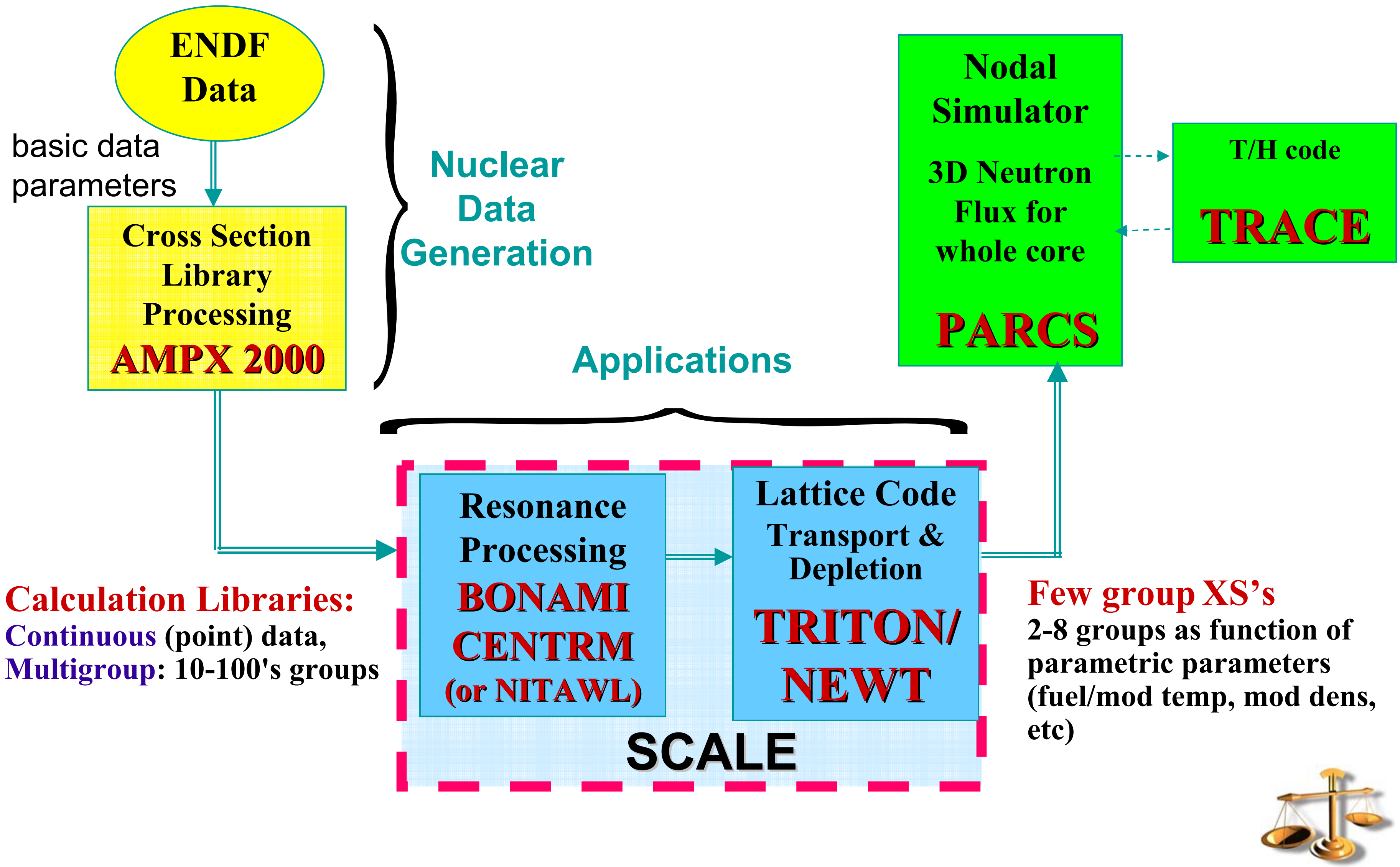
Cross Section Processing and Nuclear Data

Mark Williams

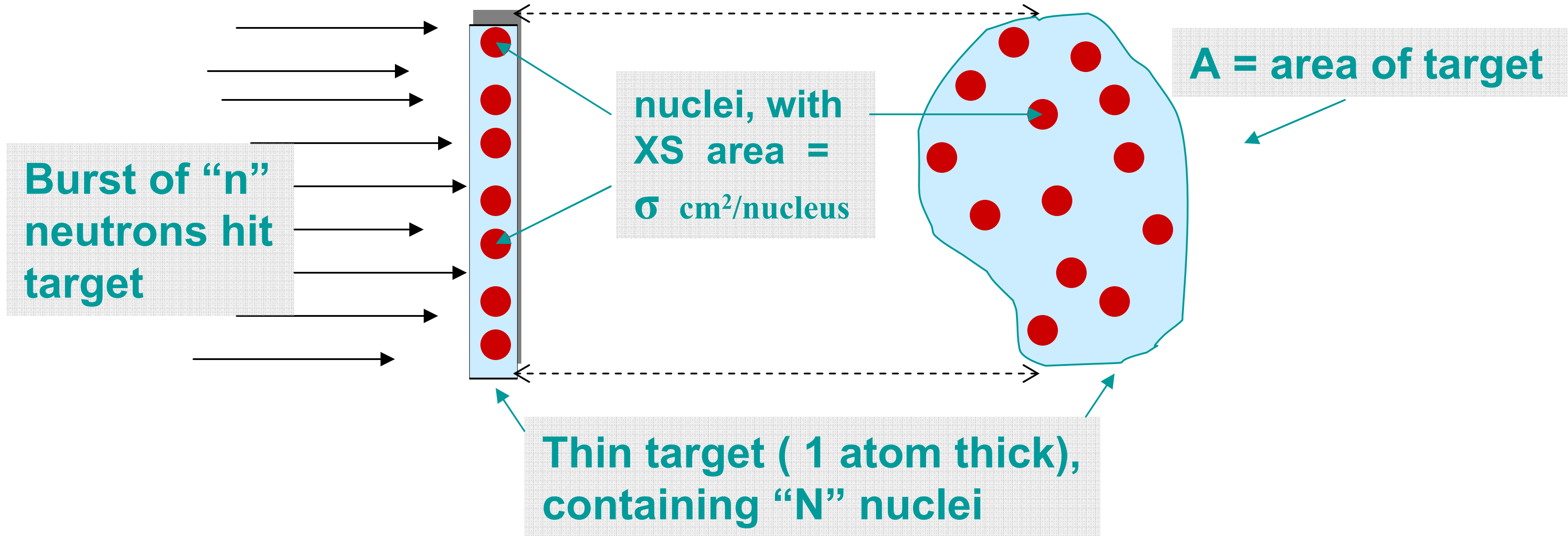
Research Staff

Oak Ridge National Laboratory

Cross-Section Processing:
The Big Picture for Reactor Analysis



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

- **Geometric Interpretation:** $R = \left(\frac{N\sigma}{A}\right) n \Rightarrow \left(\frac{R}{N}\right) = \sigma \underbrace{\left(\frac{n}{A}\right)}_{\Phi}$
  - σ = target area (*cm² per nucleus*)
  - 1 barn $=10^{-24}$ cm² ~ πR^2 => R~ 5.6×10^{-13} cm nuclear radius

- **Reaction Interpretation:**
  - generalization to account for energy-dependence of reaction rate
  - $\sigma \equiv$ reactions (*R*) per atom (*N*), per unit fluence (Φ *n/cm²*)

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

reactions per atom in target (numerator)

incident neutron fluence with energy E (denominator)

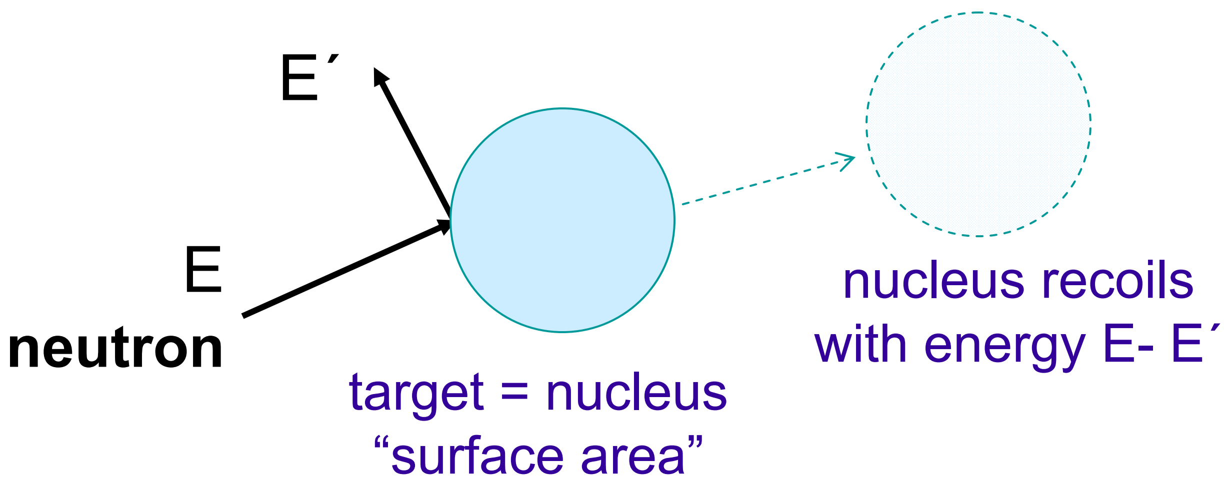
Types of Neutron Interactions

Potential Scatter Reactions

- **billiard ball type interaction =>**

  neutron bounces off “surface” of nucleus

  (n,n) elastic scatter



Types of Neutron Interactions, *continued*

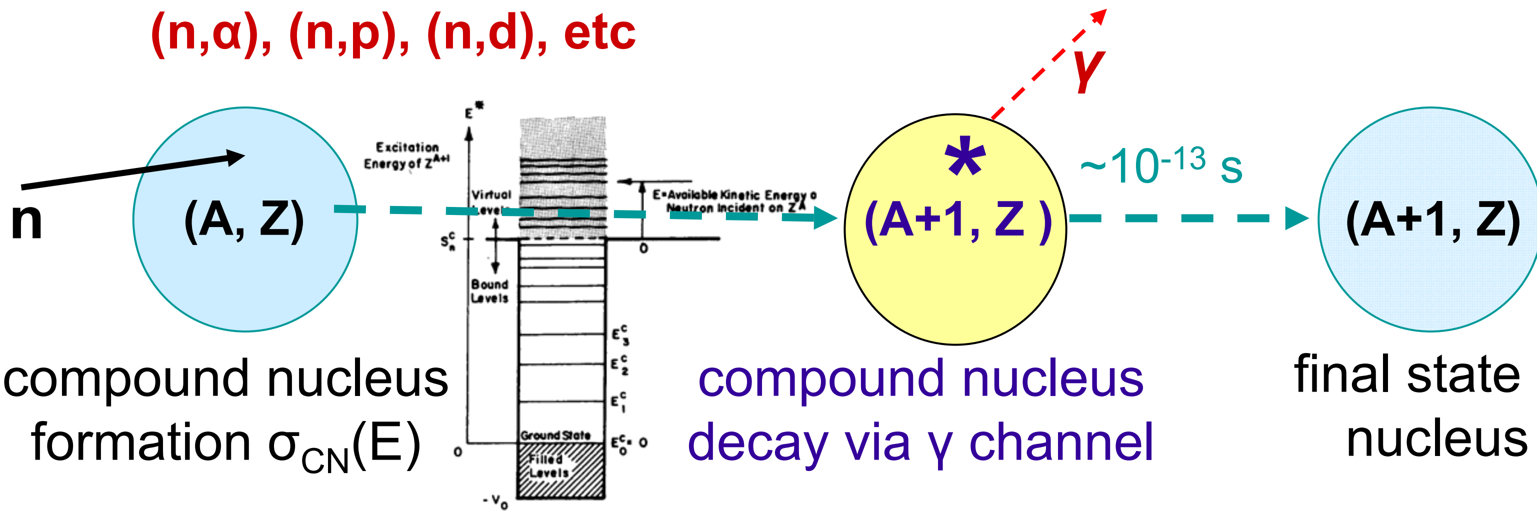
- **Compound Nucleus Reactions…** ***involves 2 steps*:**
  - neutron enters nucleus and forms excited compound state
  - compound nucleus "decays" after $\sim 10^{-13}$ sec via different "reaction-channels":

    (n,γ)   radiative capture

    (n,n´) compound elastic and inelastic

    (n,f)   fission

    (n,α), (n,p), (n,d), etc

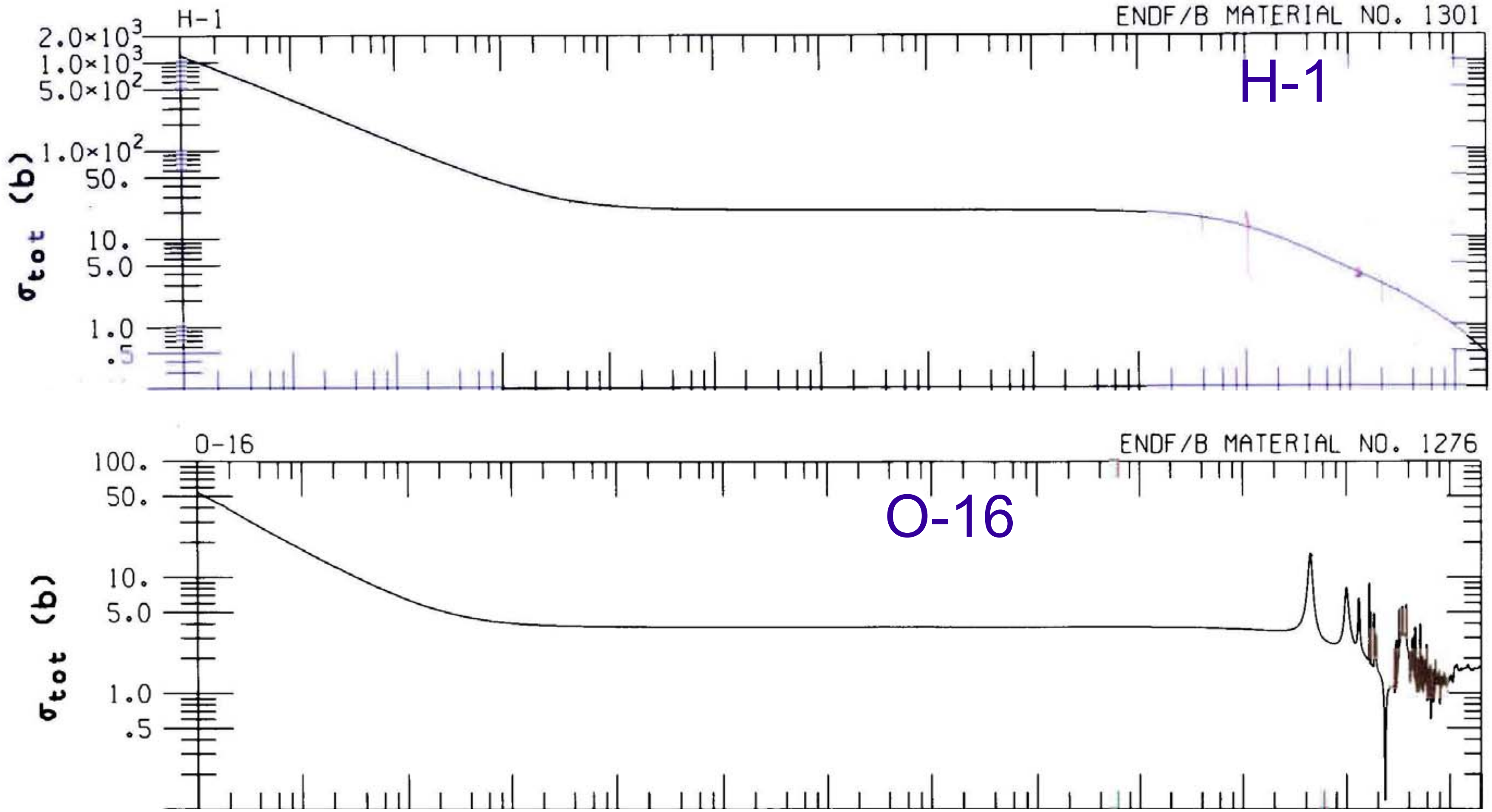


compound nucleus formation $\sigma_{CN}(E)$

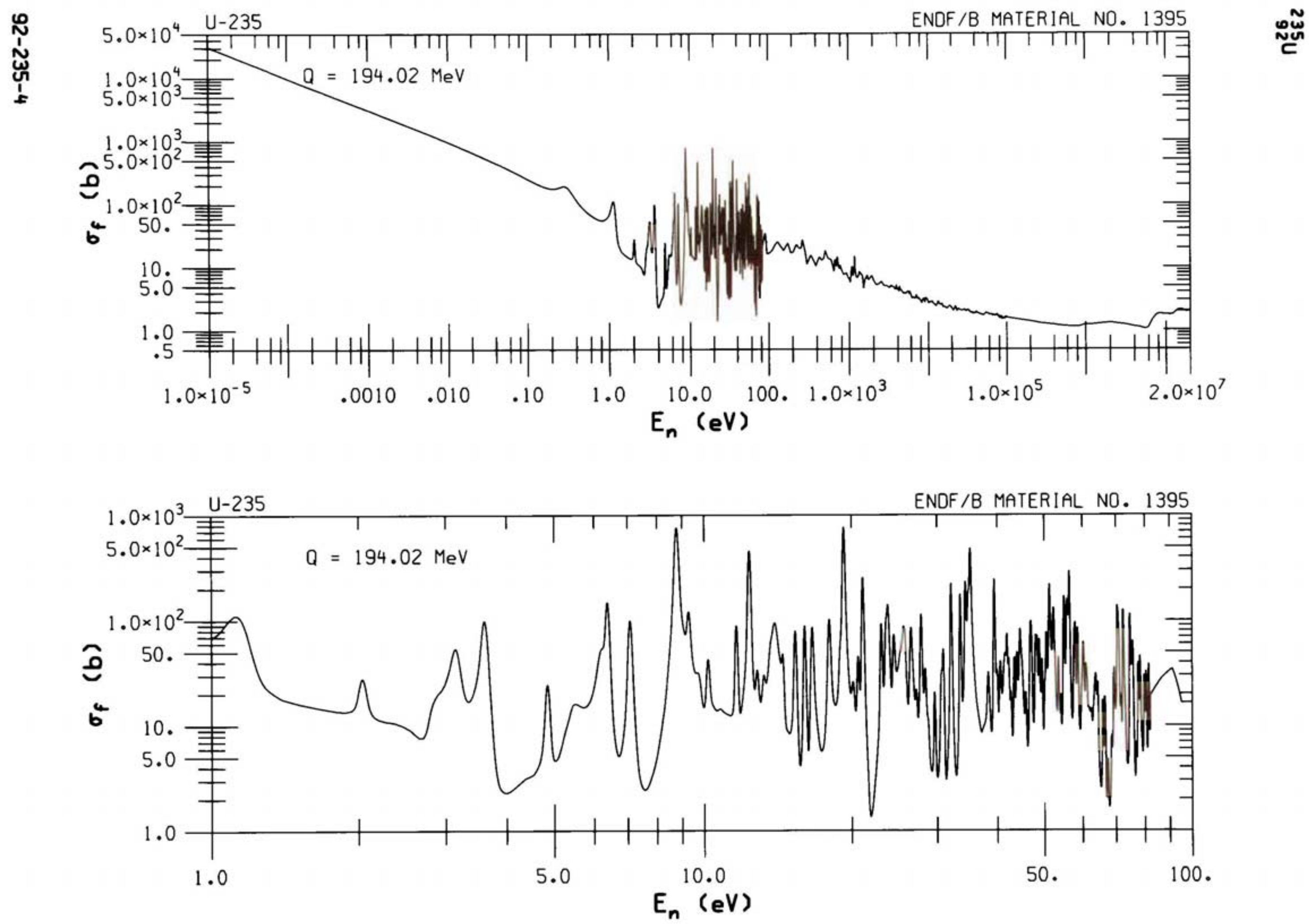
compound nucleus decay via γ channel

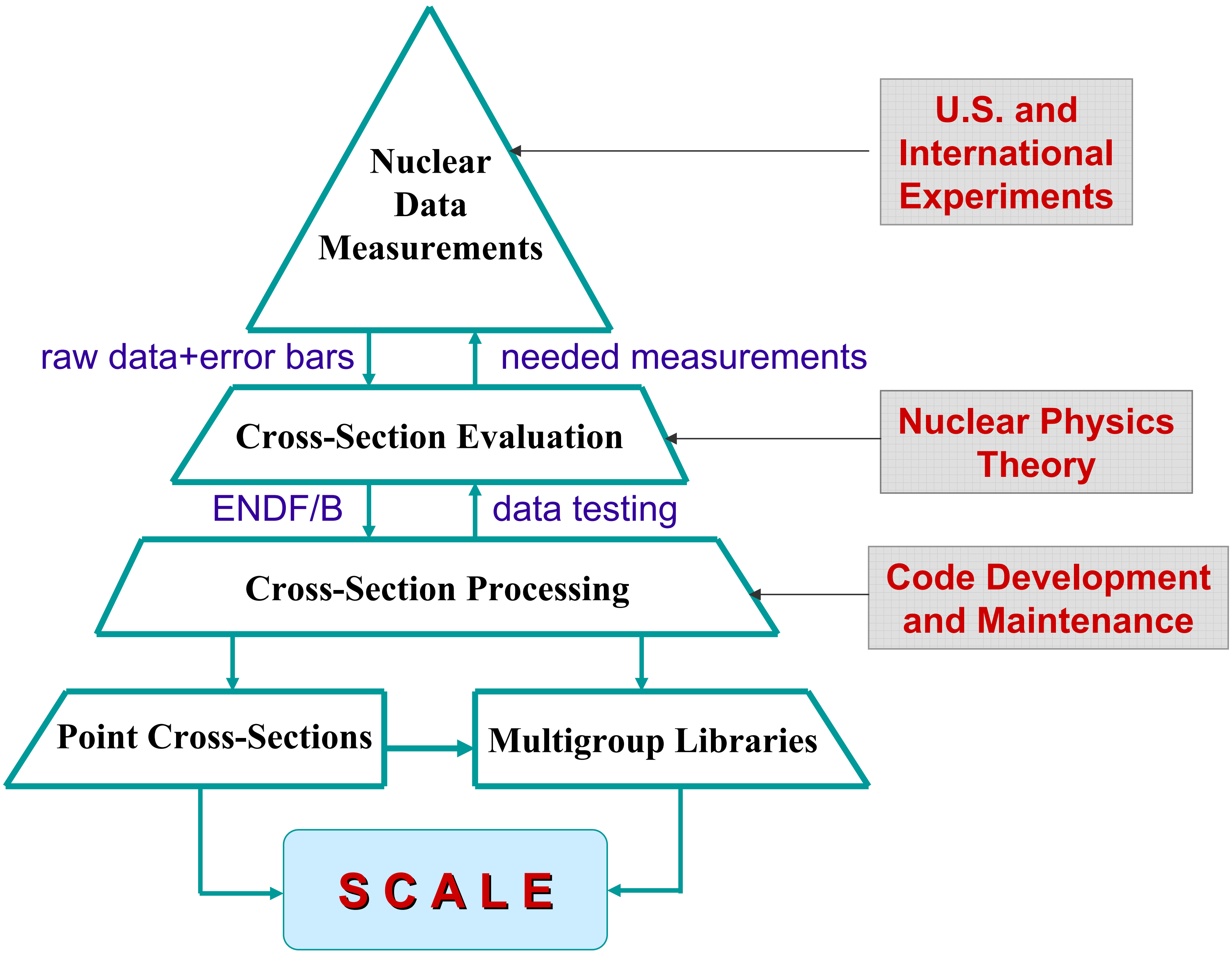
final state of nucleus

H and O Cross Sections

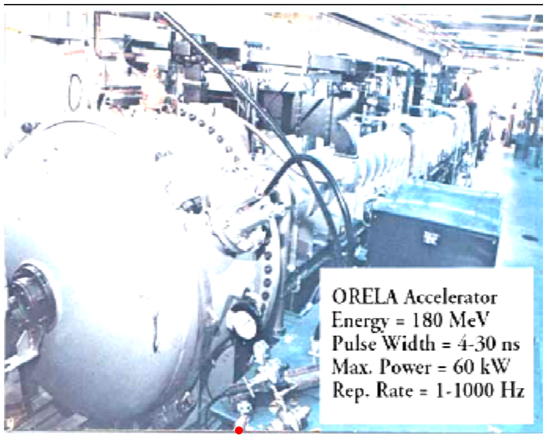


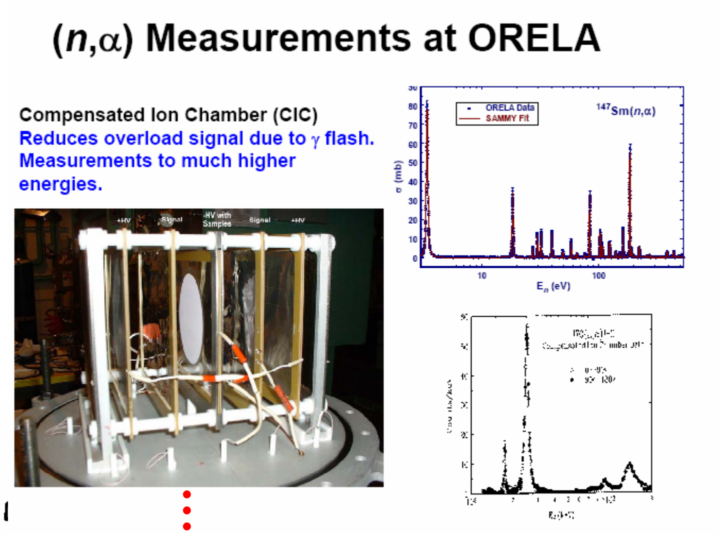
U-235 Fission Cross Section

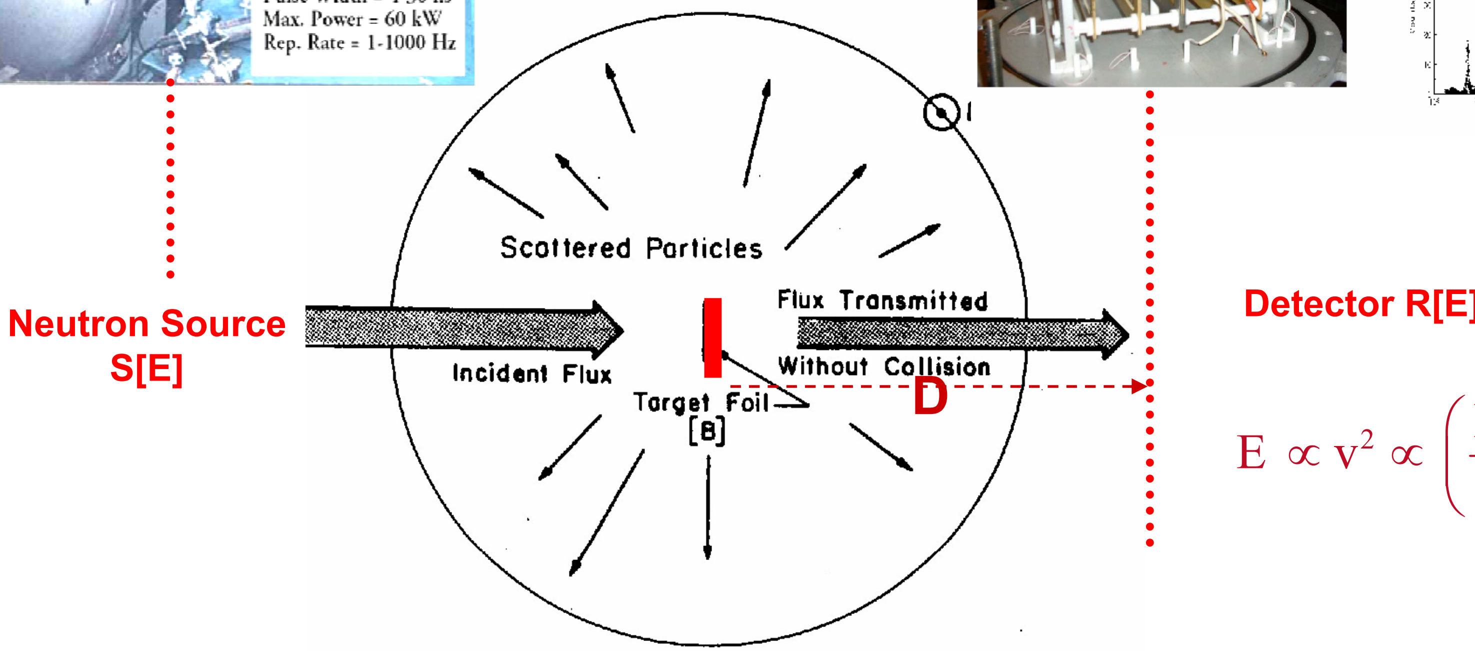



Nuclear Data Measurements
U.S. and International Experiments
raw data+error bars
needed measurements
Cross-Section Evaluation
Nuclear Physics Theory
ENDF/B
data testing
Cross-Section Processing
Code Development and Maintenance
Point Cross-Sections
Multigroup Libraries
SCALE

Experimental Measurements are Performed to Obtain XS Parameters







$$E \propto v^2 \propto \left(\frac{D}{t}\right)^2$$

Nuclear Physics Theory for Describing Resonance Reactions

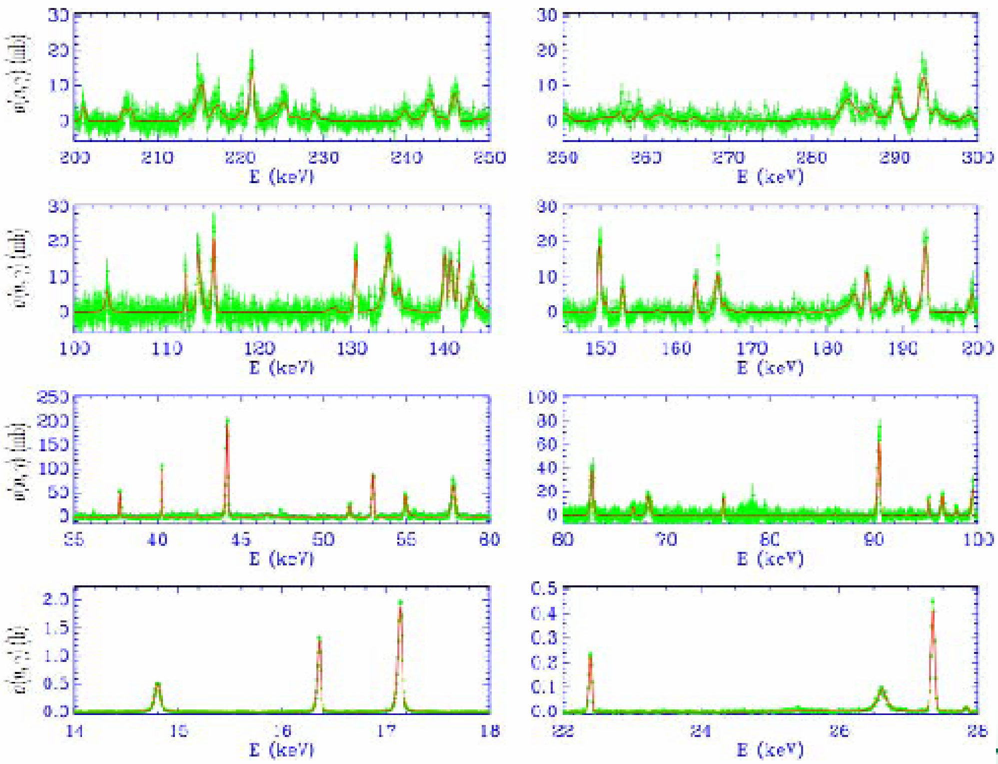
- General expression for σ vs. E can be derived from quantum mechanics: "***R-Matrix Theory***"
- "Resonance formalisms" are simpler approximations derived from general R-matrix theory:
  - **Single Level Breit Wigner (*SLBW*)**

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

  - **Multilevel Breit Wigner (*MLBW*); Reich-Moore (*RM*)**
- Resonance parameters E_r, Γ_γ , Γ_n , etc.. appearing in the expressions are found by fitting experimental measurements of XS's

Evaluators utilize measurements and nuclear models to determine best estimate for XS

Comparison of SAMMY Fits with ORELA ^{nat}Cl capture data



Evaluated database ENDF

NNDC BROOKHAVEN NATIONAL LABORATORY

Evaluated Nuclear Data File

- ENDF/B-VI.8, released in Oct 2001
- ENDF/B-VII, under development, release ~ Dec 2005

ORNL Evaluations in ENDF

	ENDF/B-VI.8	ENDF/B-VII
Total Evals	329 materials	340 materials
ORNL Evals	77 materials Structural materials Many FPs 11 actinides	< 75 materials Structural materials FPs likely replaced 12 actinides ($^{233,235,238}U$, …) 8 new covariances

Types of ENDF/B Data

File	Description	File	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

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 are available:**

AMPX-2000 (ORNL) and _NJOY_ (LANL)

- **Producing a library for radiation transport**
  - **_Pointwise_ and/or _multigroup_ libraries may be needed**
  - **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(α,β) data for thermal moderators**
    - **Perform multigroup averaging**

Multigroup (MG) Cross Section (XS) = *flux*-weighted average of XS data for a group

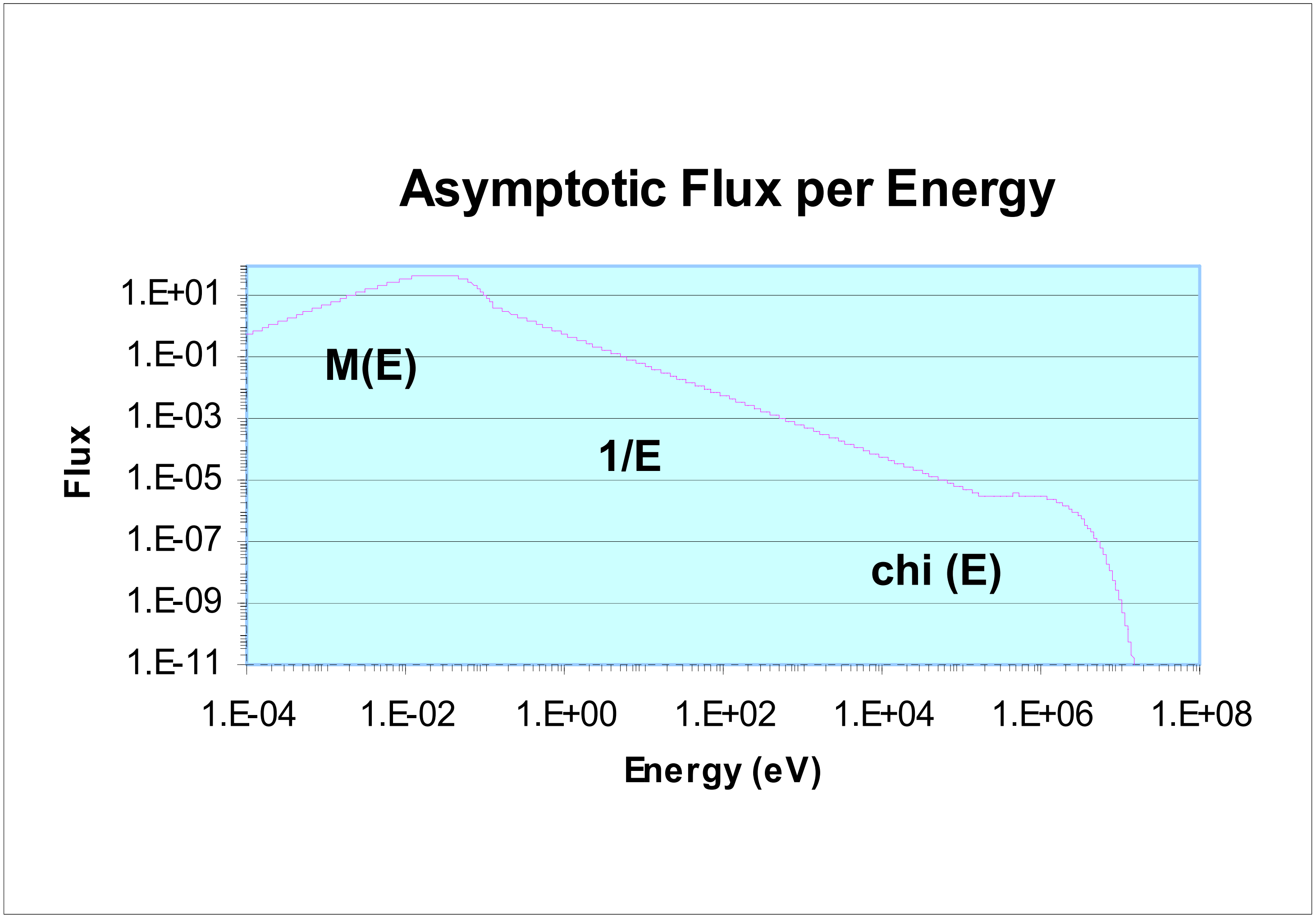
$$\sigma_g \equiv \frac{\left(R_g / N\right)}{\Phi_g} \approx \frac{\left\langle \phi(E)\,\sigma(E) \right\rangle_g}{\left\langle \phi(E) \right\rangle_g}$$

< > means integration over energy group g

- **σ(E)** = energy dependent XS from ENDF/B
- **Φ(E)** = weight-function that approximates the neutron energy spectrum in system

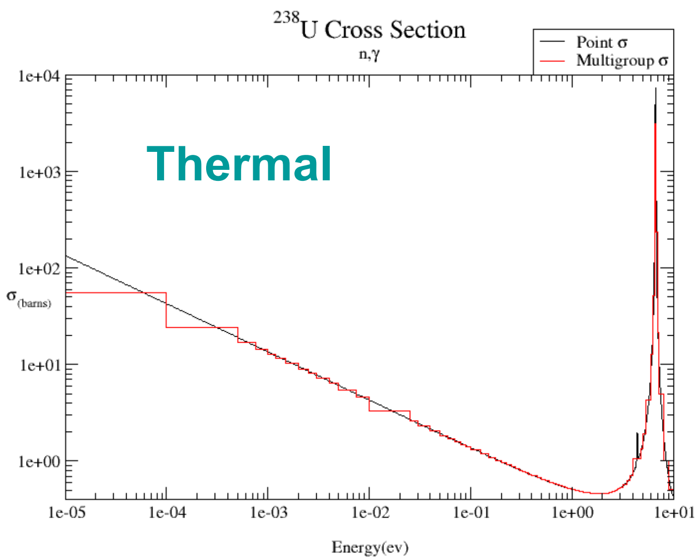
You must know the detailed answer [Φ(E)] to get the approximate answer [Φ_g] ??!

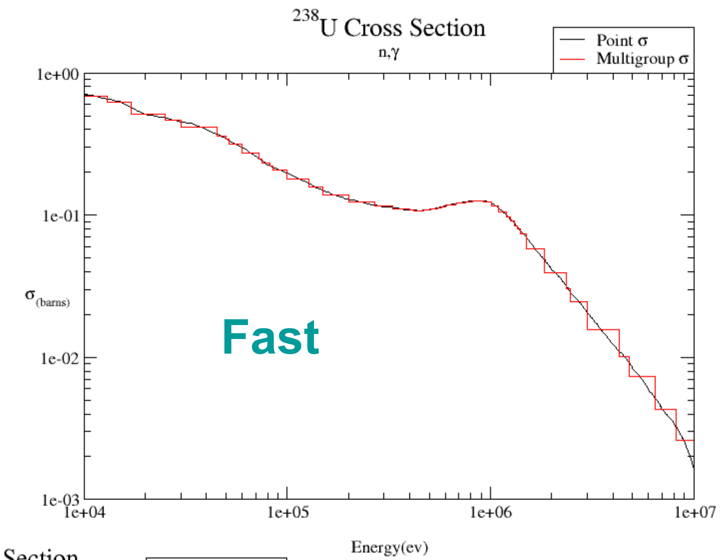
"Generic" Neutron Spectrum: Fission Source in a Moderator *(Infinitely Dilute Resonance Absorbers)*

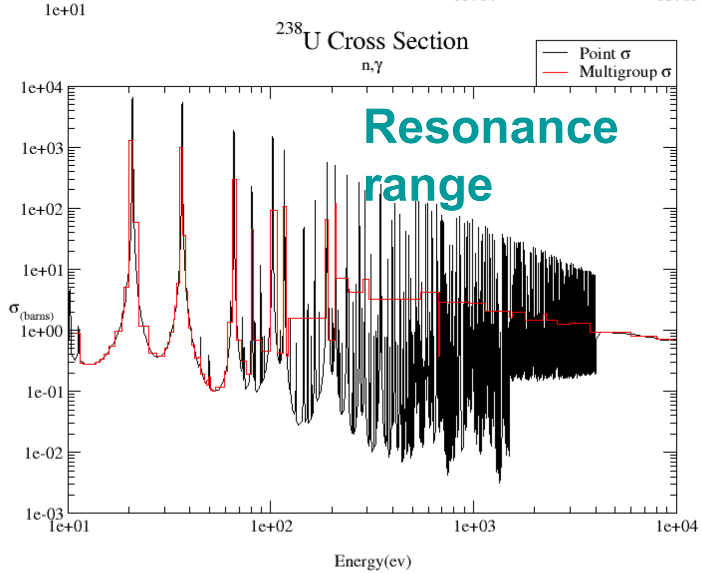


SCALE problem-independent multigroup libraries are based on generic spectrum

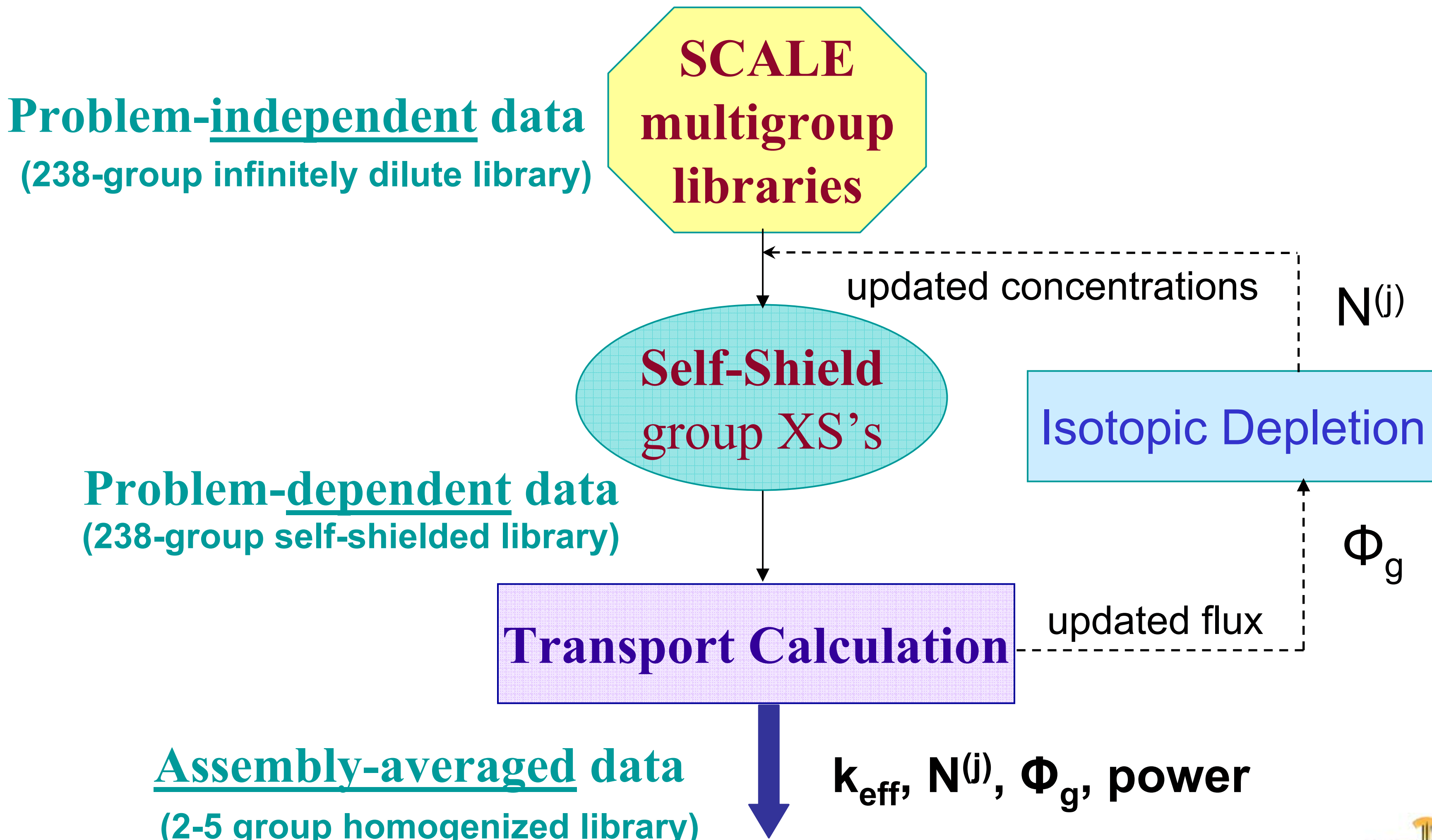
Infinitely-dilute 238-group vs PW XS's



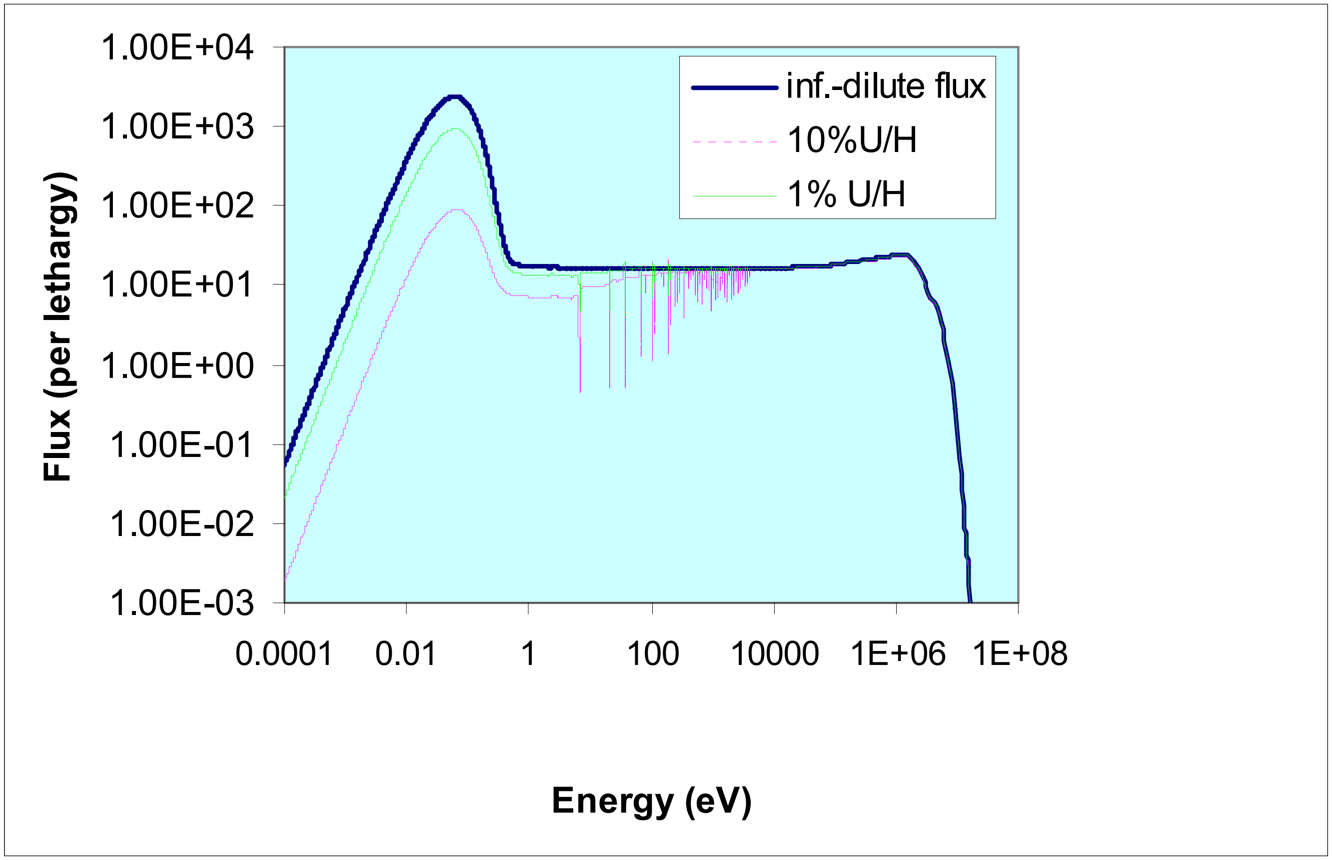




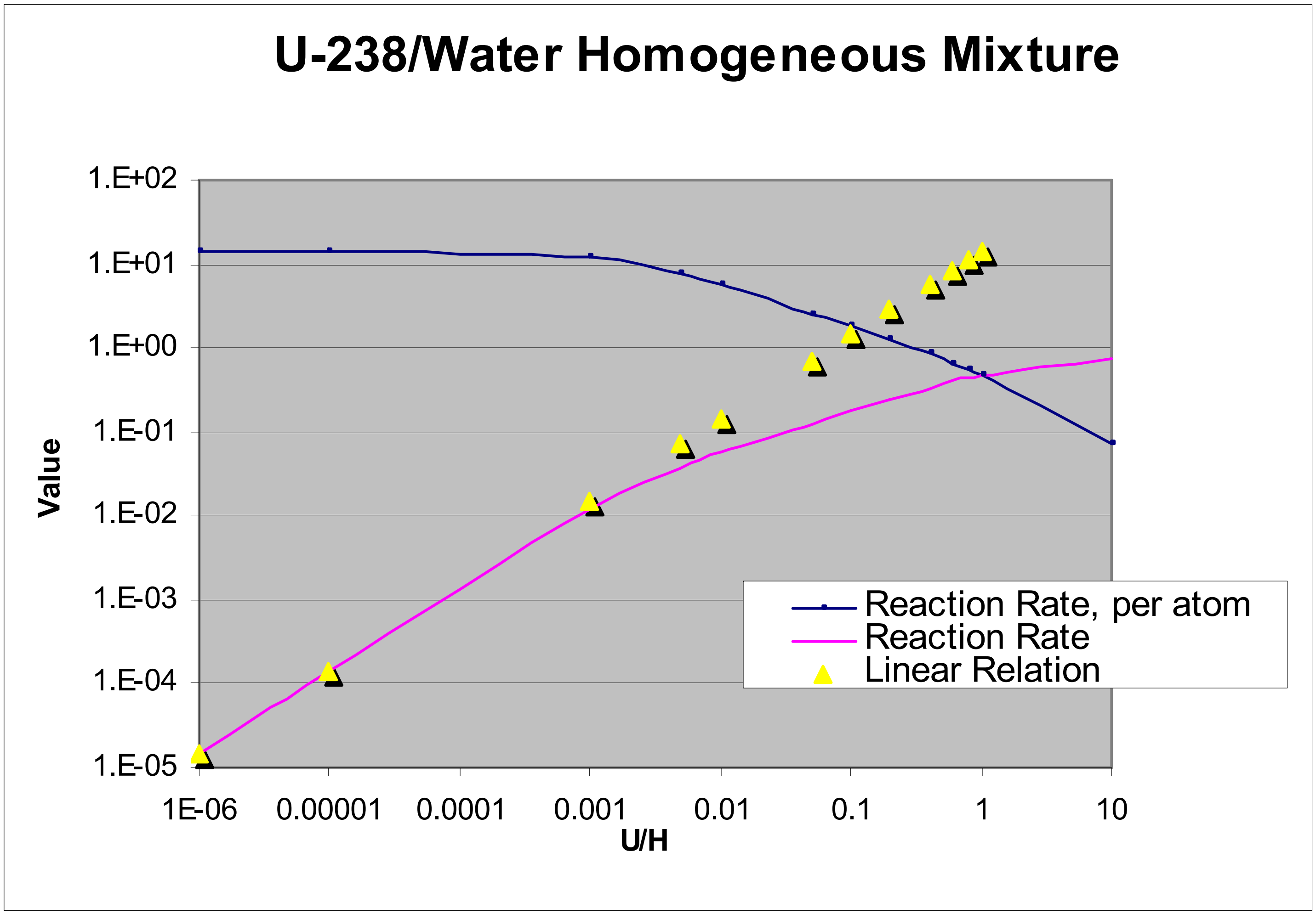
Major Components in Typical SCALE Calculation Sequence



Impact of Resonance Absorption on Neutron Spectrum



"Self-shielding" decreases reaction rate per atom→ σ_g decreases as concentration increases



Major Factors Impacting Resonance Self-Shielding in Heterogeneous Systems

- **Concentration of absorbers (N_r) + admixed moderators (Σ_m) => i.e., dilution**
- **Composition of external moderators (Σ_{M^*})**
- **Dimension/shape of absorber lumps (eg, *fuel radius*)**
- **Arrangement of lumps (eg, *pitch*)**

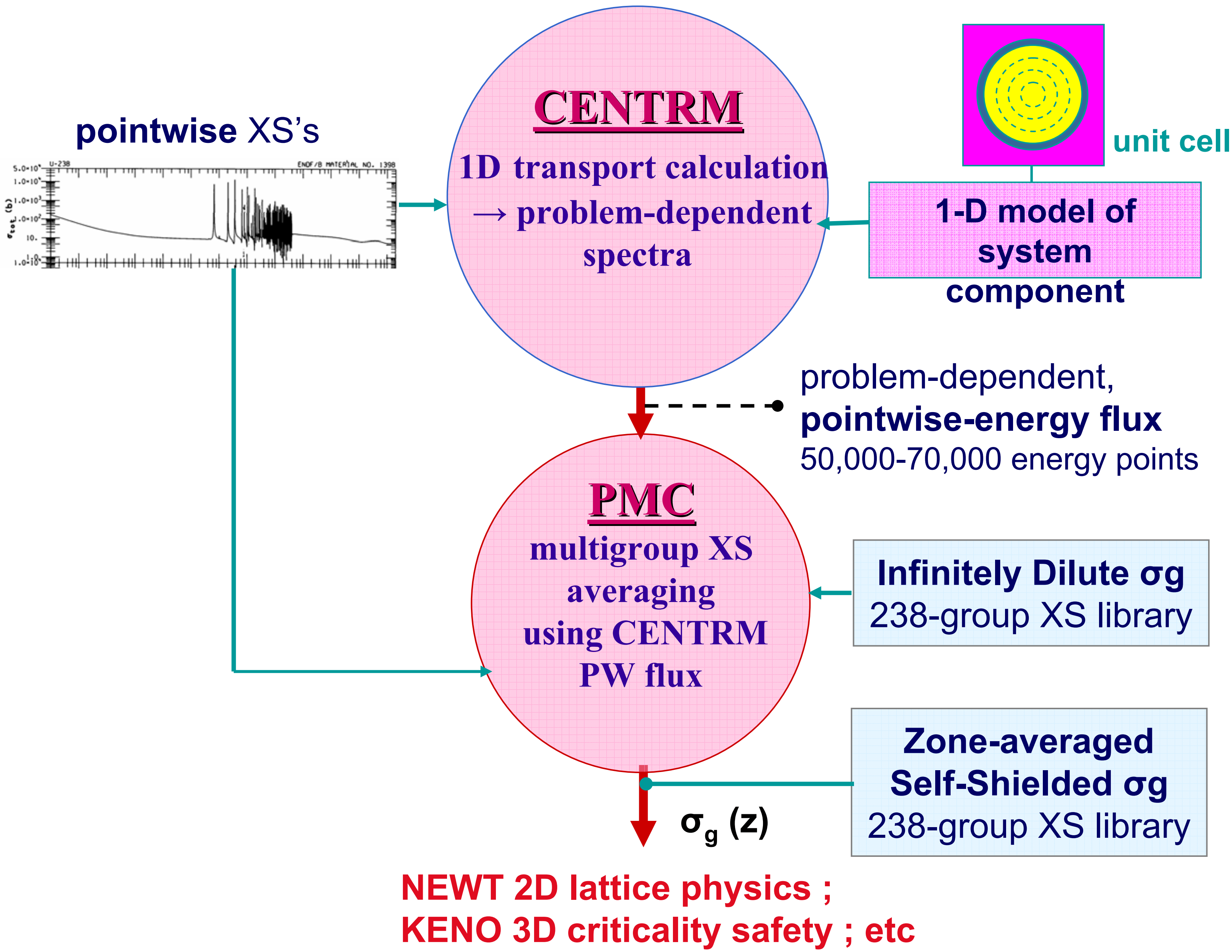
$$\sigma_g = \sigma_g(N_r , \Sigma_m, \Sigma_{M^*}, \text{lump size, pitch, etc… })$$

Self-Shielding Methods in SCALE

- **Bondarenko Method (*BONAMI*)**
  - Most approximate method; very fast
  - Only used for unresolved resonance range in SCALE

- **Nordheim 2-Region Integral Treatment (*NITAWL*)**
  - Significantly better than Bondarenko for most applications, but still has modeling restrictions.
  - Is default method in resolved range for SCALE4.0/5.0

- **Continuous Energy,1-D Sn (*CENTRM/PMC*)**
  - Most rigorous model in both energy and geometry effects
  - Becomes default method for SCALE 5.1

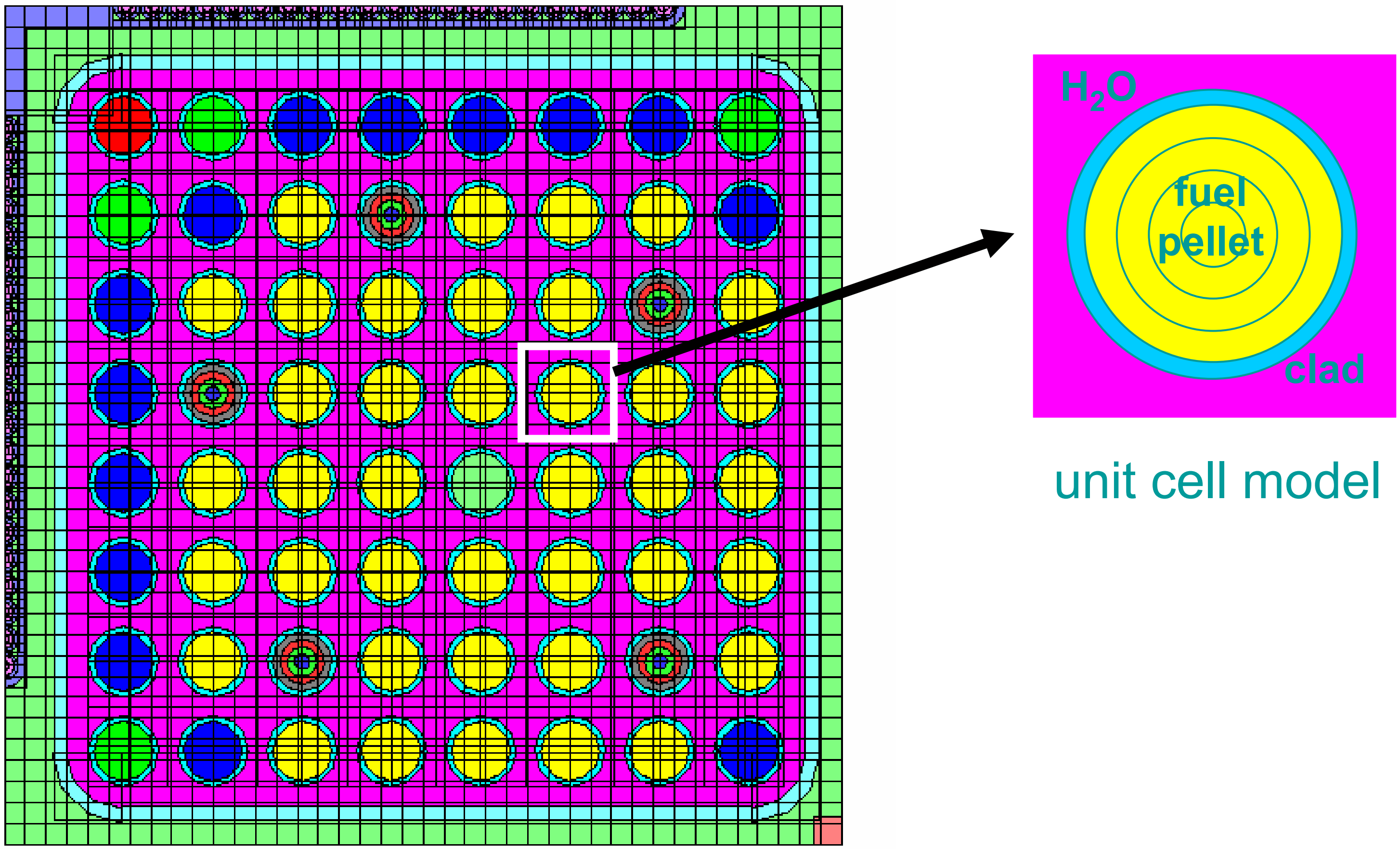

pointwise XS's
CENTRM
1D transport calculation
→ problem-dependent
spectra
unit cell
1-D model of
system
component
problem-dependent,
pointwise-energy flux
50,000-70,000 energy points
PMC
multigroup XS
averaging
using CENTRM
PW flux
Infinitely Dilute σg
238-group XS library
Zone-averaged
Self-Shielded σg
238-group XS library
σg (z)
NEWT 2D lattice physics ;
KENO 3D criticality safety ; etc

Self-Shielded XS's are Input to SCALE Multigroup Transport Codes

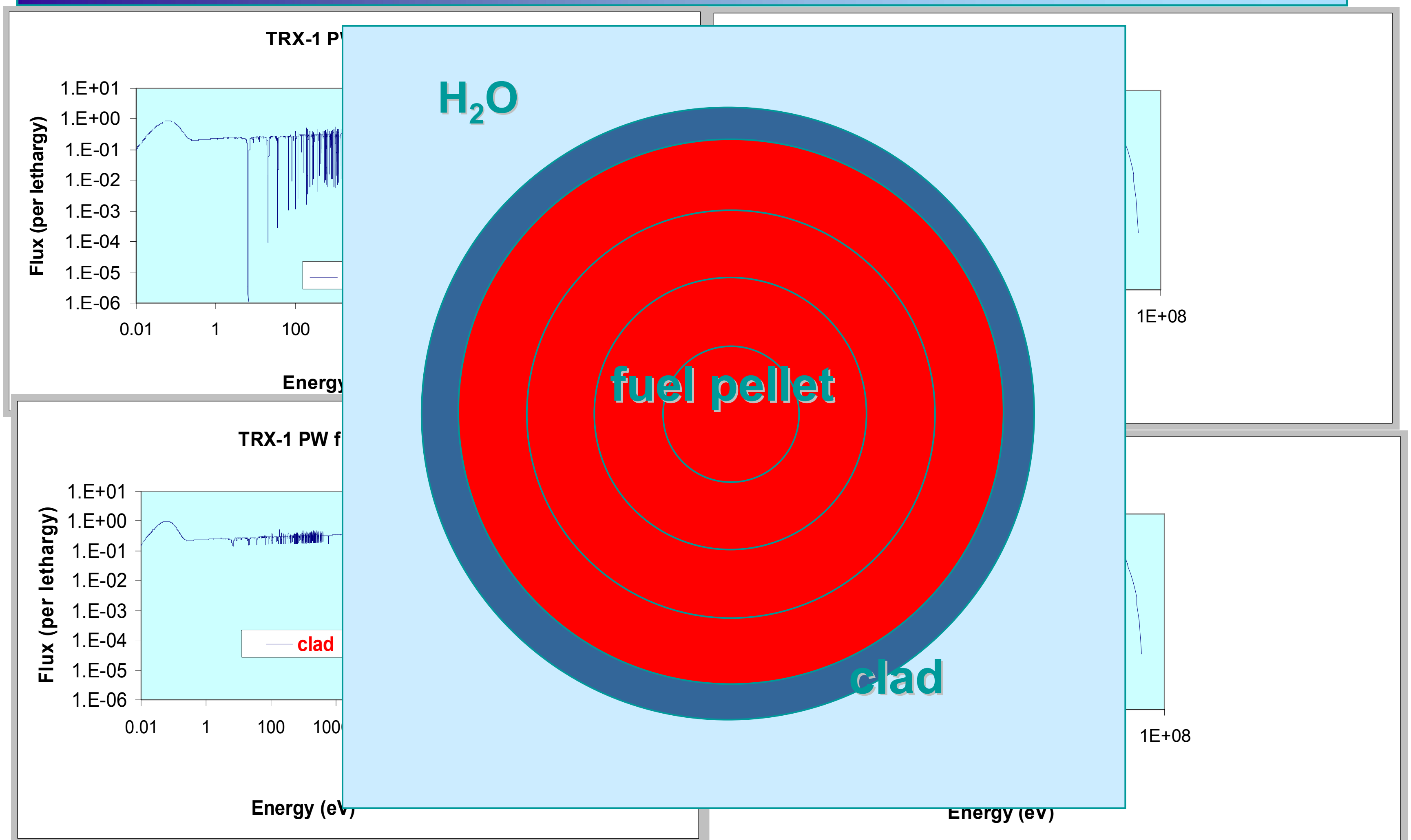
- **XSDRNPM:** 1D S_N
- **DORT/TORT:** 2D/3D S_N for shielding
- **KENO:** Monte Carlo for criticality
- **MONACO:** Monte Carlo for shielding

- **NEWT:** 2D S_N for lattice physics

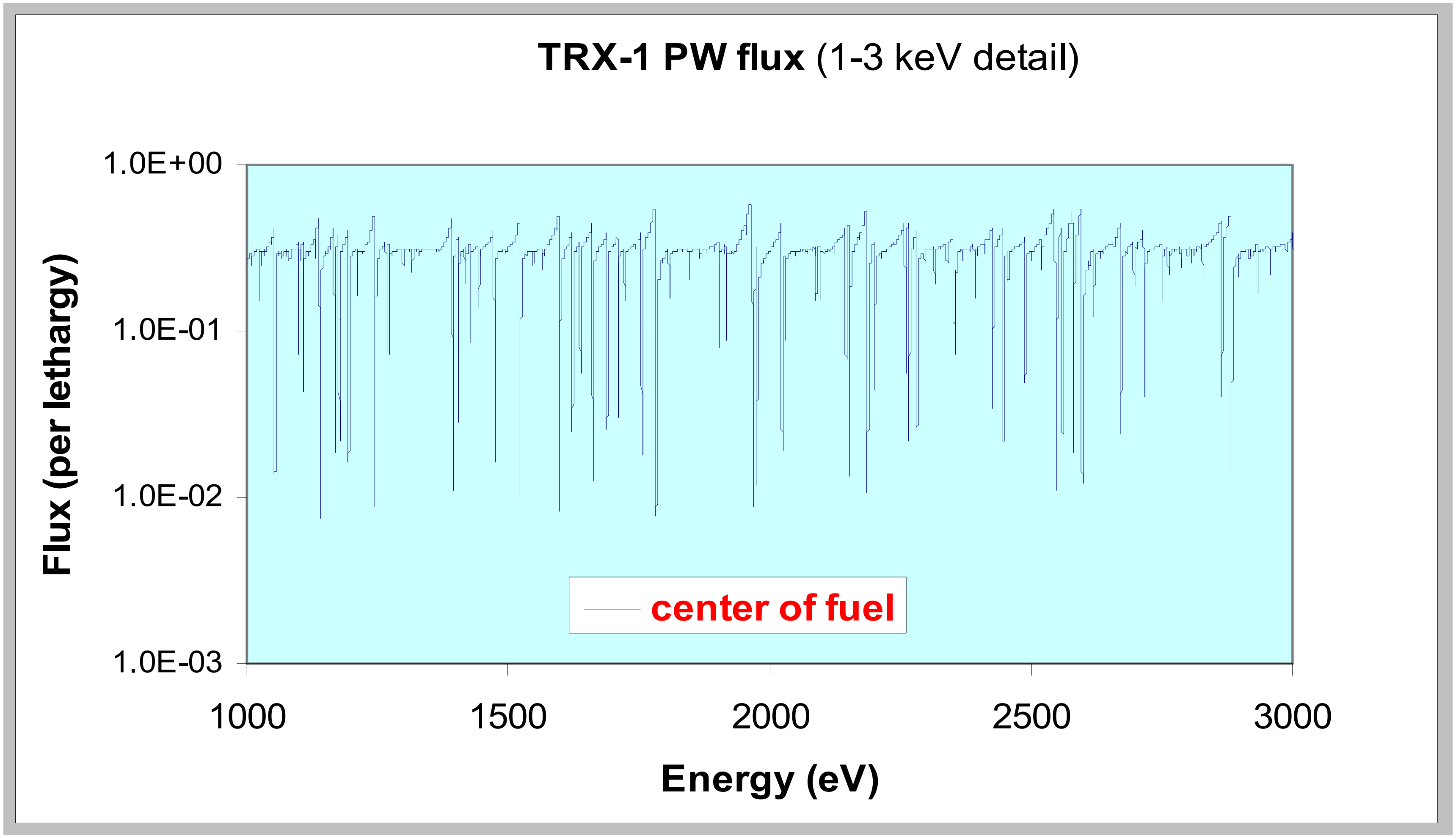
NEWT 2D Lattice Physics Model of BWR Bundle



LWR Unit Cell Spectra



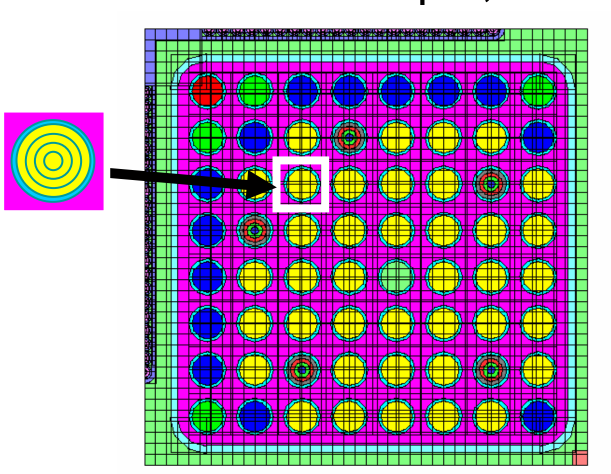
LWR Spectrum: Fine-Structure Detail



Flux Solution from 2D Newt Calculation Can Be Used For:

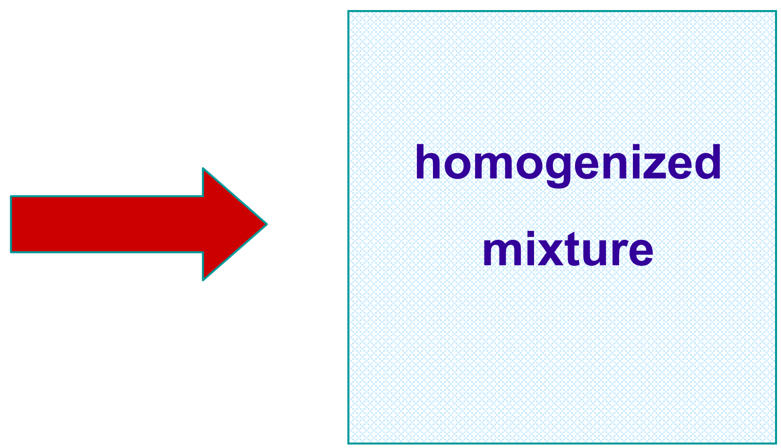
- **Spatial Averaging of XS (homogenization)**
- **Reduction in number of energy groups (collapsing)**

238-group zone-averaged XS
for each fuel pin, etc



NEWT Heterogeneous Model

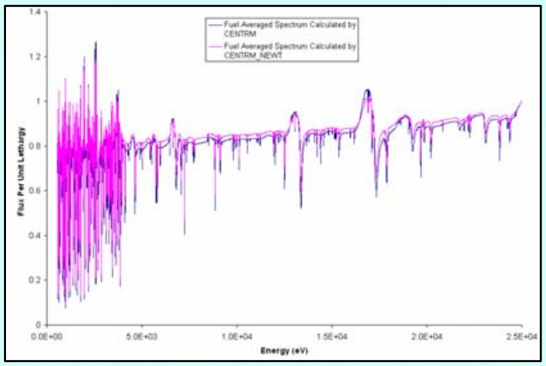
2-5 group bundle-averaged XS
for homogenized mixture



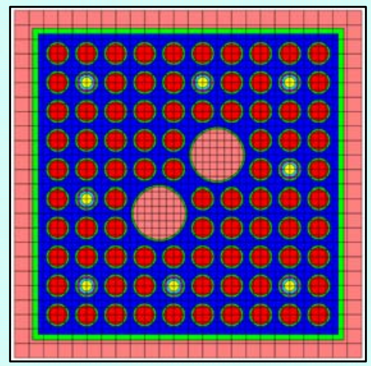
Homogeneous Model for Nodal

TRITON Lattice Physics Sequence

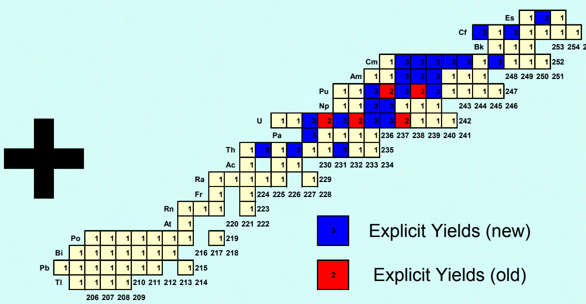
- **CENTRM: 1-D continuous energy resonance processing**
- **NEWT: 2-D flexible mesh discrete ordinates transport**
- **ORIGEN-S: detailed isotopic compositions**



+



+



CENTRM
Continuous-Energy Spectrum

NEWT
2-D General-Geometry Deterministic Transport

ORIGEN-S
Isotopic Distribution ~1600 nuclides

TRITON

Nuclear Data Summary