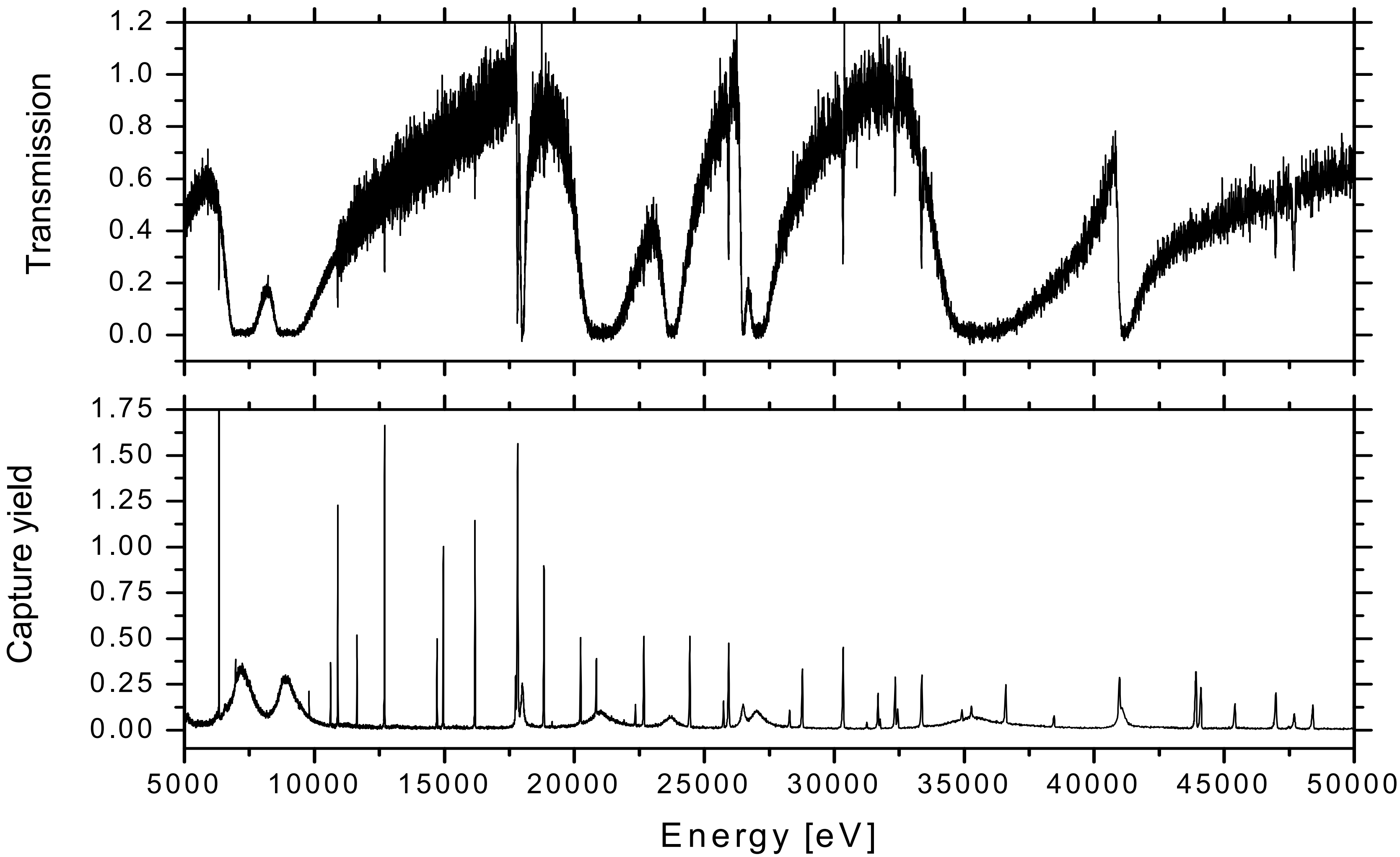
Several resonance areas too large (neutron sensitivity) in the ENDF/B-VI evaluation, resonances are missing



# FY2006 ORNL-IRMM Transmission and Capture Measurements for $^{103}$Rh in Resonance Region (GELINA Accelerator, Geel Belgium)



# FY2006 ORNL-IRMM Transmission and Capture Measurements for $^{55}Mn$ in Resonance Region (GELINA Accelerator, Geel Belgium)



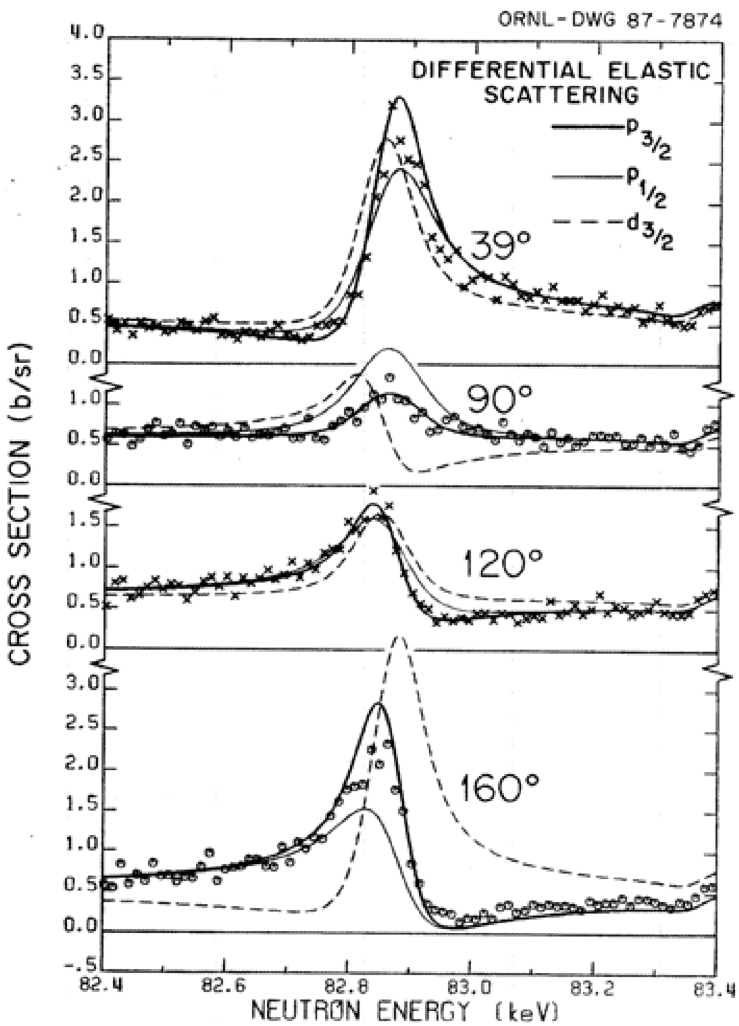
# Elastic Scattering Measurement Capabilities

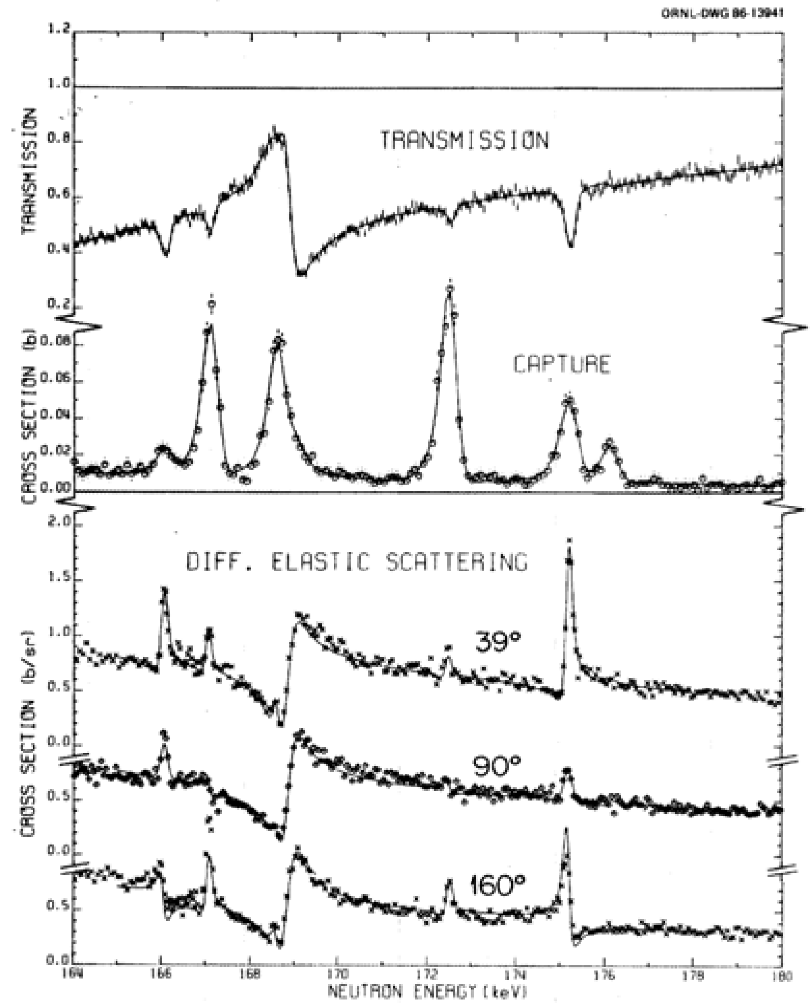
- Six neutron detectors
  - 4.32 cm diameter, 7.62 cm length NE110 cylinder
  - 8850 photomultiplier tubes connected at each end of NE110 cylinder
- Position detectors at various lab angles from target sample located in center of scattering chamber
- Previous $^{52}Cr$ measurement angles:

  39°, 55°, 90°, 120°, 140°, and 160°

Scattering Chamber Interior

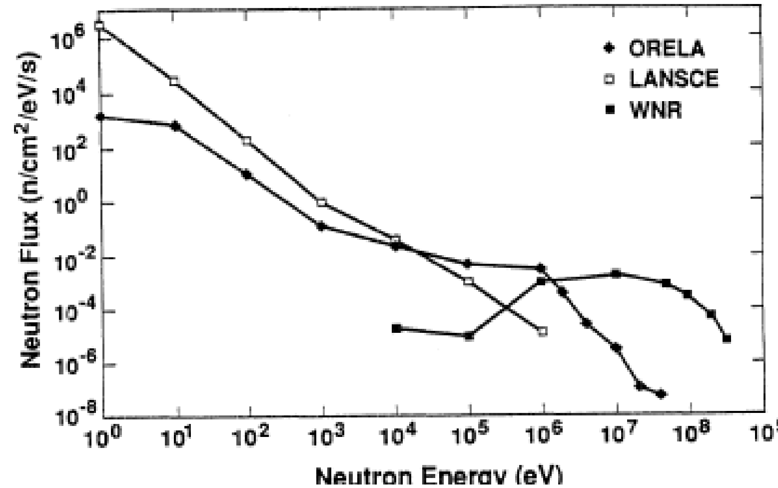
# ORELA $^{58}$Ni Measurement and SAMMY Analysis (ORNL/TM-10841 ENDF-347)



# Complementary Cross Section Measurement Capabilities

- Historically, ORELA and LANSCE have served as the primary source of measured cross-section data for U.S. ENDF/B
- ORELA and LANSCE are complementary facilities: LA-UR-90-4355
  - **LANSCE provides accurate data at “high energies” (MeV and higher)**
  - **ORELA fills the “data gap” with detailed energy resolution from eV to MeV range—intermediate energy range**
- ORELA capability unmatched in U.S.



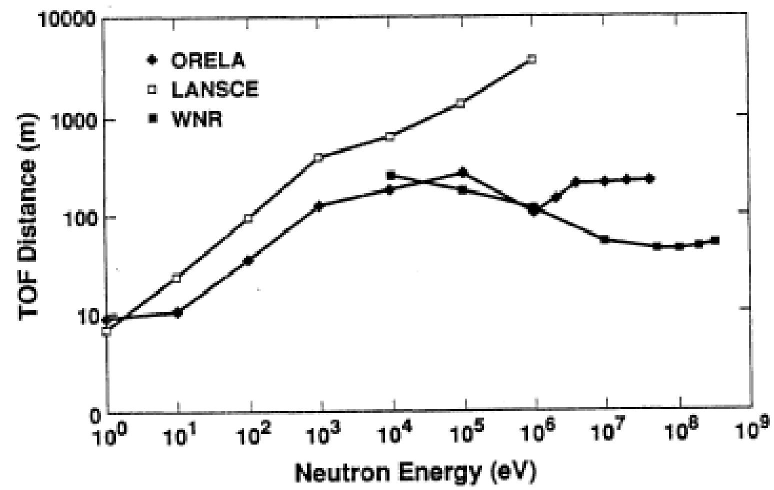



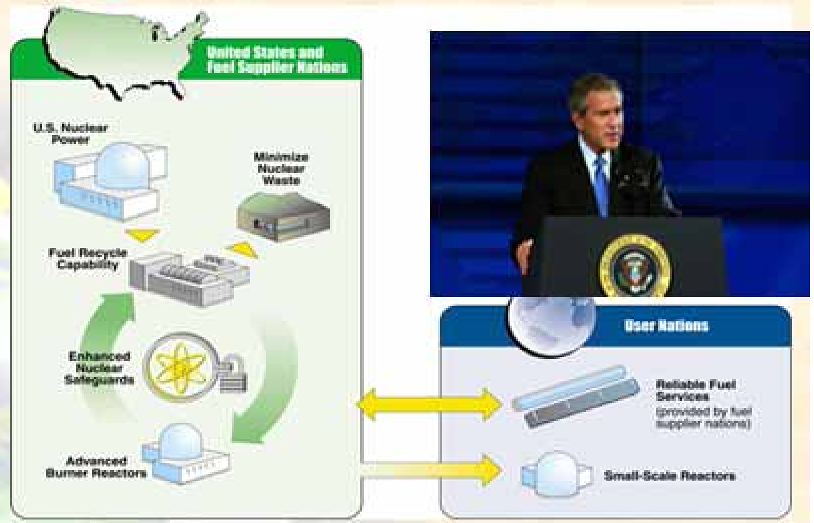

Fig. 12. TOF distance as a function of neutron energy for the resolution profile RP1 (Fig. 7) and for the three facilities: ORELA, LANSCE, and WNR, as they presently exist (A-plot).

# Haven't we measured everything yet?

## Closing the Nuclear Fuel Cycle

Example Data Needs

- Challenges
  - Build up of higher mass number isotopes of Pu, Am, and Cm
  - Transition from fluid to solid form in reprocessing establishes intermediate and thermal neutron spectra
- Nuclear data for many actinides anticipated in SNF reprocessing streams—not well known at intermediate energies
- Assess possible data needs for improving
  - Fuel exposure prediction of SNF isotopics—actinides and fission products
  - Prediction of spent fuel reactivity worth—burnup credit for transportation, efficient sizing of reprocessing equipment
  - Prediction of radiation source terms
  - Isotopes acting as chemical reagents—important for moderation and absorption
- Possible need for improved differential data from low eV to MeV region—**ORELA can address**




Improved nuclear data needs

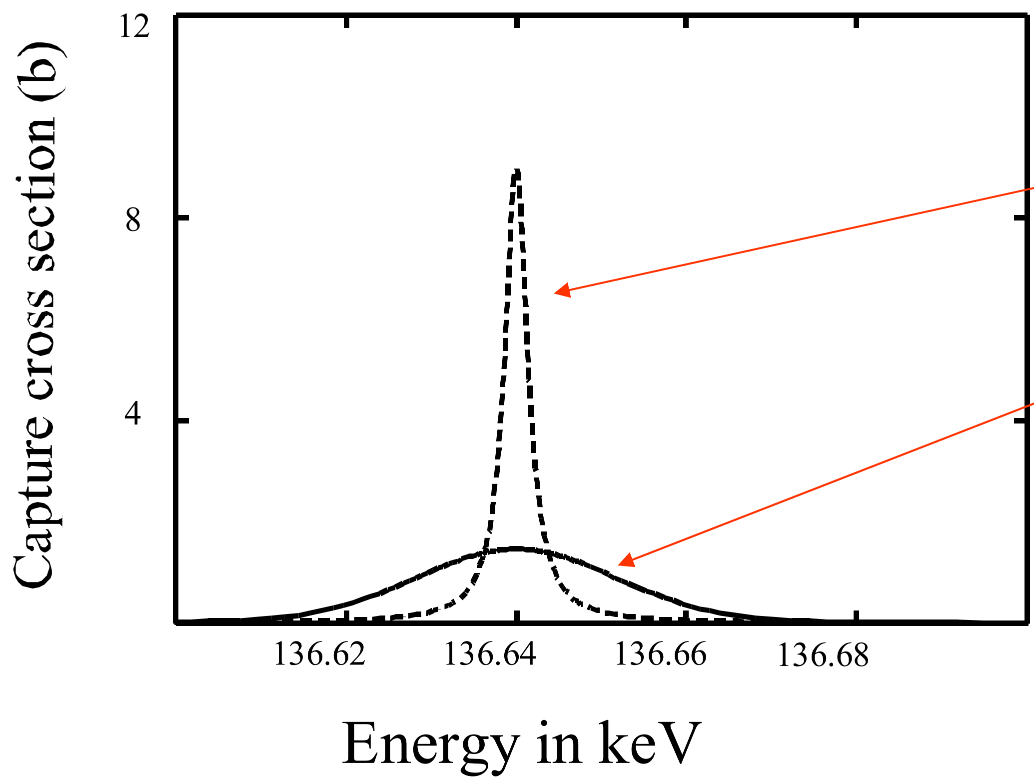
- $^{232}$Th, $^{233}$U, $^{234}$U, $^{235}$U, $^{236}$U, $^{238}$U, $^{237}$Np, $^{238,239,240,241}$Pu,
- $^{241,242m,243}$Am
- $^{242,243,244,245}$Cm,
- Pb, Bi, $^{56,57}$Fe,
- $^{58}$Ni, $^{52}$Cr, Zr, $^{15}$N, Si, C, O, Na, $^{10}$B $^{1}$H ,
- Ti (5 isotopes), $^{85}$Rb, $^{87}$Rb

# Measured Data Analyzed to Prepare Cross-Section Evaluation for ENDF

- **Measured data cannot be used directly for integral calculations**
- **Experimental data include measurement-related effects such as**
  - **Finite temperature**
  - **Finite size of samples**
  - **Finite resolution**
  - **Other machine-dependent features**
- **Each type of data must be measured separately**
  - **Capture, total, fission, reaction, …**
- **Measured data may look very different from the underlying “true” cross section**

as shown on next slide

# Doppler broadening only …




**Capture cross section for $^{58}Ni$ without Doppler broadening (dashed curve) and with Doppler broadening at 300 K (solid curve)**

# Evaluated data have advantages …

- **Evaluated data include**
  - **Theoretical understanding re shape of cross section**
  - **All available experimental information, including all available uncertainty information**
- **Evaluated data can be extrapolated**
  - **Different temperatures**
  - **Different energies (lower, higher, in-between)**
  - **Different reactions**

# ORNL: SAMMY R-Matrix Analysis Software

- **SAMMY is used to analyze measured data and produce evaluations**
- **Multilevel multichannel R-matrix code**
- **Developed at ORNL, used at ORNL and around the world for analysis of neutron-induced cross sections**
- **Includes corrections for experimental conditions**

**also can be used for charged-particle evaluations**

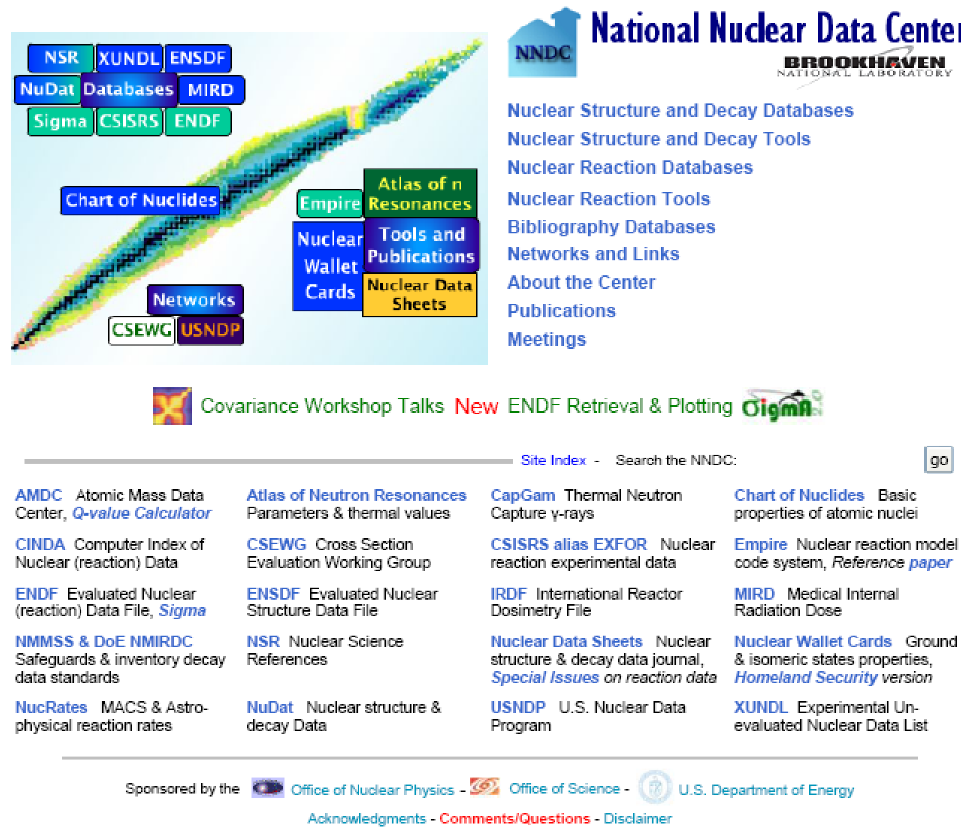
**Doppler, resolution, multiple scattering, normalization, background**

# SAMMY (cont.)

- **Capable of utilizing full off-diagonal covariance matrix for experimental data**
- **Produces full off-diagonal resonance parameter covariance matrix**
- **Creates ENDF File 2 (resonance parameter file) and File 32 (resonance parameter covariance file)**

# Evaluated Nuclear Data

- In the U.S., **Evaluated Nuclear Data File (ENDF)** System Provides Evaluated Cross-Section Data for Various Materials of Interest---Latest is ENDF/B-VII.0
- ENDF Data are Received and Distributed at Brookhaven National Laboratory
- Cross-Section Evaluation Working Group (**CSEWG**) is the ENDF/B Governing Body (i.e., Maintains/Updates ENDF/B Formats, Reviews/Approves New Evaluations, etc.)




ENDF/B data format is international standard format used by all other data projects (JEFF, JENDL, etc.)

# ENDF/B Data Overview: “MF” numbers

| File (MF) | Description | File (MF) | Description |
|---|---|---|---|
| **1** | **General Information** | 10 | Cross Sections for the Production of Radioactive Nuclides |
| **2** | **Resonance Parameters** | 11 | General Comments of Photon Production |
| **3** | **Neutron Cross Sections** | 12 | Photon Production and Multiplicities and Transition Probability Arrays |
| **4** | **Angular Dist. of Secondary Particles** | 13 | Photon Production Cross Sections |
| **5** | **Energy Dist. of Secondary Particles** | 14 | Photon Angular Distributions |
| **6** | **Coupled Energy-Angle Dist. of Secondary Particles** | 15 | Continuous Photon Energy Spectra |
| **7** | **$S(\alpha, \beta)$ Scattering Law Data** | 23 | Photon Interaction Cross Sections |
| 8 | Radioactive Decay and Fission Product Data | 27 | Atomic Form Factors or Scattering Functions |
| 9 | Multiplicities for Production of Radioactive Nuclides | 30 – 40 | Data Covariance Files |

# ENDF/B-VII Overview and Status

- Following slides taken from presentation by Pavel Oblozinsky (head of NNDC) at Advanced Fuel Cycle Workshop August 10-11, 2006, Bethesda, MD

# Nuclear data = Integration theme

Integrates NNSA, NE, Office of Science, …

Integrates experiment, theory, neutronics

Provides link to GNEP, AFC, GenIV simulations

# Cross Section Evaluation Working Group

**CSEWG** is cooperative effort of the national laboratories, industry and universities in the United States and Canada, responsible for the production of the U.S. **E**valuated **N**uclear **D**ata **F**ile, ENDF.

**Basic facts about CSEWG**

- Established in 1966
- Currently ~ 60 scientists, vigorous and active collaboration
- 20 laboratories (LANL, BNL, ANL, LLNL, ORNL,…, Westinghouse, Bettis, …)
- National Nuclear Data Center coordinates, provides support, archives the library

**Current funding of CSEWG, estimate**

| | |
|---|---|
| \$ 1mil | DOE-SC, Office of Nuclear Physics, via US Nuclear Data Program, includes \$200K allocated for AFC work in FY06 |
| \$ 7mil | DOE-NNSA (advanced simulation, criticality safety, nonproliferation), DOE-NE, also DOE naval reactor labs, NIST, industry, … |
| \$ 1mil | International contribution (NEA Paris, IAEA Vienna, …) |
| \$ 9 mil | |

# Evaluated Nuclear Data File, ENDF

## Releases of ENDF library, historical perspective:

| | | | |
|---|---|---|---|
| ENDF/B-I released | 1968 | - | CSEWG established in 1966 |
| ENDF/B-II | 1970 | 2y | |
| ENDF/B-III | 1972 | 2y | |
| ENDF/B-IV | 1974 | 2y | |
| **ENDF/B-V** | **1978** | **4y** | Early interest in covariances |
| **ENDF/B-VI** | **1990** | **12y** | Last update in 2001 |
| **ENDF/B-VII** | **2006** | **16y** | 40 years of CSEWG |
| ENDF/B-VIII | ??? | ??? | |

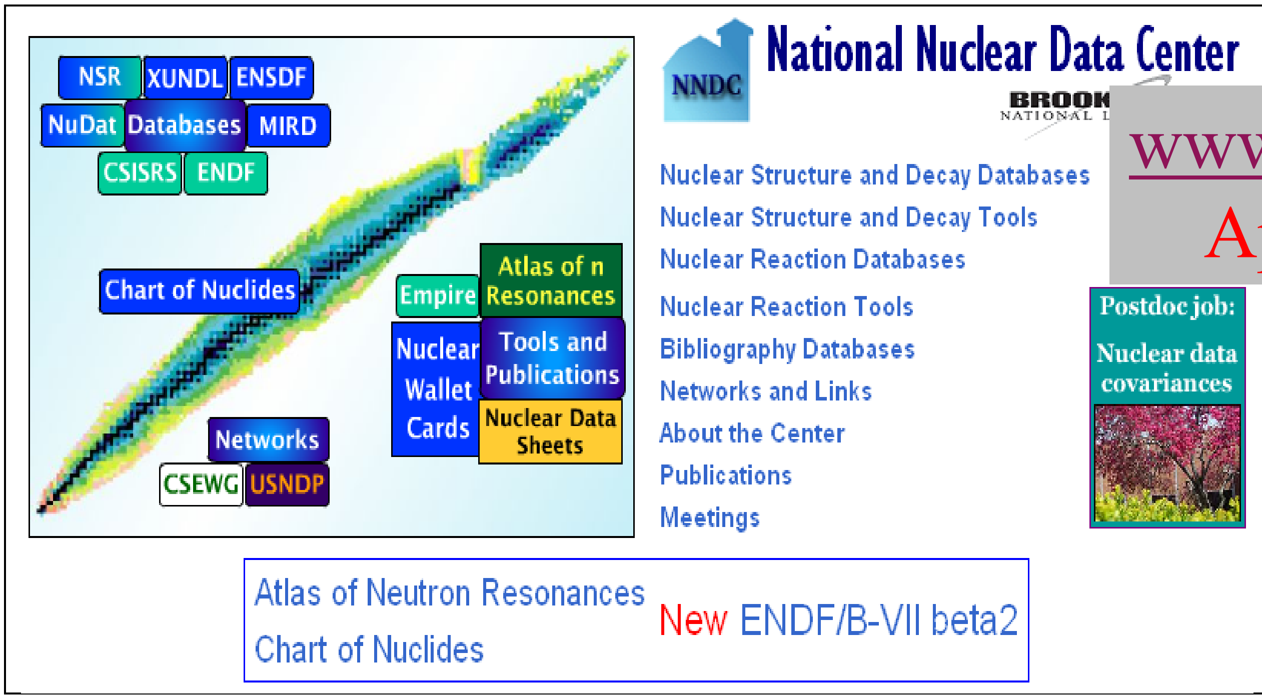
Development of the ENDF/B-VII library started modestly at the end of 2001.
No one assumed that there will be so much interest in its release in 2006.
ENDF data retrievals from the NNDC web service increased by **150%** in 2006.

CSEWG understands historical opportunity, and long-term impact of ENDF/B-VII.
CSEWG is highly motivated to produce the best library ever.

But: Limited funding for AFC applications → Many AFC needs not addressed.

# ENDF/B-VII: Status of the library

- April 2006: Beta2 version released, followed by extensive testing and validation against integral experiments
- June 2006: CSEWG validation meeting, major improvement compared to ENDF/B-VI
- Sep. 2006: Beta3 release, followed by the final round of testing
- Nov. 2006: Official release of ENDF/B-VII.0




www.nndc.bnl.gov
April 25, 2006

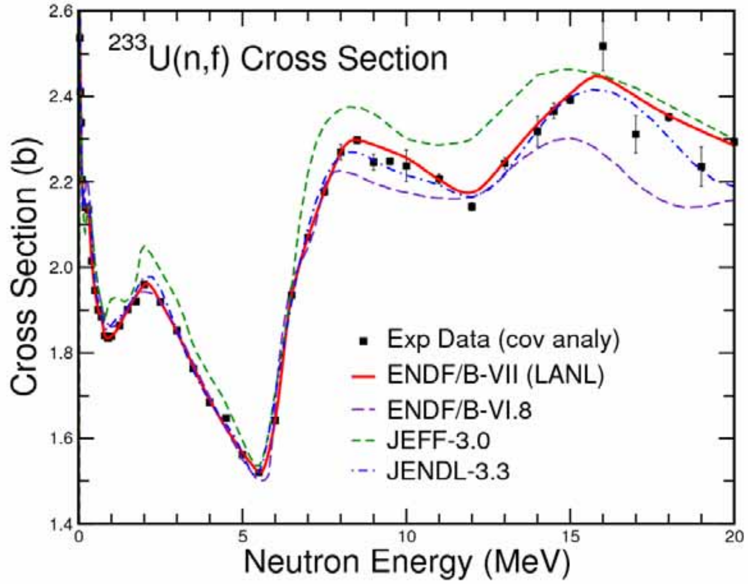
# ENDF/B-VII: Contents of the library

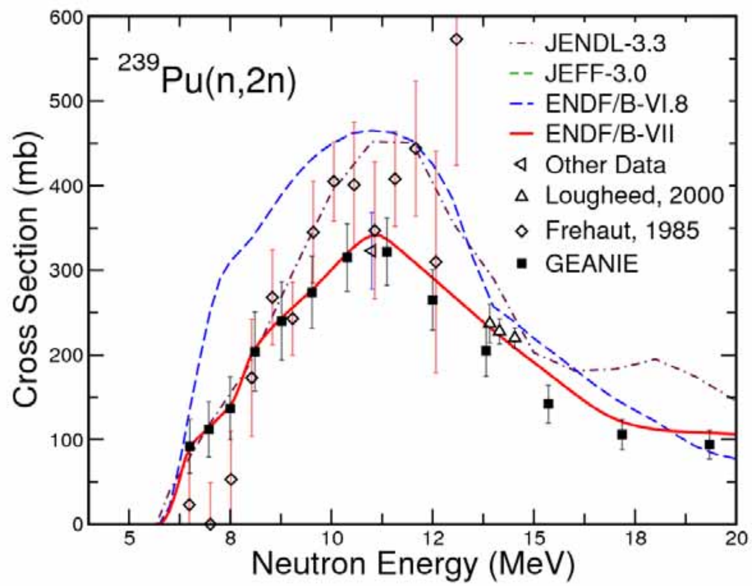
- General purpose library: Reactor design, advanced fuel cycles, waste transmutation, nonproliferation, national & homeland security, nuclear medicine, shielding, physics facility design, …
- Contents: 14 sublibraries (2 - new, 7 - many improvements, 5 – unchanged)

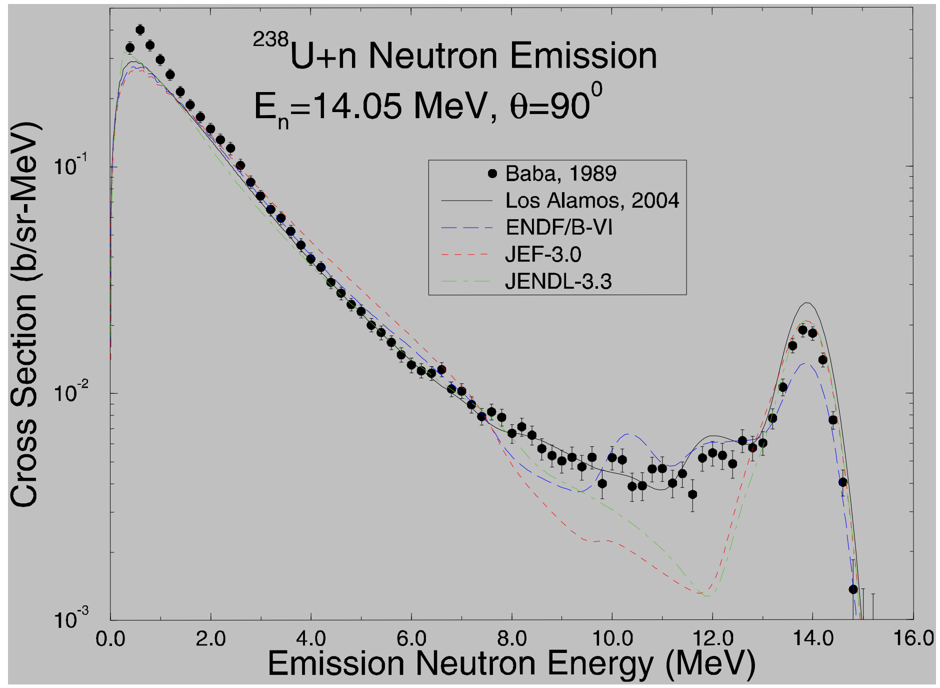
| No. | Sublibrary | Materials in B-VII | Materials in B-VI | Comment |
|---|---|---|---|---|
| 1 | Photonuclear reactions | **163** | - | **New sublibrary** |
| 2 | Photo-atomic | **100** | 100 | Taken from VI.8 |
| 3 | Radioactive decay | **3830** | 979 | **New evaluations** |
| 4 | Spontaneous fission yields | **9** | 9 | Taken from VI.8 |
| 5 | Atomic relaxation | **100** | 100 | Taken from VI.8 |
| 6 | **Neutron reactions** | **387** | **328** | **Many new evaluations** |
| 7 | Neutron fission yields | **31** | 31 | Taken from VI.8 |
| 8 | Thermal neutron scattering | **20** | 15 | **Some new evaluations** |
| 9 | Standards | **8** | 8 | **New evaluations** |
| 10 | Electro-atomic | **100** | 100 | Taken from VI.8 |
| 11 | Proton reactions | **48** | 35 | Some new evaluations |
| 12 | Deuteron reactions | **5** | 2 | Some new evaluations |
| 13 | Triton reactions | **3** | 1 | Some new evaluations |
| 14 | He-3 reactions | **2** | 1 | Some new evaluations |
| | **Full library** | **4812** | 1709 | |

# ENDF/B-VII: Neutron cross sections

## Major improvements in actinides (LANL – fast neutrons, ORNL – resonances)



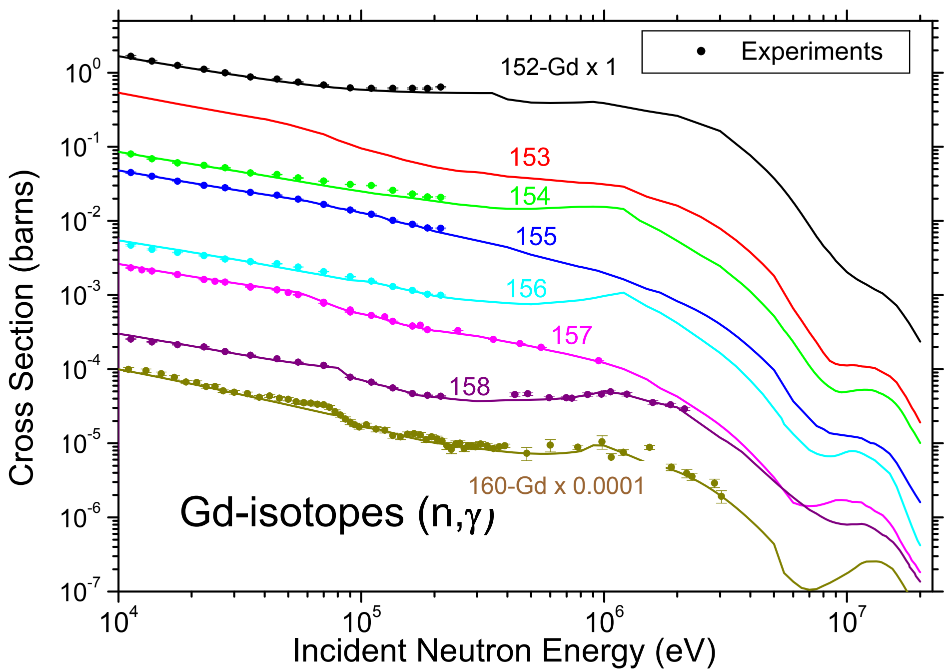



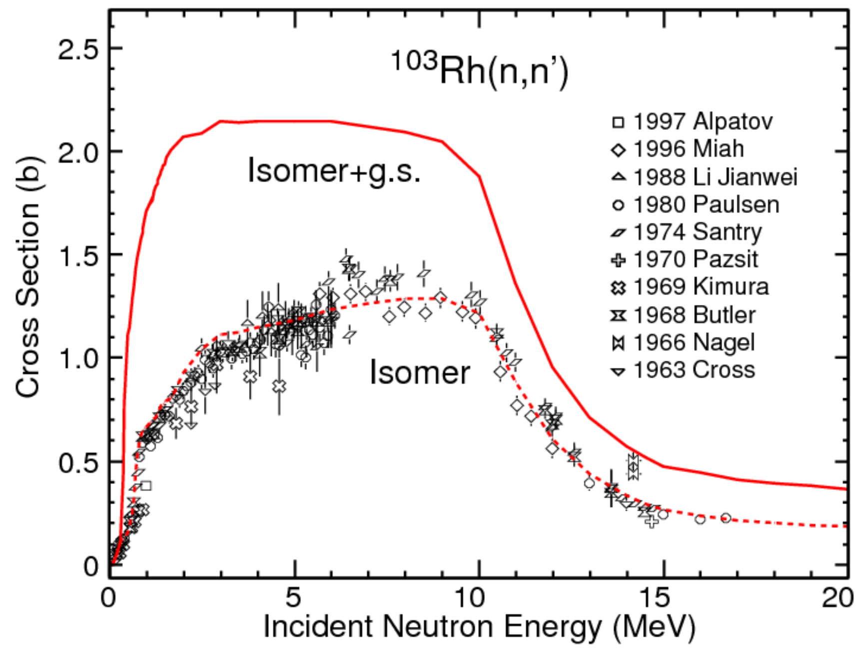




233U: Fission much improved
238U: Neutron spectrum much improved below elastic peak
239Pu: (n,2n) problem solved
Many other improvements, based on advanced modeling, …

# ENDF/B-VII: Neutron cross sections

## Major improvements in fission products (BNL, international)




Gd-isotopes: New evaluations for criticality safety applications, include covariances by BNL-LANL-ORNL.
70 materials ($^{103}$Rh, …): New evaluations, advanced modeling.
Other materials: Best non-US evaluations adopted.

# ENDF/B-VII: Quality Assurance

**Quality Assurance** is of key importance in the library development, it is done by careful comparison of the library against hundreds of integral benchmark experiments (benchmarking and validation).

**Criticality benchmarks:**

- main fissionable isotope (low enriched U, high enriched U, …)
- physical form of fissile material (metal, compound, solution)
- neutron spectrum (thermal, intermediate, fast)

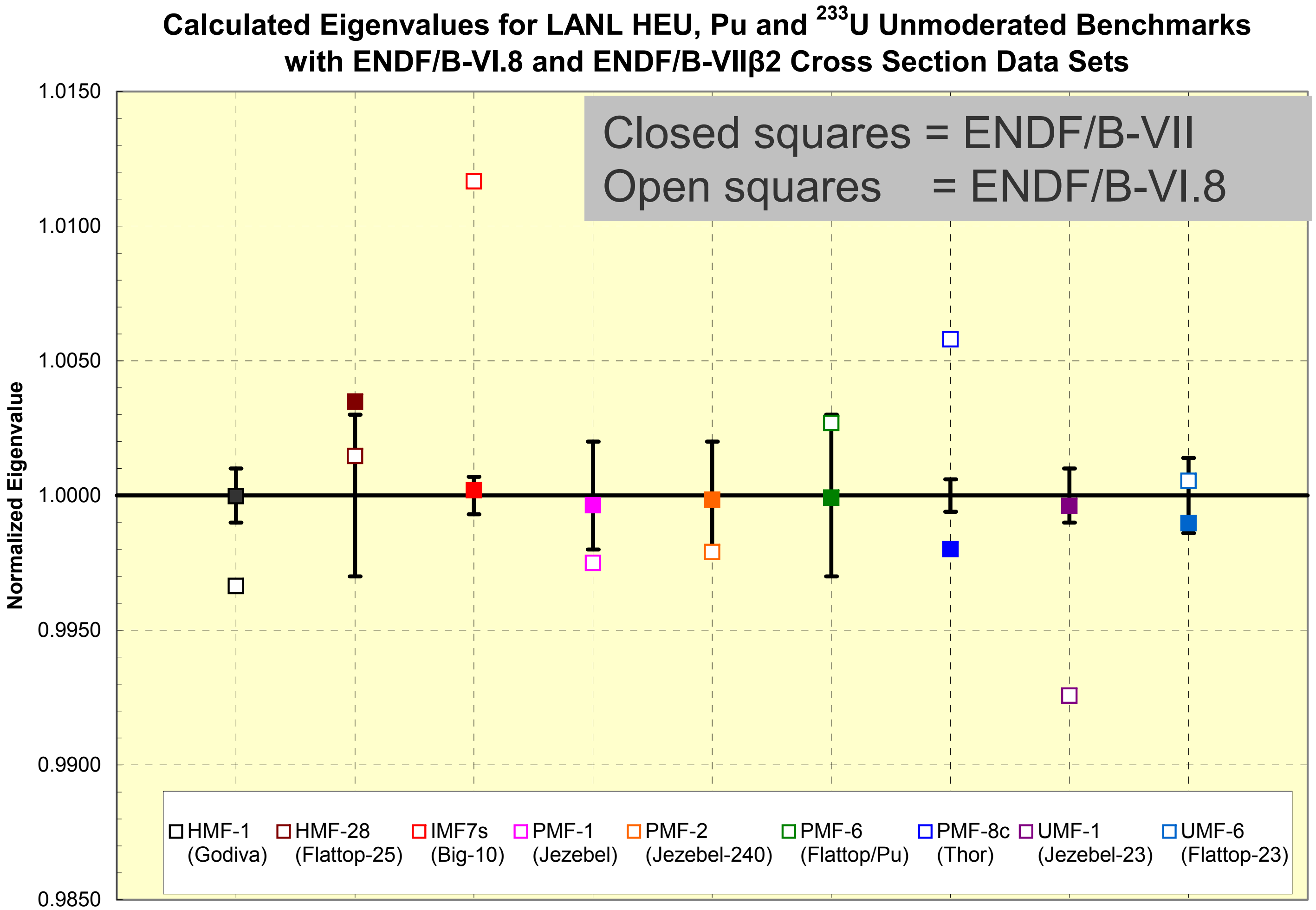
**Validation is complex process, multiple pathways:**

- US laboratories (LANL, KAPL, ANL, …, Westinghouse, Bettis,… )
- Europe (Petten, Cadarache), independent testing
- Use of independent tools (simulation codes MCNP – Los Alamos, TRIPOLI - Cadarache)

**Preliminary results are encouraging, some statements:**

"… major improvement…, significantly improved…, better than any previous data set…, mother of all nuclear data libraries…"

# Quality Assurance: Example of Integral Validation




Fast U and Pu benchmarks:

Considerable improvement for all benchmarks.

## ENDF/B-VII: Covariance data

### Although very important for simulations, little covariance data are available

**Covariances**

Covariances are given in a form of matrix that include uncertainties (e.g., for cross section at a given incident neutron energy) and correlations (e.g, between cross sections at different neutron incident energies).

**ENDF/B-VII should contain quality covariances only:**

Covariances mostly produced in1970-ties for ENDF/B-V, little done since then.
CSEWG decided to keep quality data only.
About 90% of old covariances were removed, based on ANL analysis.
Only partial covariances for 13 materials migrated from B-VI to ENDF/B-VII.

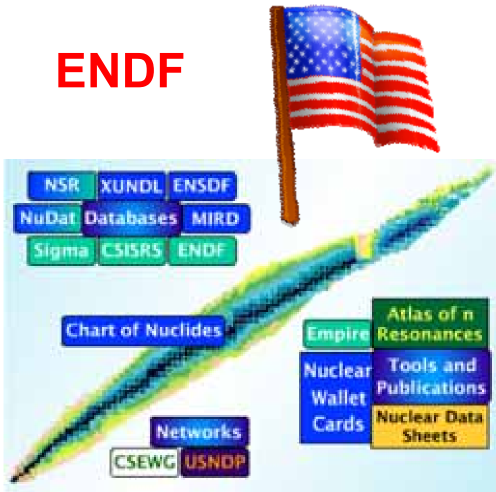
**New covariances for 9 materials:**

152,153,154,155,156,157,158,160-Gd (produced by BNL-LANL-ORNL)
232-Th (IAEA international project, resonance region by ORNL)

**ENDF/B-VII: Covariances only for 22 materials out of total 393 materials.**

# Nuclear Data is an International Effort

ENDF



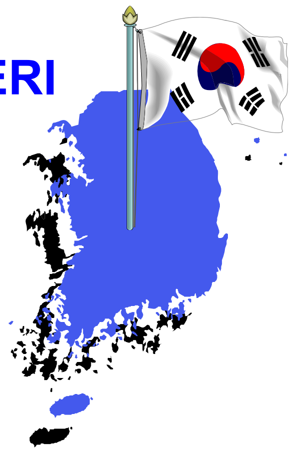

AEN NEA Agence pour l'énergie nucléaire
Nuclear Energy Agency
OECD

**Working Party for Evaluation Cooperation (WPEC)**

JEFF

JENDL


KAERI



International Atomic Energy Agency
Nuclear Data Services

BROND


CENDL

# General Considerations for Library Production

- **Radiation transport codes do not utilize ENDF evaluations directly**
  - ENDF data are "processed" by codes to generate libraries for transport codes
  - Two independent processing codes systems available to ENDF/B Data: *AMPX* (ORNL) and *NJOY* (LANL)

- **Producing a library for radiation transport**
  - Data present in evaluation dictates processing procedures
  - Operations for processing a nuclide evaluation:
    - Perform resonance reconstruction from resonance parameters
    - Perform temperature-dependent Doppler broadening for resonances
    - Calculate Energy-Angle Distributions of Secondary Particles
    - Process $S(\alpha,\beta)$ Data for Thermal Moderators
    - Calculate Weighting Spectrum for Multigroup Averaging
    - Generate cross section libraries
      - Pointwise libraries
      - Multigroup libraries (1-D and 2D transfer matrices)

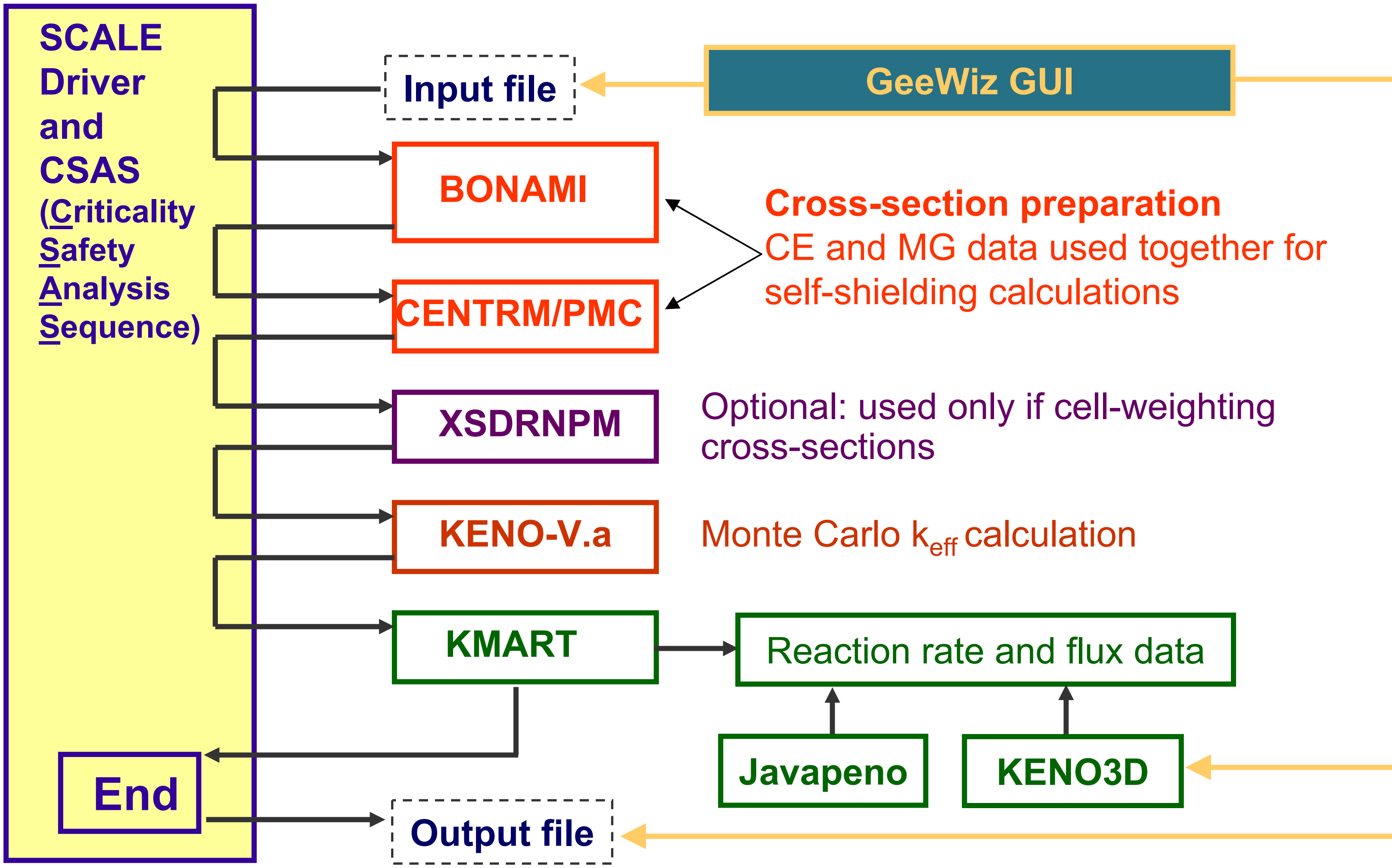
# AMPX Cross-Section Processing System

- SCALE relies on AMPX for data libraries—Independent from NJOY
  - **MG and CE cross-section data**
  - **Data processing procedures including problem-dependent resonance self-shielding**
  - **Cross-section uncertainty data to support S/U methods in SCALE**
- AMPX Processes ENDF/B Formats
  - **Generate Temperature-Dependent Pointwise Cross Sections**
  - **Provide Resonance Self-Shielding for RRR and URR**
  - **Probability Table Generation for URR**
  - **Energy and Angle Distributions for Secondary Particles**
  - **Process S(α,β) Data for Thermal Moderators**
  - **Generate free-gas S(α,β) Data for Non-Thermal Moderators**
  - **Process Particle-Yield Data**
  - **Generate Pointwise Weighting Spectra**
  - **Multigroup Averaging Operations**
  - **Process Cross-Section Uncertainty Data for TSUNAMI**
  - **Automated Cross-Section Library Production—Process Multiple Nuclides**

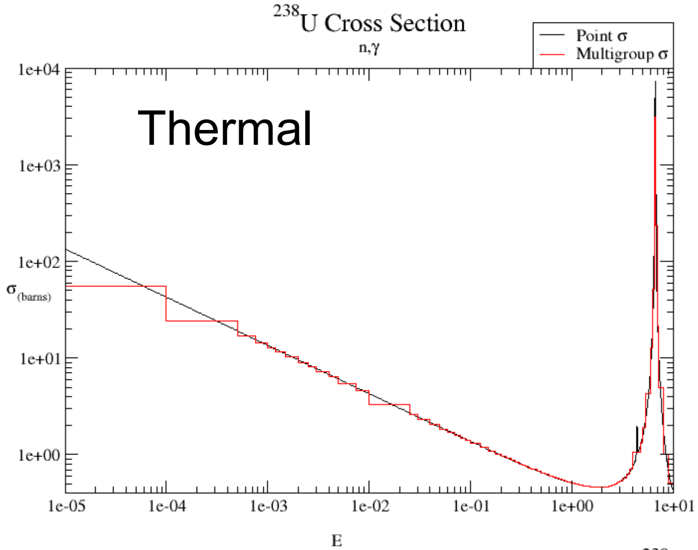
# Cross Section (XS) Library Formats in SCALE

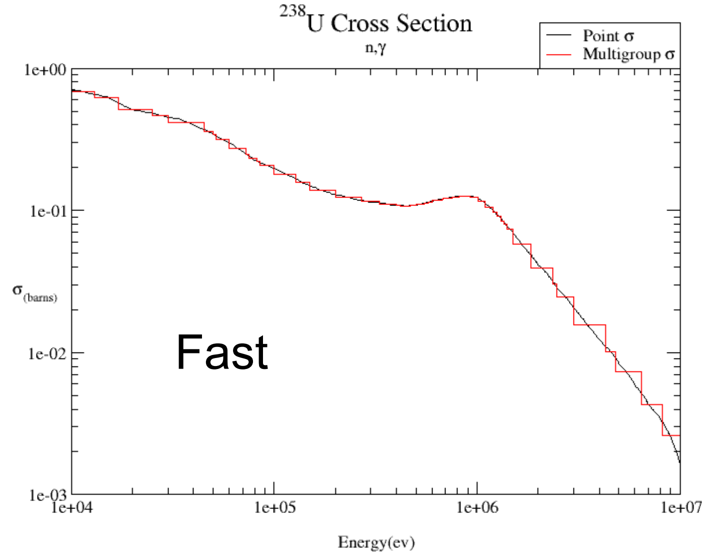
- Multigroup (MG) Libraries
  - AMPX Master Library (general)
    - Very general, include temperature-dependent cross-section data and resonance data
    - Distributed with SCALE
    - Used as a basis for creating an AMPX working format library that is problem-dependent
  - Working Library (e.g., Used by XSDRNPM and KENO)
    - Problem-dependent data generated by processing master library with BONAMI and NITAWL or CENTRM/PMC
- Continuous Energy (CE) Libraries
  - CENTRM
    - CE deterministic library distributed with SCALE
    - Used by CENTRM/PMC to self-shield multigroup data
  - CE-KENO
    - CE Monte Carlo library processed from same ENDF/B evaluations as ENDF/B-VI multigroup and CENTRM libraries

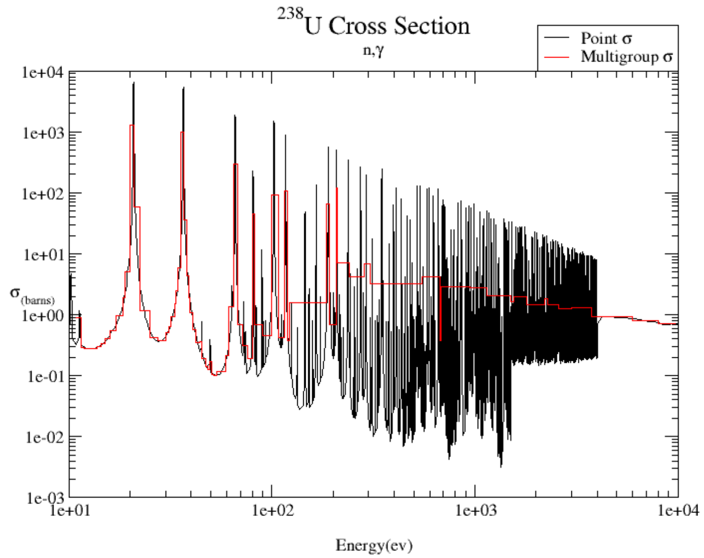
# SCALE Problem-Dependent Resonance Self-Shielding for MG Transport Calculations



# Comparison of 238-Group versus CE Data for $^{238}U$ Capture (n,$\gamma$)

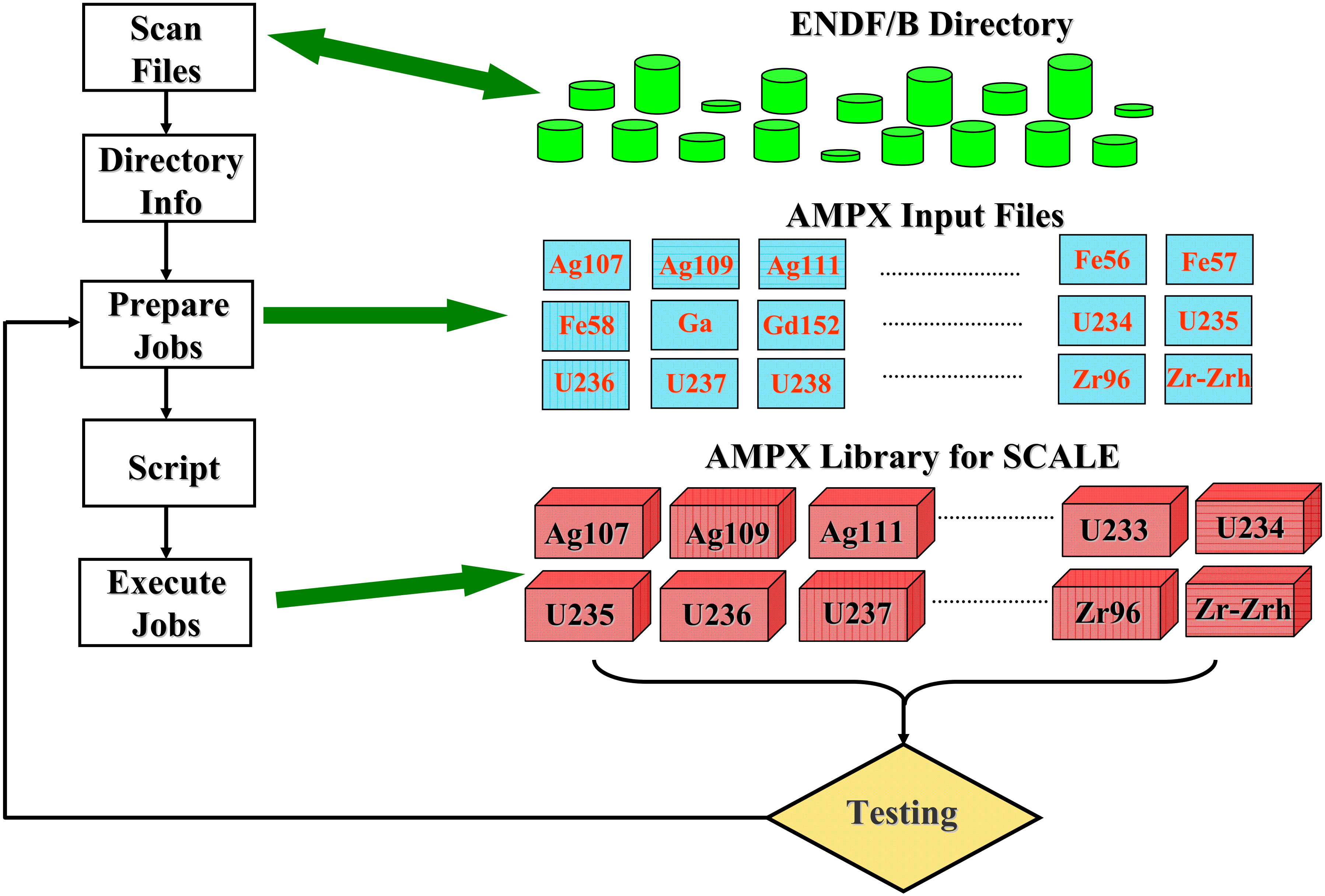


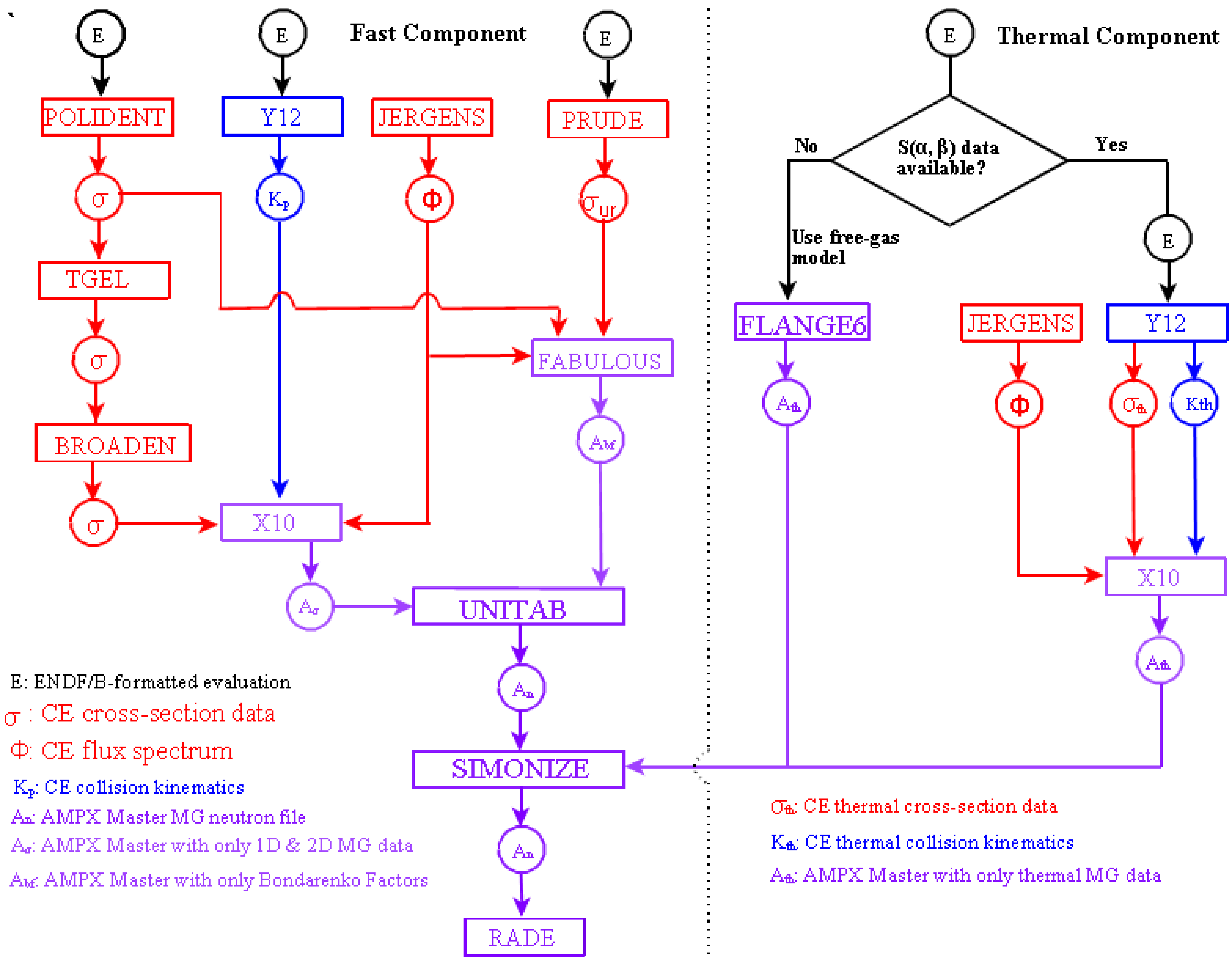




Resonance range

# SCALE Library Production Overview



# MG Library Generation for ENDF/B Nuclide



# Nuances of Producing Cross-Section Libraries

- Significant effort required to produce a cross-section library
- Assumptions and/or input options can have an impact on transport calculations
  - **Energy-mesh generation for resonance reconstruction**
  - **Resonance self-shielding using full-range Bondarenko factors**
  - **Weighting spectrum used to generate multigroup library**
  - **Etc.**
- What is impact on calculated results (e.g., $k_{eff}$, dose, etc.)?
- Depends on the problem
- Example: coarse energy-mesh tolerance for pointwise cross sections

# Nuances of Producing Cross-Section Libraries

- Energy Grid for Resonance Reconstruction
  - **ENDF/B Provides Resonance Parameters for Nuclides with Resonance Structure (e.g., SLBW, MLBW, Reich-Moore, etc.)**
  - **Processing Code Must Reconstruct Pointwise Data from Parameters**
  - **ENDF/B does not Provide Energy Mesh for Resonance Reconstruction**
  - **Processing Code Must Determine Suitable Energy Mesh**
  - **Calculate Cross Sections on Energy Grid using Specified Formalism**
  - **Energy-Mesh Generation Tolerance can Impact Results**
- Consider OECD/NEA Benchmark 20 Problem
  - **U(2.5)$O_2$ Spherical Fuel Pellets Partially Dissolved in Borated $UO_2$ Solution**
  - **Different Triangular Pitch Configuration of Pellets**
  - **Boron Concentration 1500 ppm**
  - **Problem Evaluates Different Levels of Dissolution**

# OECD/NEA Benchmark 20 Problem

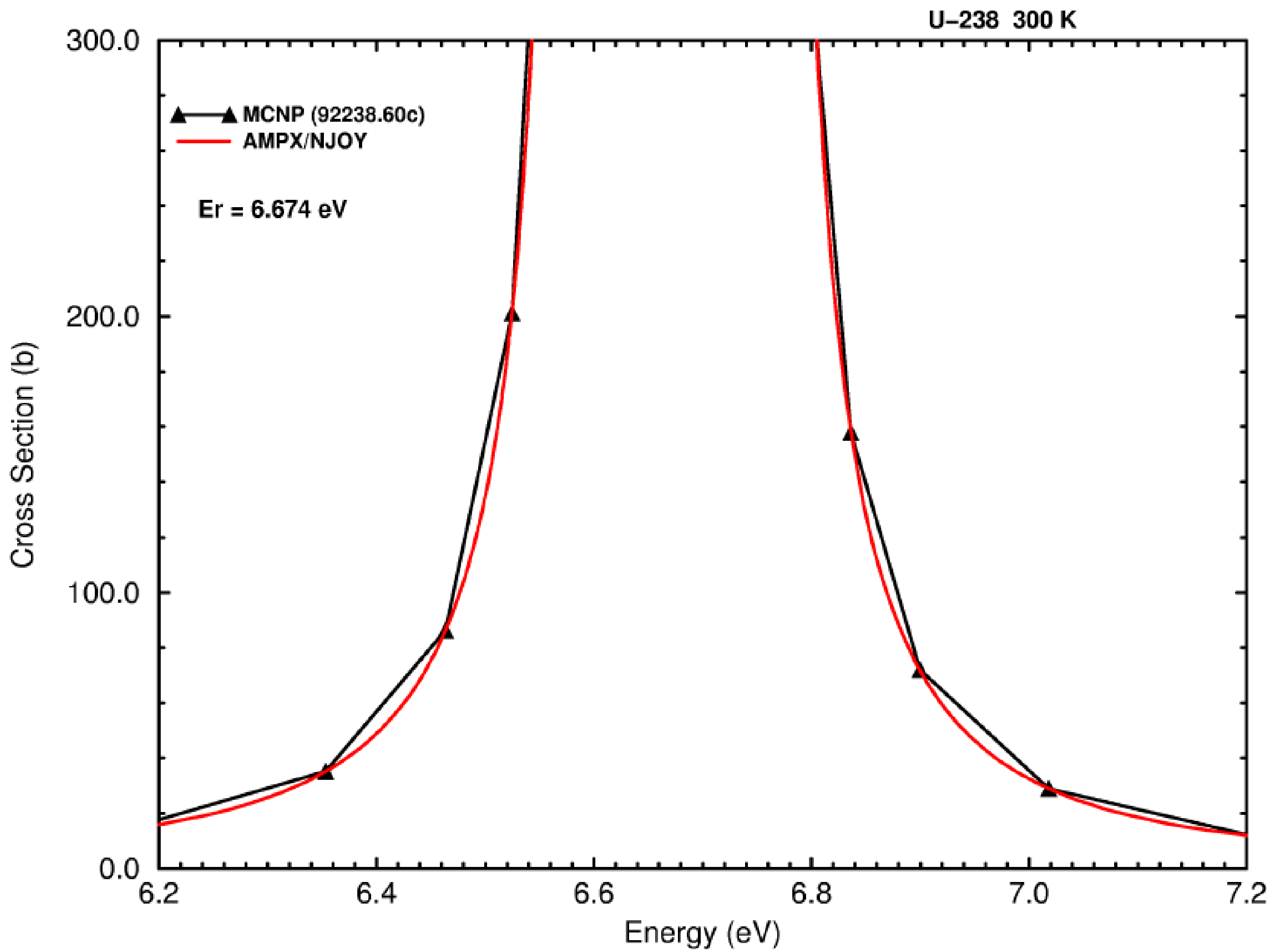
## ENDF/B-VI

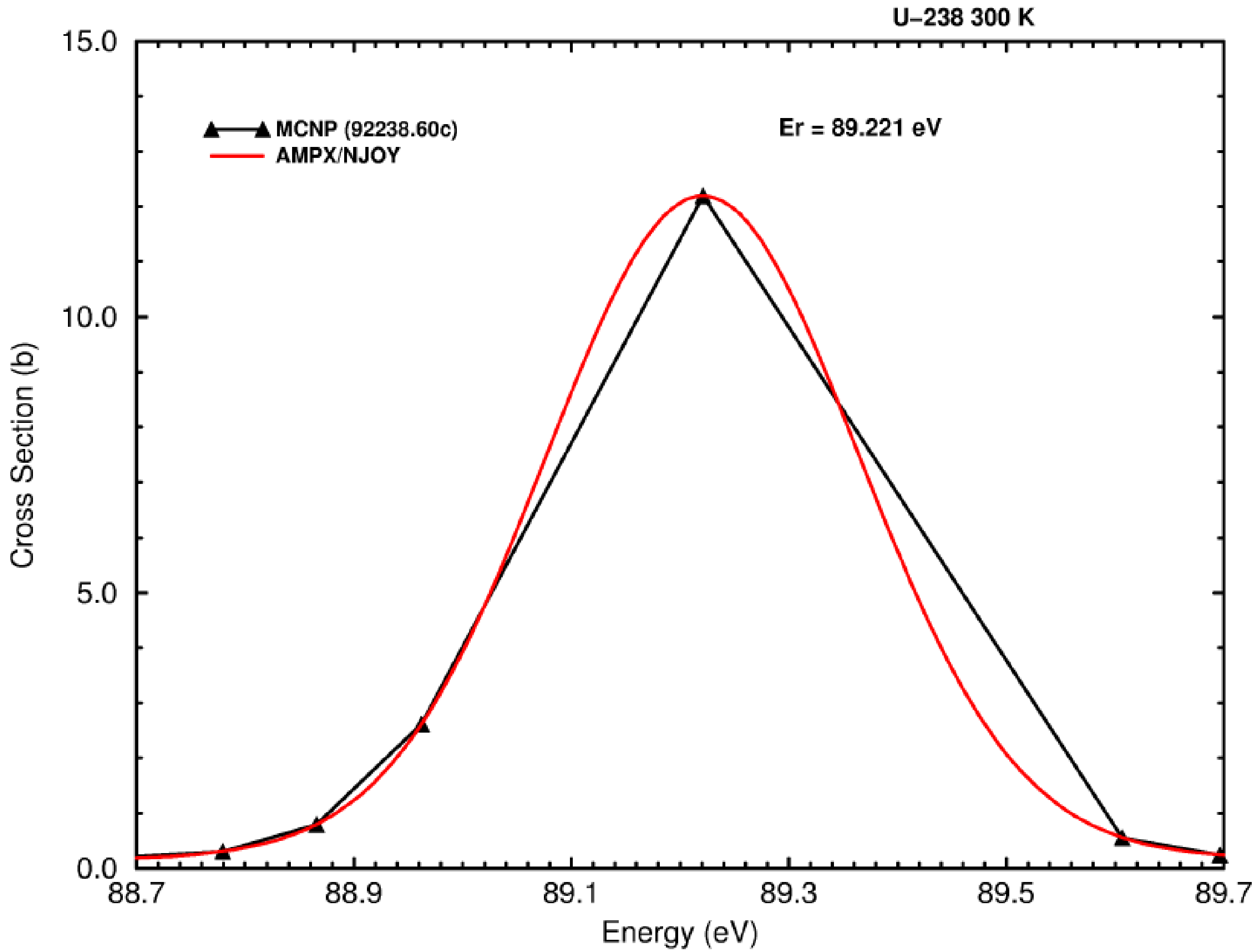
Libraries based on same ENDF/B-VI evaluations

Boron 1500 ppm

| ID | Tri. Pitch (cm) | $UO_2$ wt% in Pellet | XSDRN CENTRM | MCNP (NJOY) U-238 tol = 0.01 | MCNP (AMPX/NJOY) U-238 tol = 0.001 |
|---|---|---|---|---|---|
| 1b | 1.0297 | 100 | 1.0936 | 1.0954 ± 0.0012 | 1.0998 ± 0.0011 |
| 1d | | 75 | 1.0711 | 1.0663 ± 0.0011 | 1.0736 ± 0.0011 |
| 1f | | 50 | 1.0643 | 1.0571 ± 0.0012 | 1.0657 ± 0.0011 |
| 2b | 1.0943 | 100 | 1.1296 | 1.1299 ± 0.0012 | 1.1364 ± 0.0011 |
| 2d | | 75 | 1.1011 | 1.0962 ± 0.0012 | 1.1026 ± 0.0012 |
| 2f | | 50 | 1.0941 | 1.0882 ± 0.0012 | 1.0964 ± 0.0011 |
| 3b | 1.1788 | 100 | 1.1253 | 1.1250 ± 0.0011 | 1.1294 ± 0.0012 |
| 3d | | 75 | 1.0934 | 1.0920 ± 0.0012 | 1.0939 ± 0.0011 |
| 3f | | 50 | 1.0872 | 1.0796 ± 0.0012 | 1.0854 ± 0.0011 |

You can encounter pitfalls with continuous-energy calculations—Check the data!!!


U–238 300 K
MCNP (92238.60c)
AMPX/NJOY
Er = 6.674 eV
300.0
200.0
100.0
0.0
Cross Section (b)
6.2
6.4
6.6
6.8
7.0
7.2
Energy (eV)


U-238 300 K
MCNP (92238.60c)
AMPX/NJOY
Er = 89.221 eV
Cross Section (b)
Energy (eV)
15.0
10.0
5.0
0.0
88.7
88.9
89.1
89.3
89.5
89.7

# OECD/NEA Benchmark 20 Problem

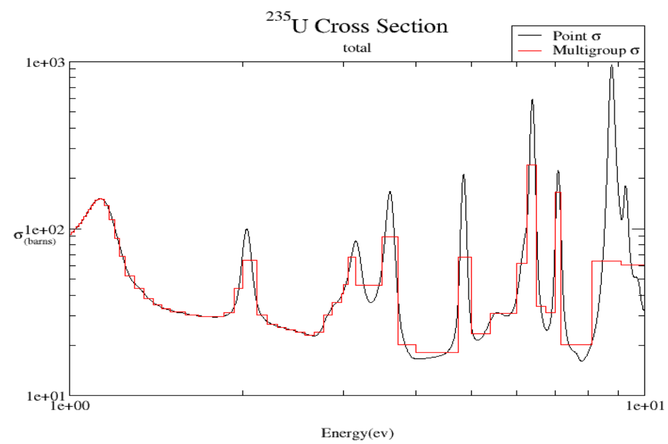
## ENDF/B-VI

Boron 1500 ppm

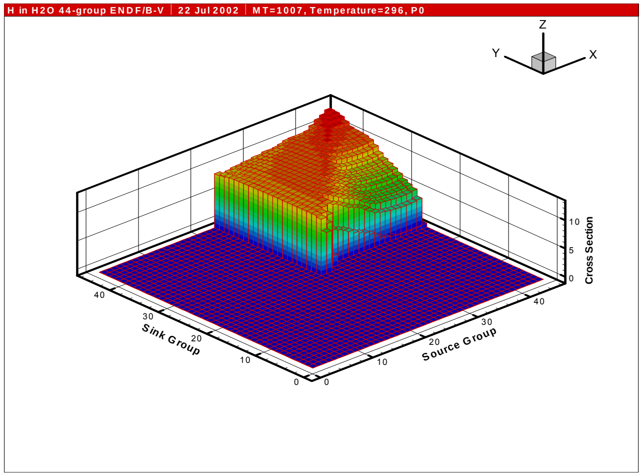
| ID | Tri. Pitch (cm) | $UO_2$ wt% in Pellet | XSDRN CENTRM | **MCNP (NJOY) $^{238}$U tol=0.001** | MCNP (AMPX/NJOY) $^{238}$U tol=0.001 |
|---|---|---|---|---|---|
| 1b | 1.0297 | 100 | 1.0936 | **1.1014 ± 0.0011** | 1.0998 ± 0.0011 |
| 1d | | 75 | 1.0711 | **1.0742 ± 0.0012** | 1.0736 ± 0.0011 |
| 1f | | 50 | 1.0643 | **1.0643 ± 0.0012** | 1.0657 ± 0.0011 |
| 2b | 1.0943 | 100 | 1.1296 | **1.1354 ± 0.0012** | 1.1364 ± 0.0011 |
| 2d | | 75 | 1.1011 | **1.1001 ± 0.0012** | 1.1026 ± 0.0012 |
| 2f | | 50 | 1.0941 | **1.0933 ± 0.0012** | 1.0964 ± 0.0011 |
| 3b | 1.1788 | 100 | 1.1253 | **1.1281 ± 0.0011** | 1.1294 ± 0.0012 |
| 3d | | 75 | 1.0934 | **1.0931 ± 0.0012** | 1.0939 ± 0.0011 |
| 3f | | 50 | 1.0872 | **1.0860 ± 0.0012** | 1.0854 ± 0.0011 |

# Library Generation & Testing for SCALE 6

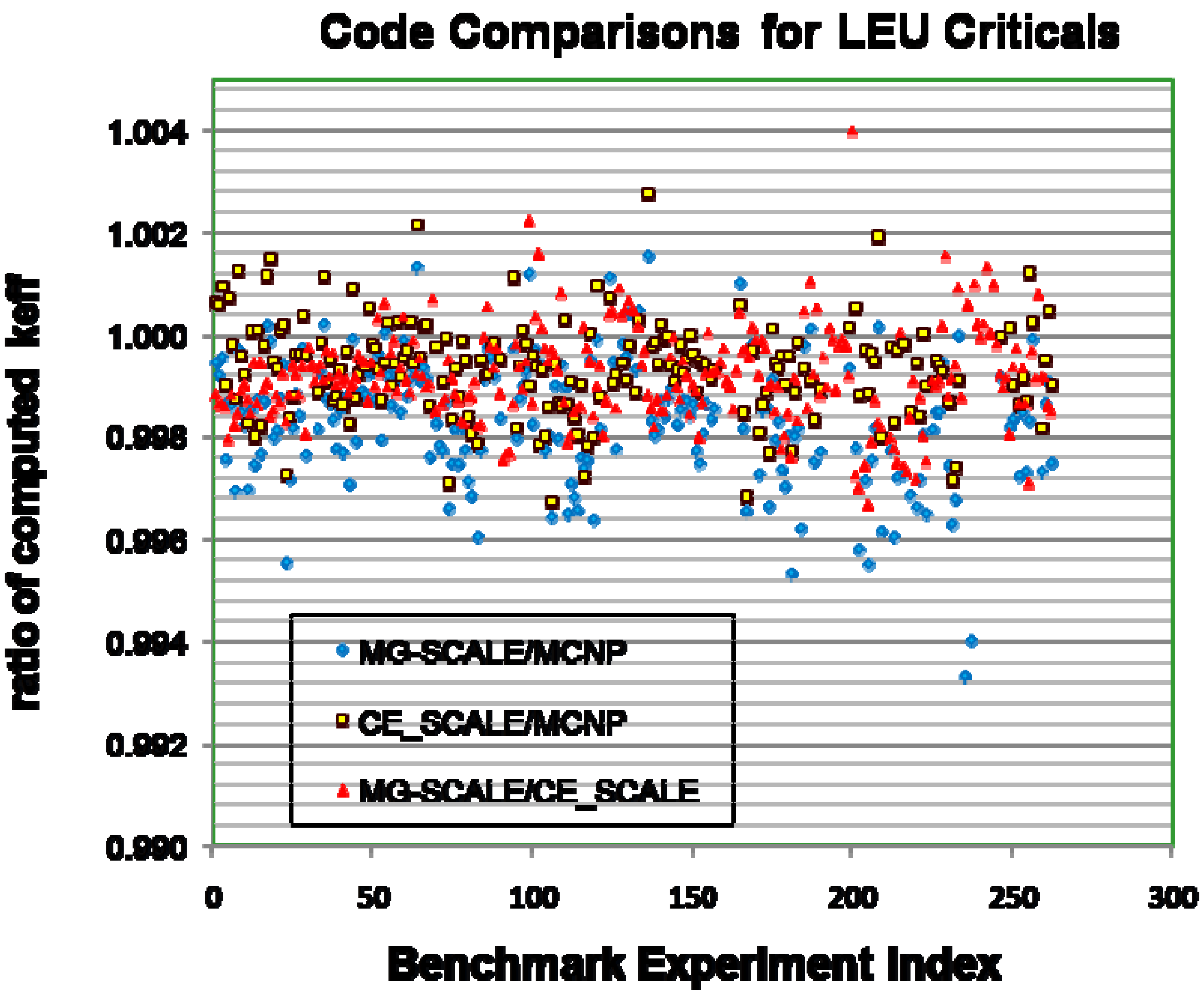
- AMPX used to process ENDF/B-VI.8 and ENDF/B-VII.0 evaluations
- New Libraries:
  - 238-group ENDF/B-VI.8 and B-VII.0
  - 200n47g ENDF/B-VI.8 and B-VII.0
  - 27n19g ENDF/B-VII.0
  - CE ENDF/B-VI.8 and ENDF/B-VII.0
    - CE-KENO and CENTRM
  - Recommend covariance data library
    - Evaluated and approximate covariance data
    - Covariance data for all ENDF/B nuclides (neutron)
- Tested with ~1300 criticality benchmark cases
- Performed shielding V&V with Mavric/MONACO




$H_2O$ Incoherent Inelastic Scattering

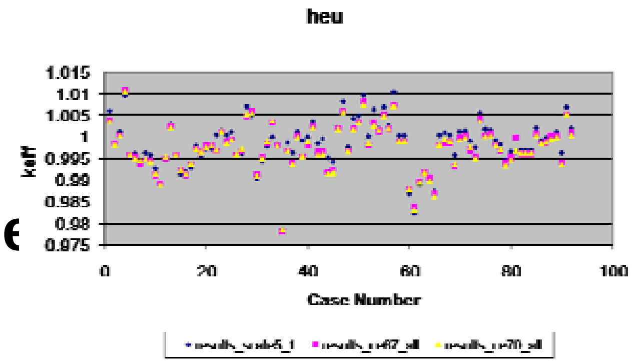


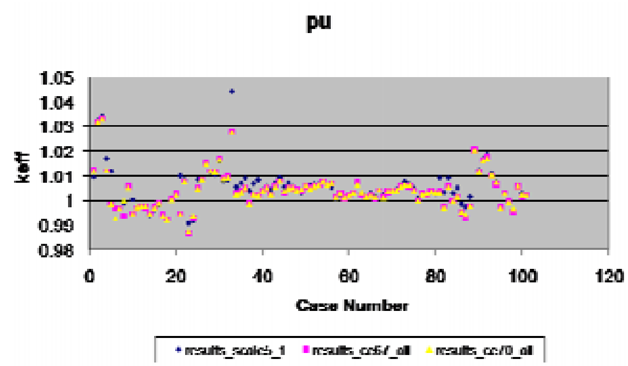
# Comparison of MG-KENO,CE-KENO, MCNP

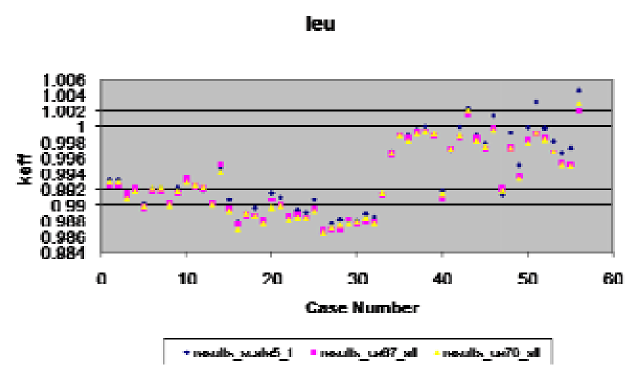


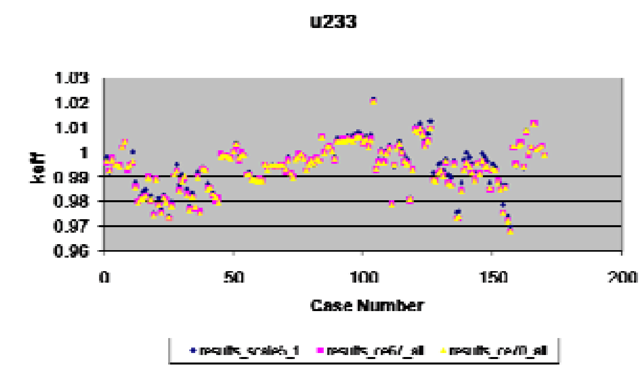
# SCALE Validation with Critical Experiments

- **~1300 critical experiments have been used for validation**
  - **433 highly enriched U cases**
  - **87 intermediate enriched U case**
  - **319 low enriched U cases**
  - **143 Pu cases**
  - **101 MOX cases**

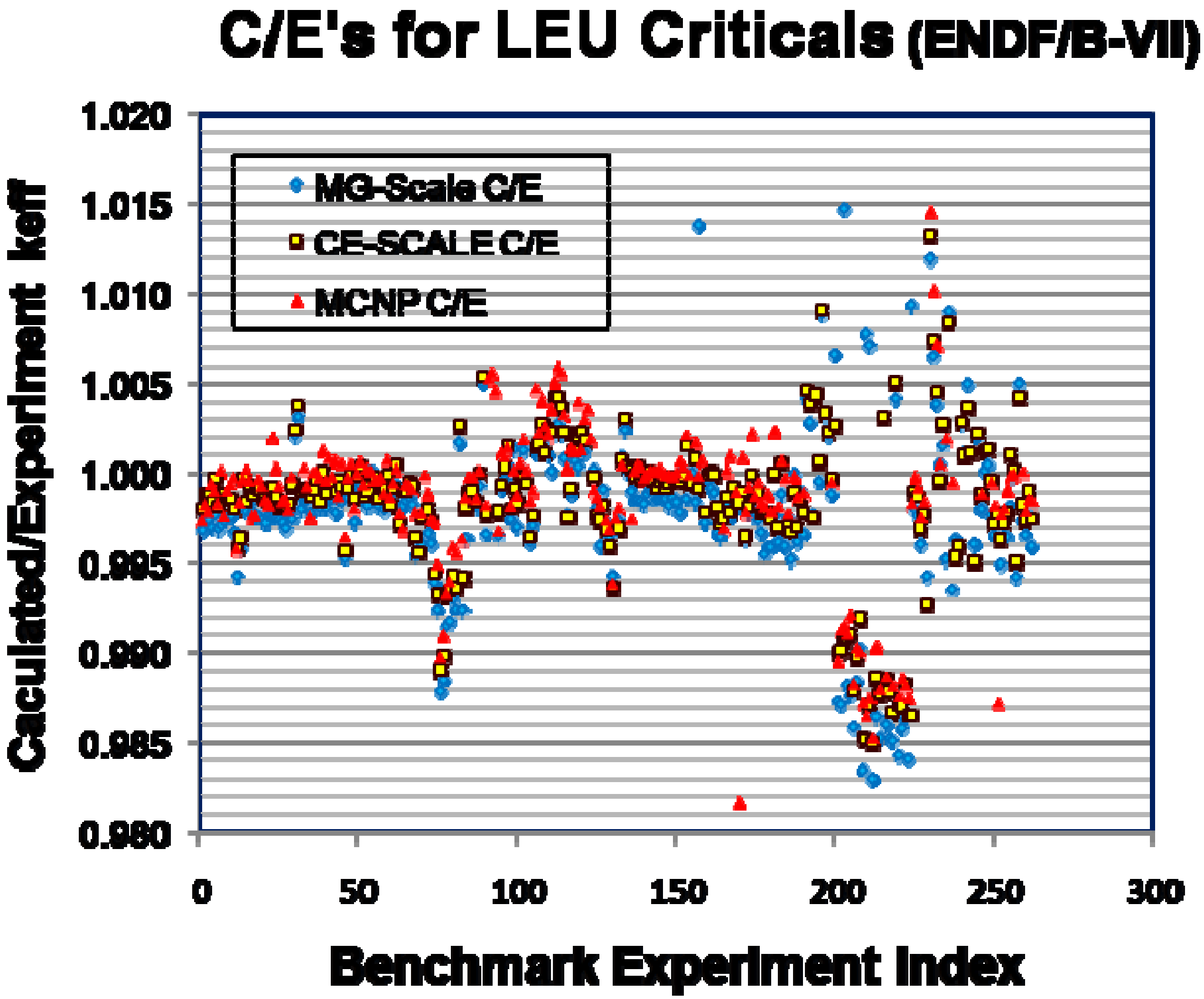


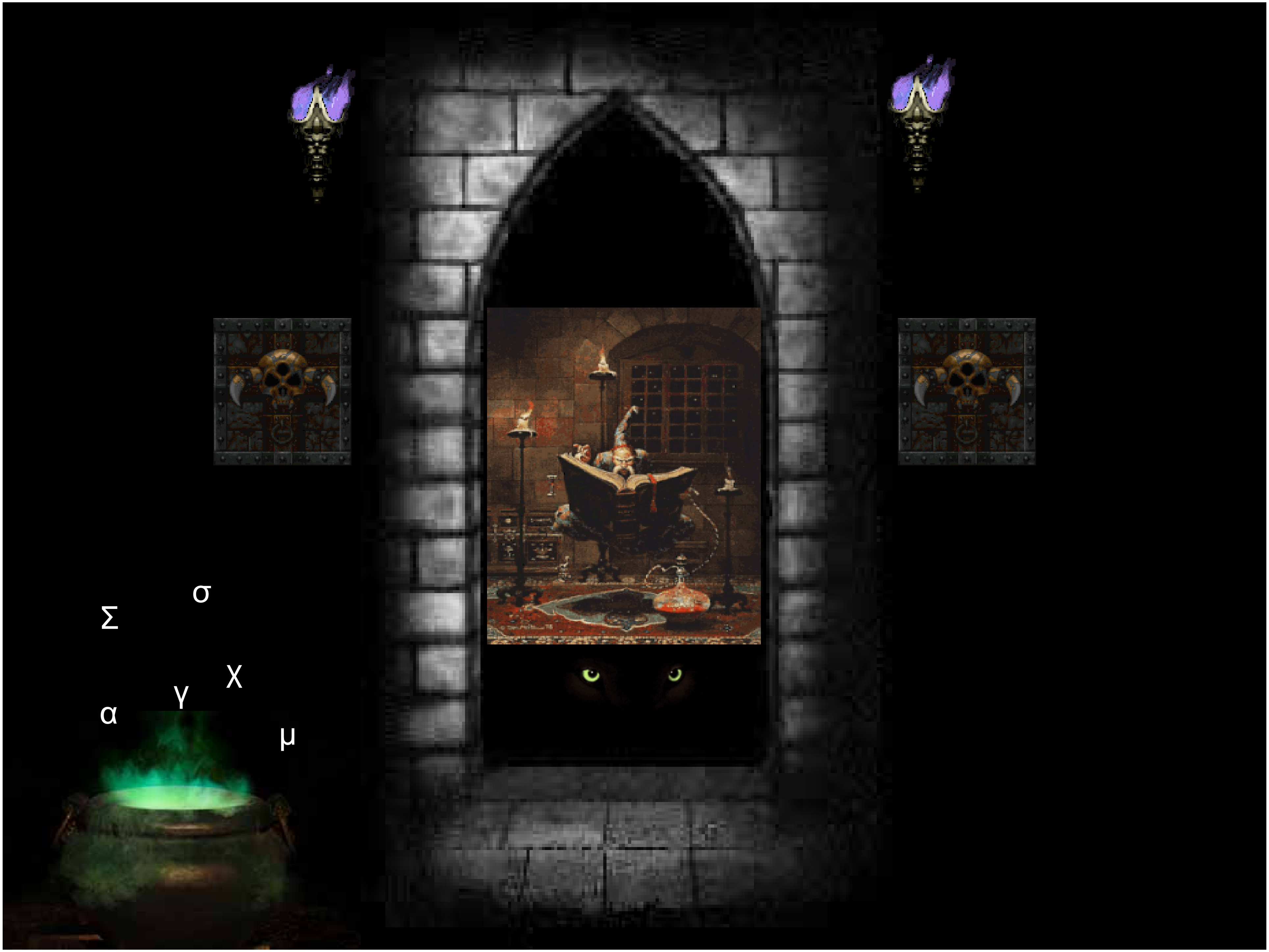



# ENDF/B-VII Keff Results for LEU Criticals




σ
Σ
χ
γ
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