

Introduction into cross section functionalization

ORNL is managed by UT-Battelle, LLC for the US Department of Energy



U.S. DEPARTMENT OF
ENERGY

Overview

- Diffusion Equation & Coefficients
- Cross Sections
- Practical use of the lattice calculation
- How cross sections can be used
- Comparison of XS interpolation schemes
- PMAXS, as a compromise

<https://www.ornl.gov/scale/training>

Coupled Neutron / Nuclide and Temperature/ Fluid Field Equations

- Neutron transport equation (Boltzmann)

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \Omega \cdot \nabla \phi(r, E, \Omega, t) + \Sigma_t(r, E) \phi(r, E, \Omega, t) = \frac{1}{4\pi} S_f(r, E, t) + \int \int_{\Omega' E'} \Sigma_s(r, E' \rightarrow E, \Omega' \rightarrow \Omega) \phi(r, E', \Omega', t) dE' d\Omega'$$

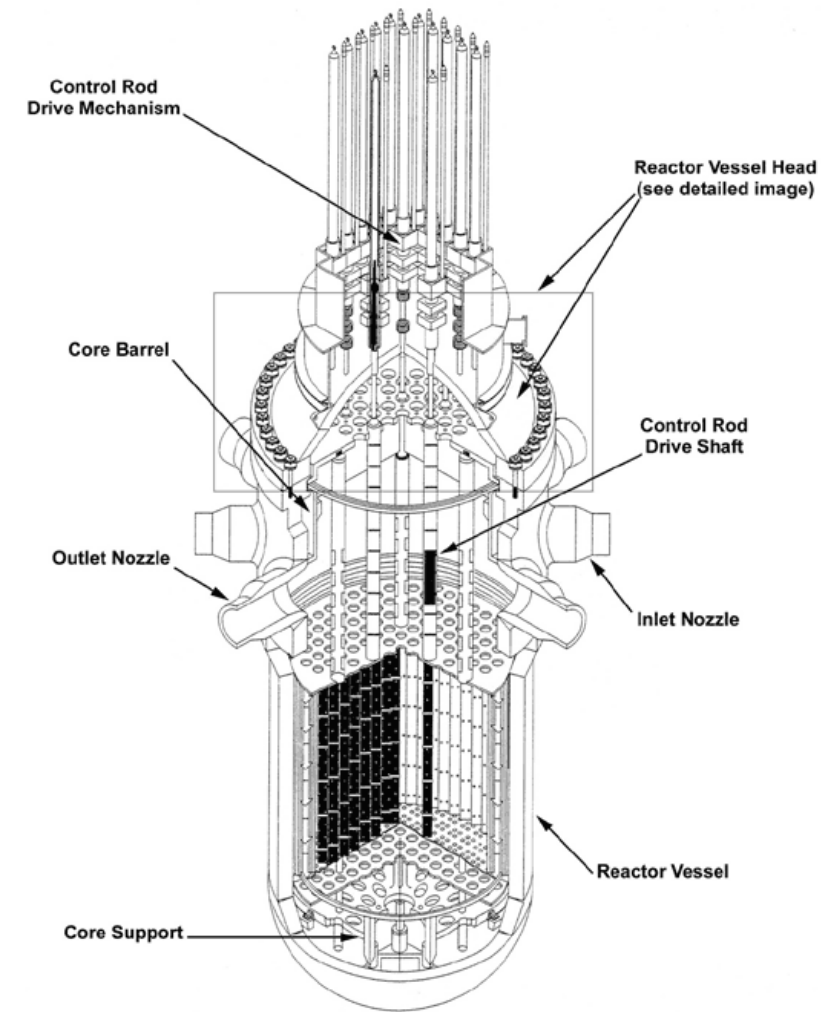
- Multigroup Neutron Diffusion Equation

$$\nabla \cdot \vec{J}_g(\vec{r}, E) + \Sigma_{rg} \phi_g(\vec{r}, E) = \lambda \chi_g \sum_{g'=1}^G \nu \Sigma_{fg'} \phi_{g'}(\vec{r}, E) + \sum_{g'=1}^G \Sigma_{sg'g} \phi_{g'}(\vec{r}, E)$$

- Nuclide depletion equation (Bateman)

$$\frac{dN_i}{dt} = \sum_{j=1}^m l_{ij} \lambda_j N_j + \bar{\Phi} \sum_{k=1}^m f_{ik} \sigma_k N_k - (\lambda_i + \bar{\Phi} \sigma_i) N_i \quad (i = 1, \dots, m)$$

Typical Pressurized Water Reactor



<https://www.nrc.gov/reactors/operating/ops-experience/vessel-head-degradation/vessel-head-degradation-files/pwr-rx-vessel.html>

Cross Sections, which ones we need

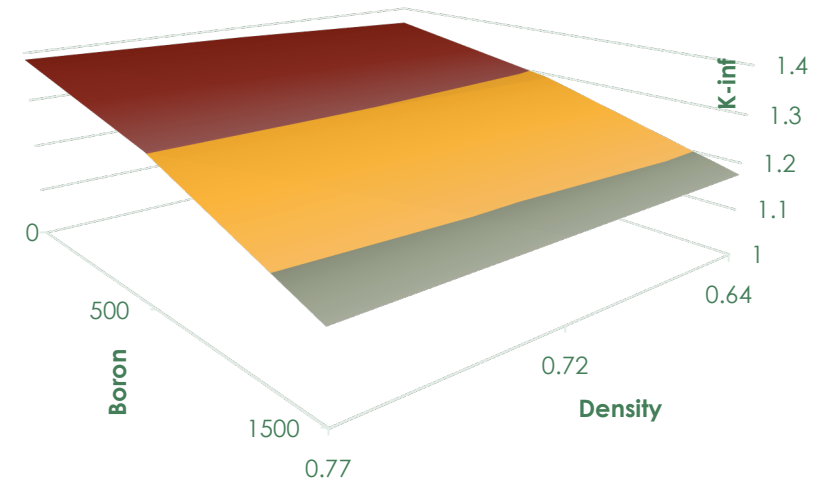
- Primary XS used in diffusion, normally 2 groups (thermal & fast)
 - Absorption, Nu-Fission, Kappa-Fission
 - Transport (Diffusion)
 - Scattering Matrix
- Secondary XS-like data
 - Assembly Discontinuity Factors
- Kinetics Data
 - Beta, Lambda, Neutron Velocity

Cross Section Dependence

- Macro cross sections

$$\Sigma = \sigma N$$

- Sigma depends on Temperature
 - Water and Fuel
- N varies with material density
 - Water density
 - With depletion, direct effect as well
- How to functionalize the cross section against the underlying physical variables?



Discussion of XS Models

- Linear Cross Section Interpolation + Fixup (H₂O Density)
 - PARCS Native XS Model
- Multi-dimensional Table (Piece-Wise Linear Interpolation Model)
 - Format for many numerical benchmarks, PBTT, MSLB
- Higher Order Non-Linear Interpolation
 - Multiple tables
 - PMAXS System

Original PARCS “Native” XS Model: Partial Derivatives

$$\begin{aligned}\Sigma(\alpha, T_f, T_m, D_m, S_b) = & \Sigma^r + \alpha \Delta \Sigma^{cr} + \frac{\partial \Sigma}{\partial \sqrt{T_f}} \Delta \sqrt{T_f} + \frac{\partial \Sigma}{\partial T_m} \Delta T_m \\ & + \frac{\partial \Sigma}{\partial S_b} \Delta S_b + \frac{\partial \Sigma}{\partial D_m} \Delta D_m + \frac{\partial^2 \Sigma}{\partial D_m^2} (\Delta D_m)^2\end{aligned}$$

Σ^r : XS at unrodded reference state

$\Delta \Sigma^{cr}$: Control rod XS;

α : rodded fraction;

T_f : Fuel temperature;
temperature

T_m : moderator

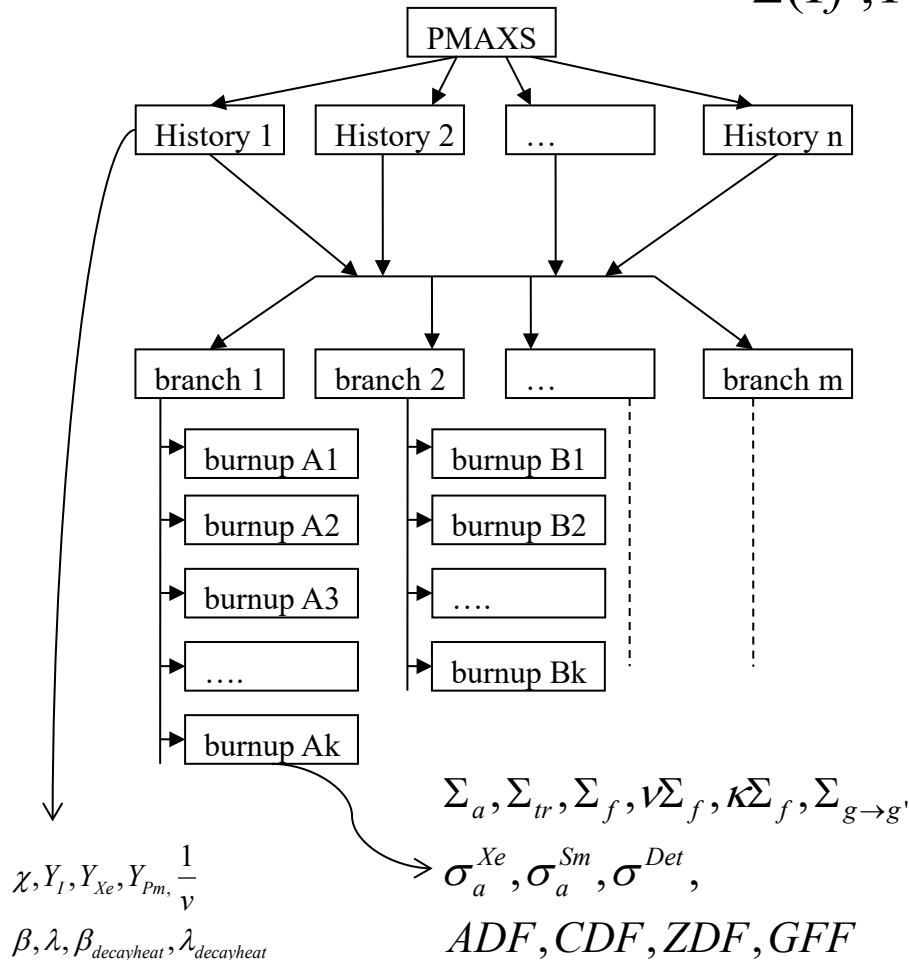
S_b : Soluble Boron Concentration; D_m : moderator Density

- Most data points can be contained: 7
 - 1 reference state
 - 2 moderator branches
 - 1 branches for each of other variables: Cr, Tf, Tm, Sb

Multi-Dimensional Piece-Wise Linear Interpolation (NEMTAB)

$$\Sigma(Tf, Tm, Dm, Sb, \alpha) = (1 - \alpha)\Sigma^{unrod}(Tf, Tm, Dm, Sb) + \alpha\Sigma^{roded}(Tf, Tm, Dm, Sb)$$

$$\begin{aligned}\Sigma^i(Tf, Tm, Dm, Sb) &= \frac{Tf - Tf^b}{Tf^a - Tf^b} \Sigma^i(Tf^a, Tm, Dm, Sb) \\ &+ \frac{Tf^a - Tf}{Tf^a - Tf^b} \Sigma^i(Tf^b, Tm, Dm, Sb) \\ &+ \dots\end{aligned}$$



```
* NEM-Cross Section Table Input
*
*   T Fuel      Rho Mod.   Boron ppm.   T Mod.
*       5         6         0         0
*
*****      X-Section set #      1
1
*
*   Group No. 1
*
*****      Diffusion Coefficient Table
*
.5000000E+03 .7602200E+03 .8672700E+03 .9218800E+03 .1500000E+04
.6413994E+03 .7114275E+03 .7694675E+03 .7724436E+03 .7813064E+03
.8100986E+03 .1467049E+01 .1469641E+01 .1470751E+01 .1471347E+01
.1477128E+01 .1401975E+01 .1404351E+01 .1405441E+01 .1405939E+01
.1411216E+01 .1353822E+01 .1356107E+01 .1357086E+01 .1357581E+01
.1362596E+01 .1352366E+01 .1354638E+01 .1355630E+01 .1356125E+01
.1361236E+01 .1345620E+01 .1347891E+01 .1348843E+01 .1349338E+01
.1354390E+01 .1322122E+01 .1324319E+01 .1325308E+01 .1325803E+01
.1330615E+01
*
*****      Total Absorption X-Section Table
```

Comparison of Models

- The Partial derivatives model is most efficient, but not as accurate
 - It is only first order for variables other than moderator density, and no cross-term effect between variables.
 - No way to treat history information or burnup
- Multi-dimensional table less efficient, but more accurate
 - Piece-wise linear interpolation is more accurate than global linear approximation.
 - It contains also cross-term effect between variables and can also be extended for history information.
- Multiple tables is a compromise between the partial derivatives model and multi-dimensional tables in efficiency and accuracy. It gains the efficiency by ignoring some cross-terms

Conclusions

- Where does PMAXS fit into these schemes?
- Goals of PMAXS: Balance accuracy and speed
 - Utilize partial derivatives
 - No constraint on underlying physics
 - Flexibility for multiple branches / cross terms
 - Straightforward treatment for burnup and history
- Interpolation order can be changed for reactor type
 - LWR, SFR, HTR
 - Use TC for PWR cases and use DC for BWR cases (2024)

Acknowledgments

This presentation was primarily authored by Andrew Ward from the University of Michigan, with contributions from ORNL staff.