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Processing and Utilization of Nuclear Reaction Data for Advanced Gas Cooled Reactor (AGCR) Applications

Ivanov K.

IAEA
Vienna
AUSTRIA

PENNSTATE
Department of Mechanical and Nuclear Engineering
Reactor Dynamics and Fuel Management Group

Processing and Utilization of Nuclear Reaction Data for Advanced Gas Cooled Reactor (AGCR) Applications

Lecture 3 – Analysis and Uncertainties

K. Ivanov, F. Puente-Espel

The Pennsylvania State University

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OUTLINE

- Introduction
  - Overview of the NJOY code
- Reference Monte Carlo analysis
  - Continuous energy cross-section generation
  - Thermal energy cross-section generation
  - Results of applying the generated cross-sections
- Few-group structures and reactor analysis
- Cross-section uncertainty propagation
- Conclusions

Overview of the NJOY Code

- ✓ The NJOY code is a nuclear data processing system which produces PointWise and GroupWise cross sections from the Evaluated Nuclear Data File (ENDF).

- ✓ The code converts the evaluated nuclear data into libraries useful for application calculations in nuclear engineering problems.

- ✓ The data is converted from the ENDF format to the PointWise Evaluated Nuclear Data File (PENDF) format and GroupWise Evaluated Nuclear Data File (GENDF) format.

Overview of the NJOY Code

- ✓ The ENDF data is freely obtainable from various source such as national laboratories and data banks. In this work, the ENDF data was downloaded from the Los Alamos National Laboratory website.

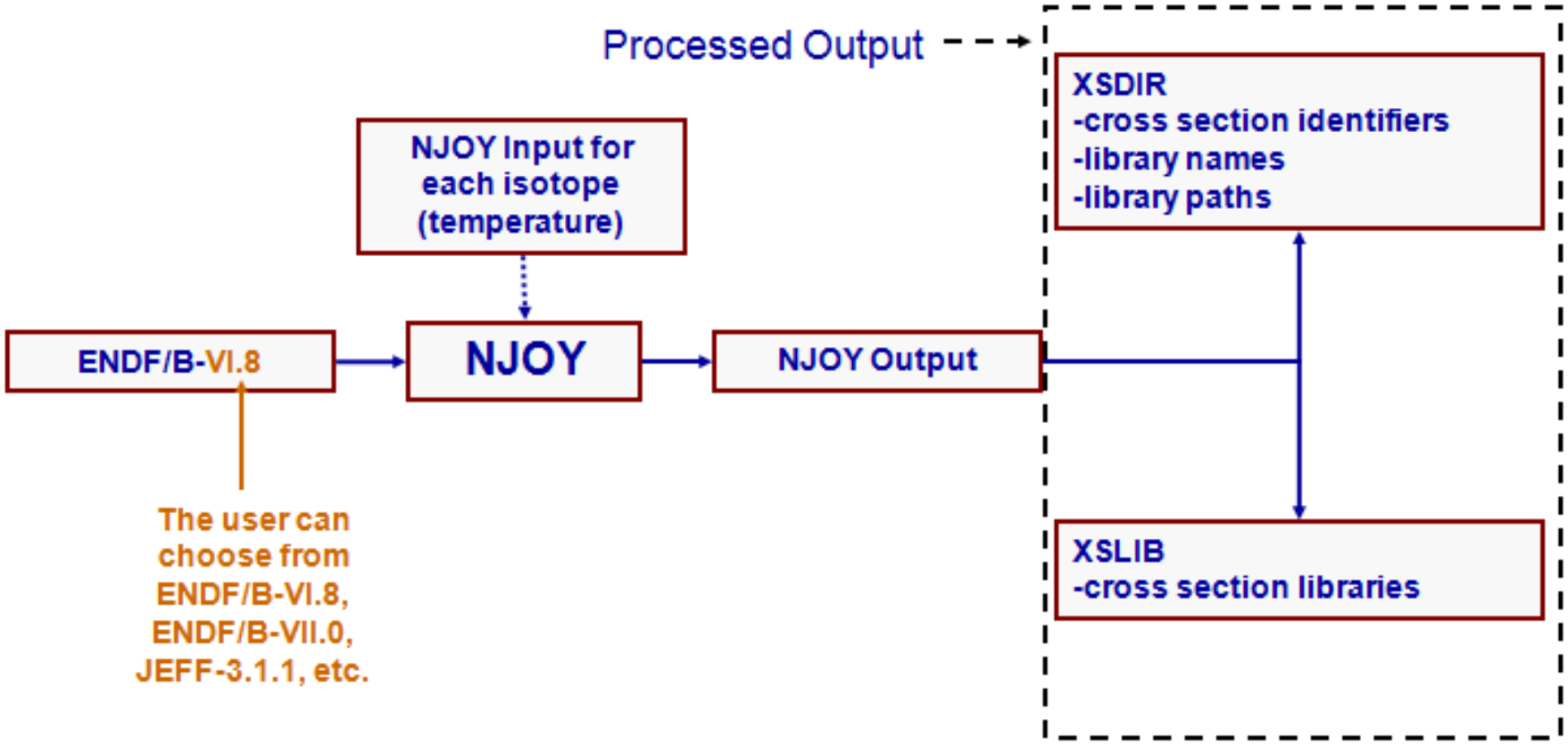
- ✓ The NJOY code consists of a number of modules. Each module operates as a separate computer program, processing a well-defined task.

- ✓ This feature makes it possible to choose only the modules that are relevant to a specific problem. The modules are linked by input and output files.

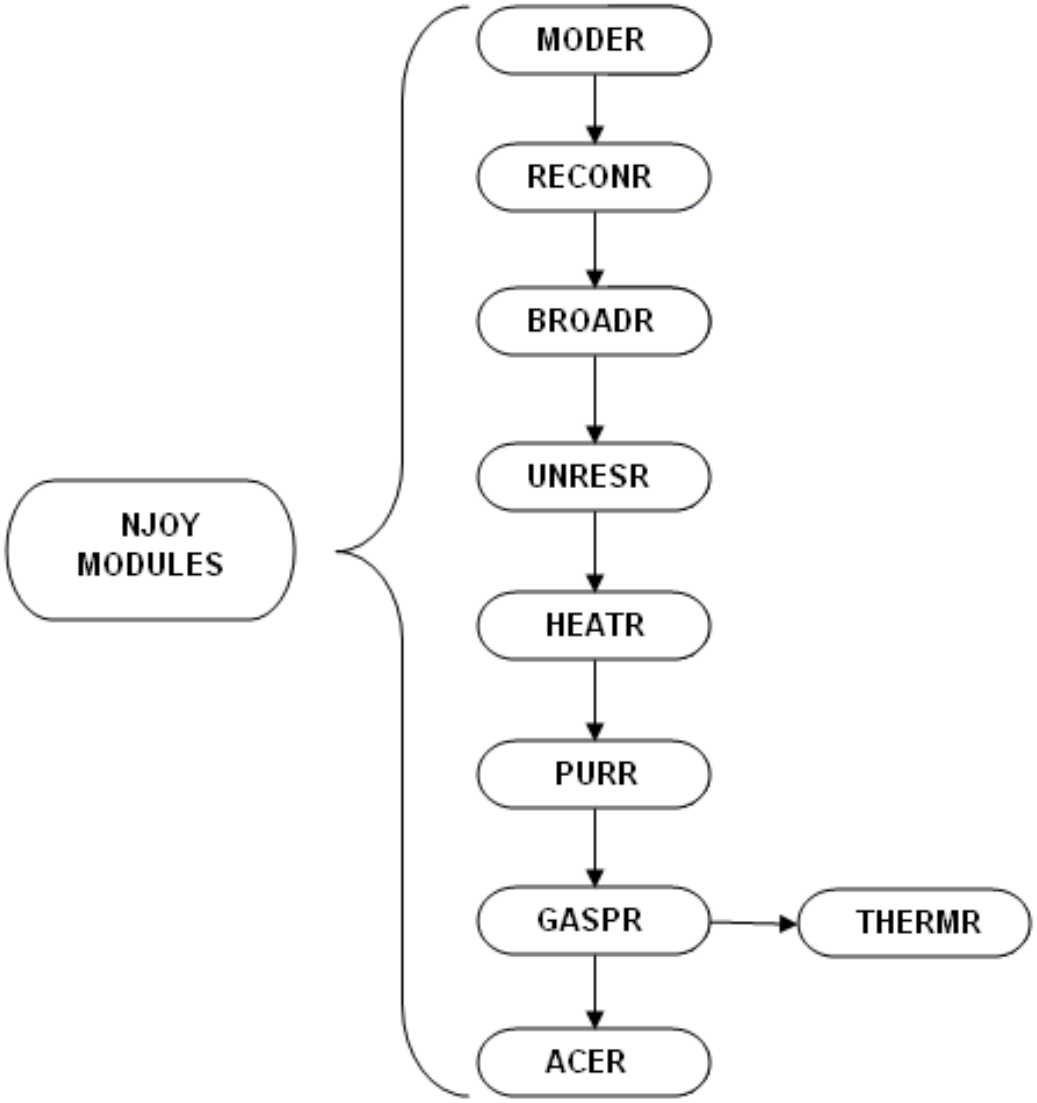
Continuous Energy Cross Sections Generation

Continuous XS

- The standard procedure for the generation of continuous energy cross-sections at different temperatures and using different evaluated nuclear date files is time-consuming and tedious.



Continuous XS



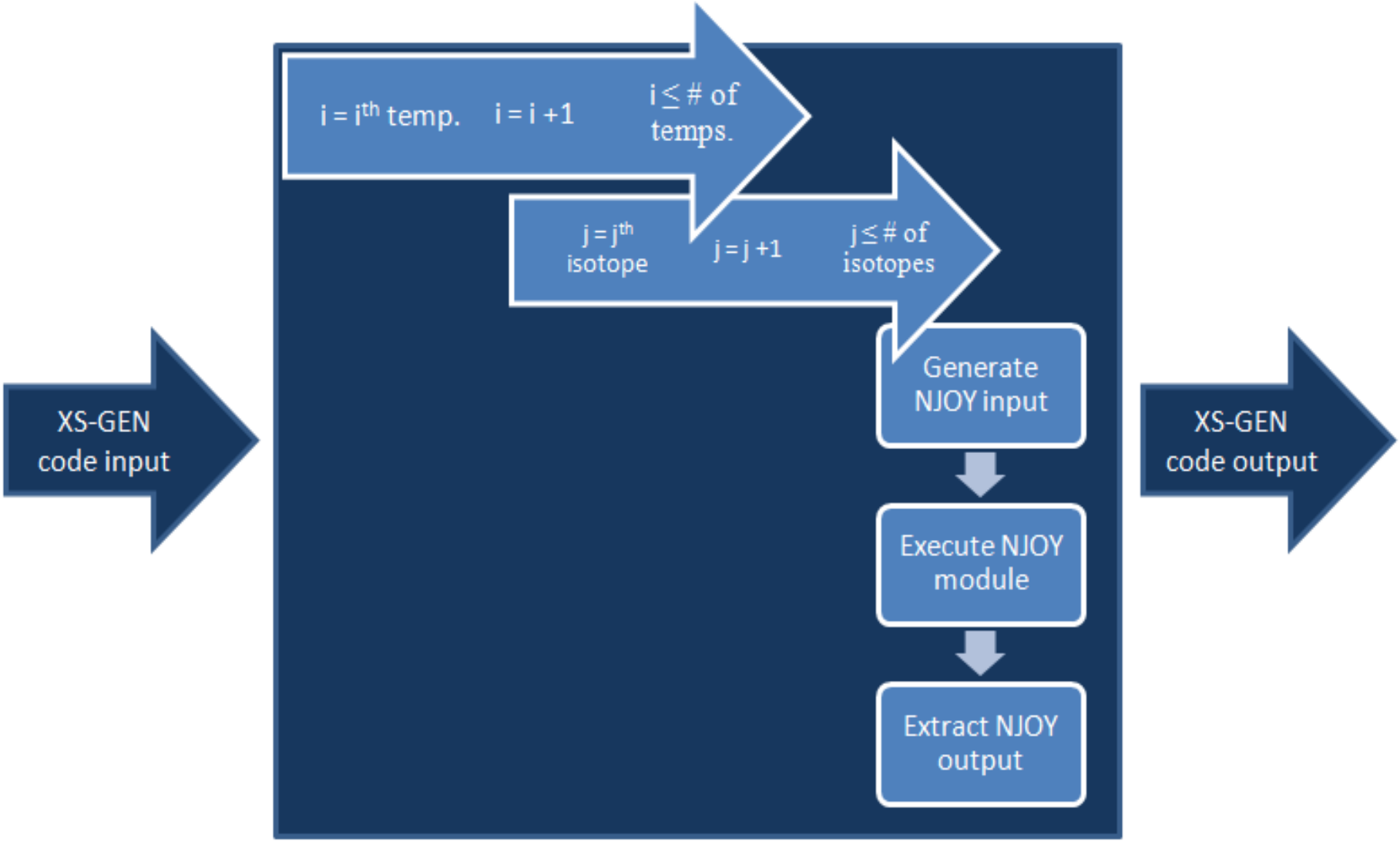
Continuous XS

- An automated tool for the generation of cross-section libraries was developed as part of the hybrid Monte Carlo-based coupled core calculations.

- The duration of the procedure has been significantly reduced. This automated tool performs the most time consuming tasks of the cross-sections generation process.

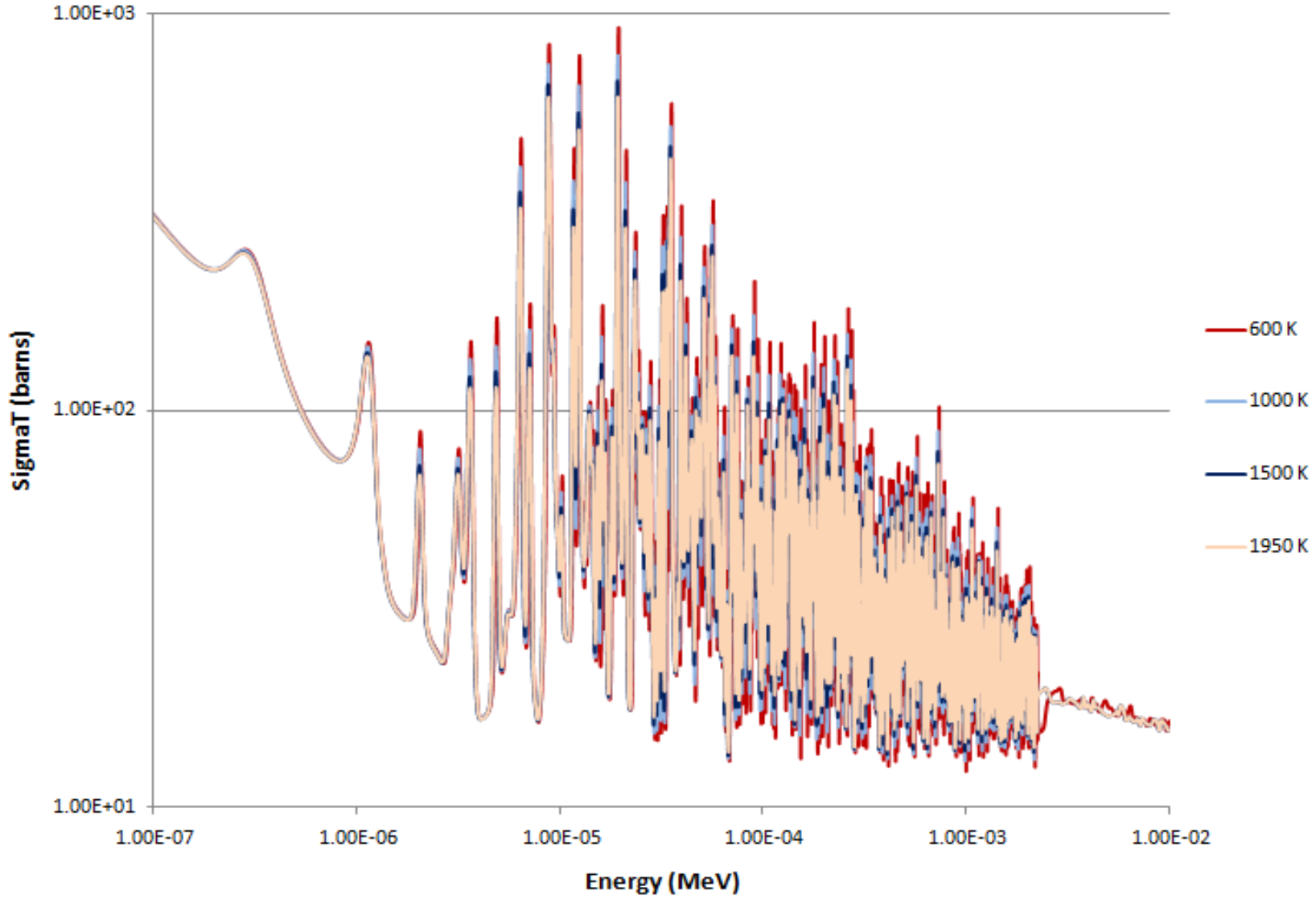
- This tool is used together with the automated cross-section temperature interpolation capability for intermediate points.

Continuous XS



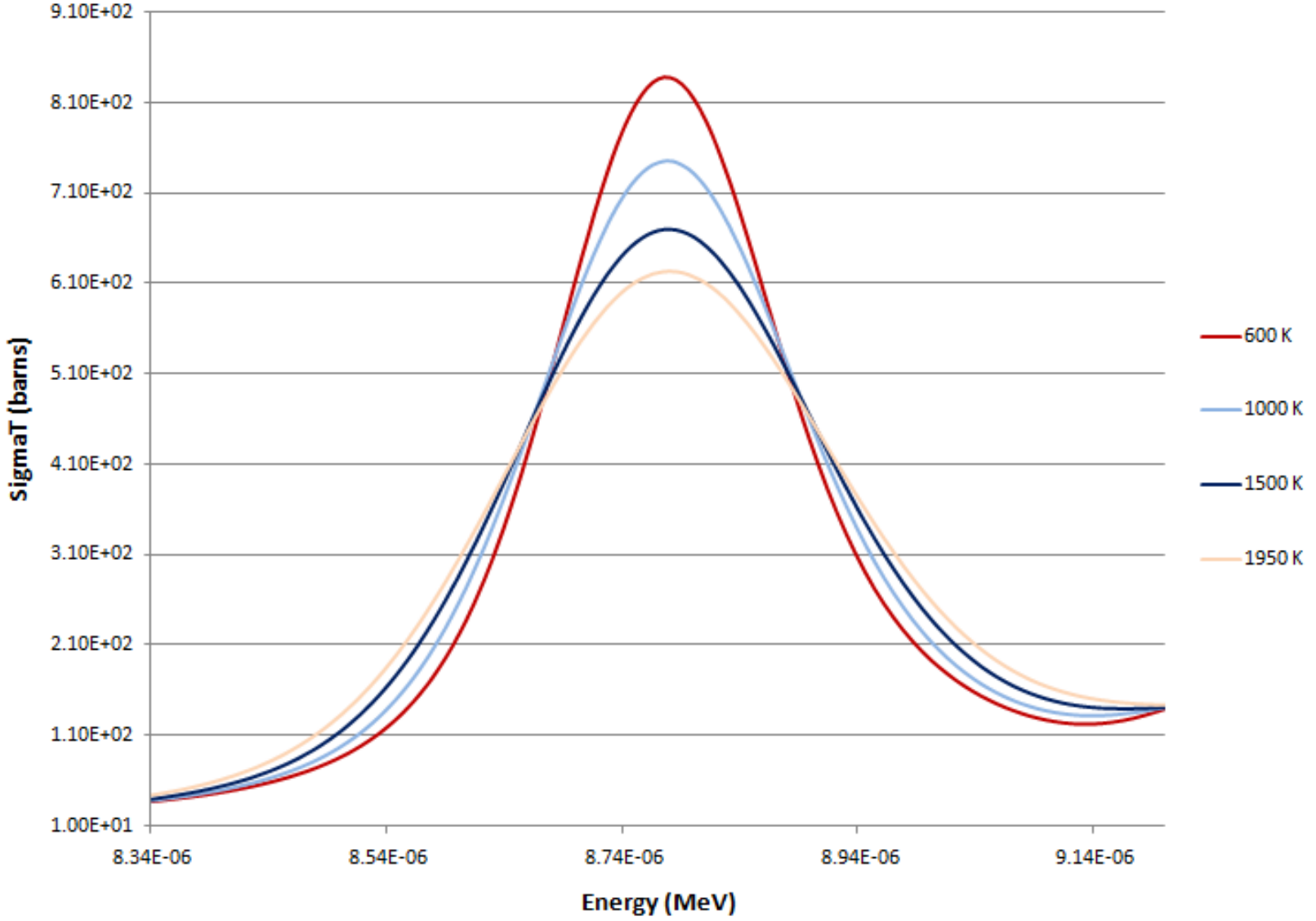
Continuous XS

- *Effect of temperature on the total cross section (SigmaT) of U-235*



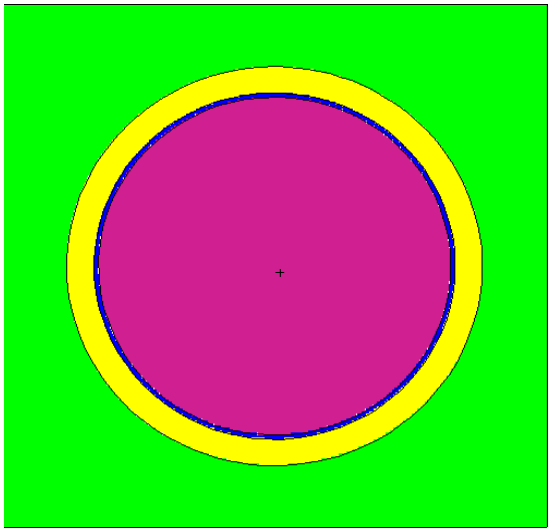
Continuous XS

- *Effect of temperature on the total cross section (SigmaT) of U-235*



Continuous XS

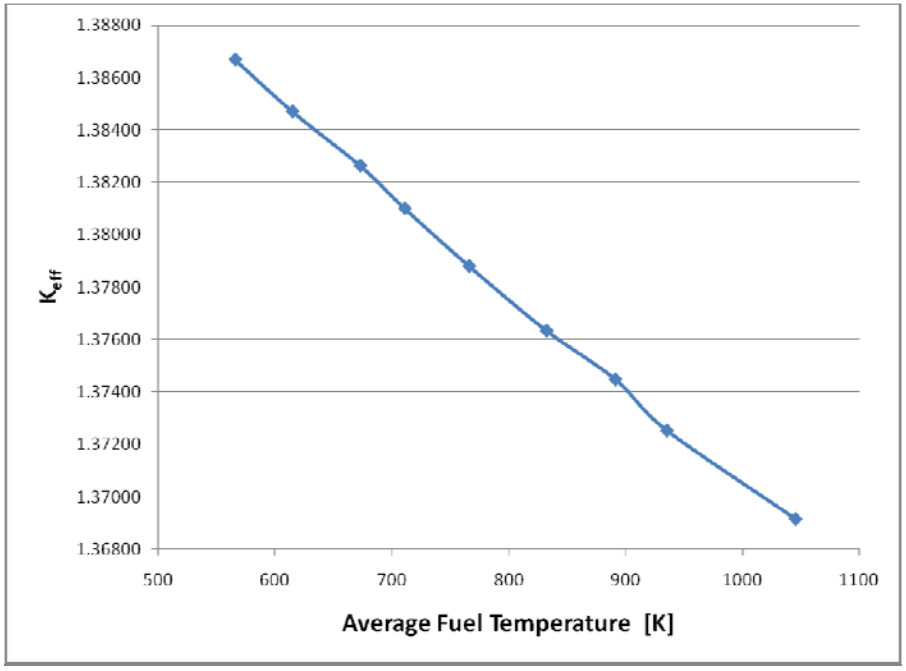
- ***MCNP5 k_{eff} results using different temperature-dependent cross section libraries***



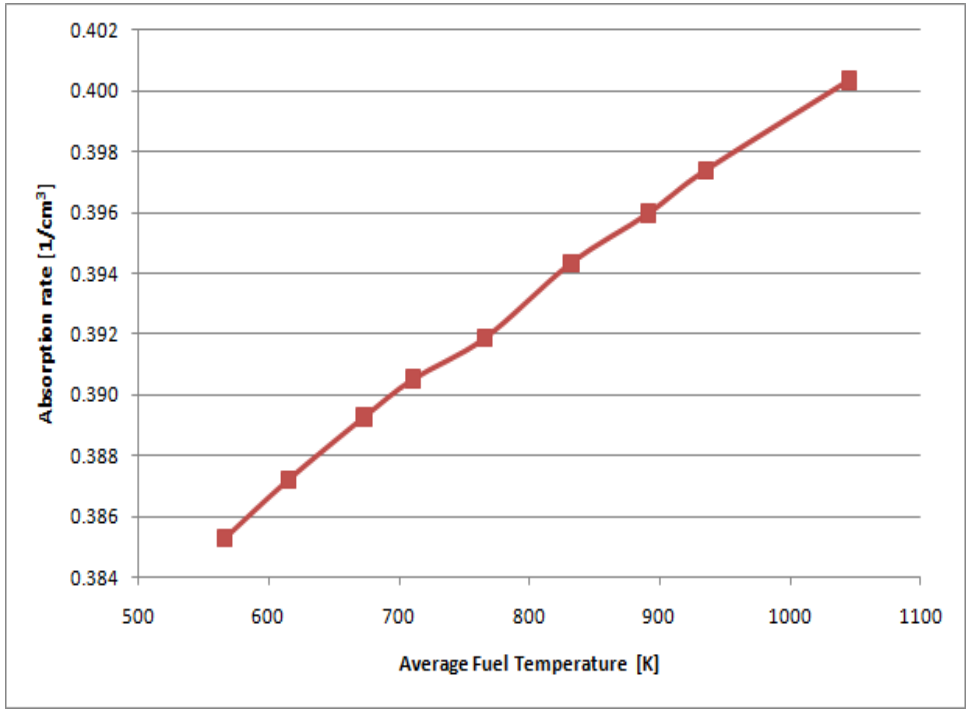
Temperature [K]	k_{eff}	Standard Deviation
566	1.38669	0.00026
615	1.38471	0.00026
673	1.38264	0.00025
711	1.38101	0.00025
766	1.37881	0.00025
832	1.37635	0.00025
891	1.37449	0.00026
935	1.37254	0.00026
1045	1.36916	0.00027

Continuous XS

- *K_{eff} of the pin cell model as a function of average fuel temperature*



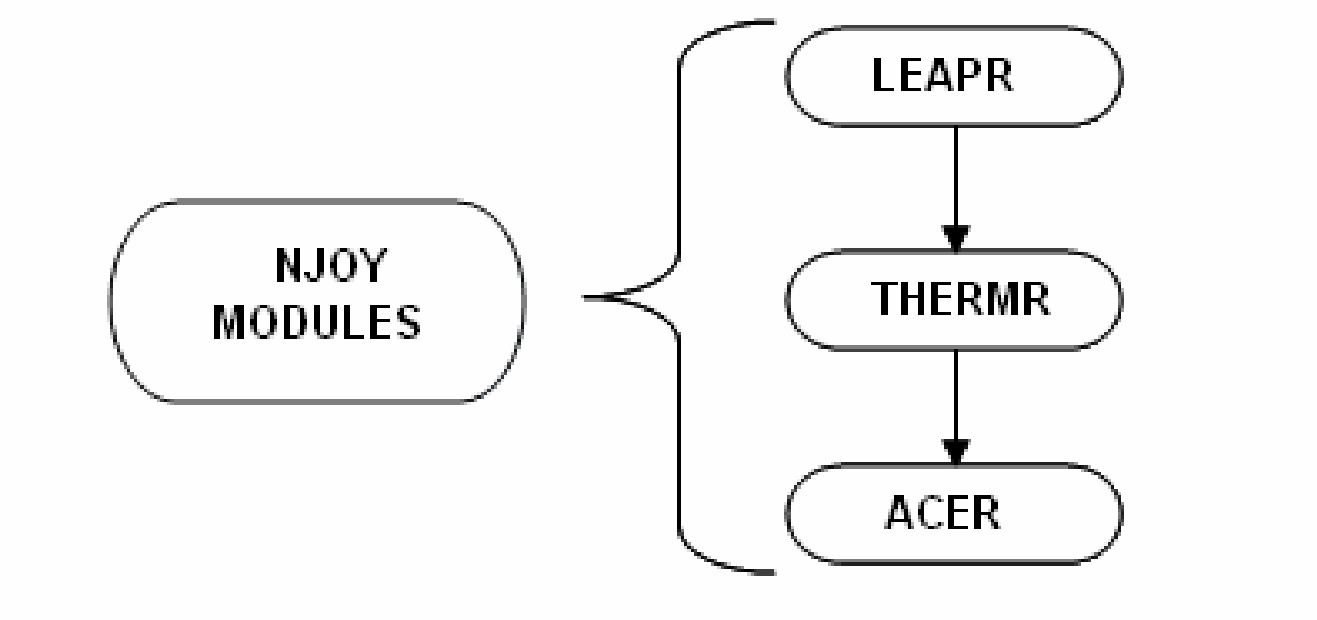
- *Absorption rate in the pin cell model as a function of temperature*



Thermal Scattering Cross Sections Generation

Thermal Scattering XS

- *NJOY modules for generation of thermal neutron scattering data*



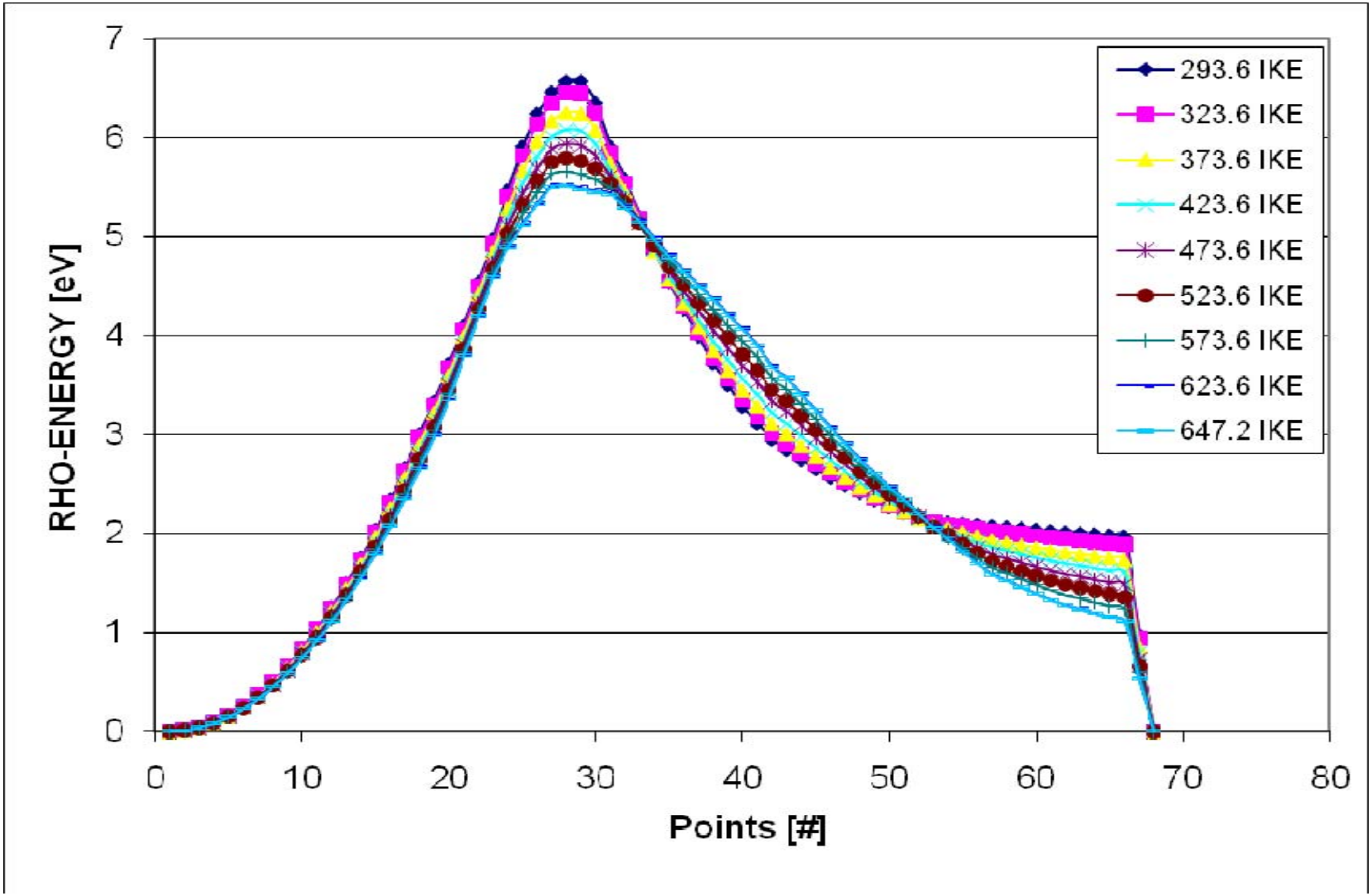
Thermal Scattering XS

The thermal neutron scattering cross section theory, contained in the LEAPR module, can be broadly divided into three different parts:

- ✓ **Inelastic**
  - ✓ **It is important for all materials, incoherent as well as coherent fall in this class and is described by the scattering law S(α,β).**
- ✓ **Incoherent elastic**
  - ✓ **It is important for hydrogenous solids. It depends on the sum of noninterfereing waves from all the particles of the system. Considering the properties of the materials, the scattering from hydrogen is almost completely incoherent.**
- ✓ **Coherent elastic**
  - ✓ **It is important for crystalline solids such as graphite, beryllium or UO_2. It includes the effects from waves that are able to interfere with each other. Considering the properties of the materials, the scattering from carbon and oxygen is almost completely coherent.**

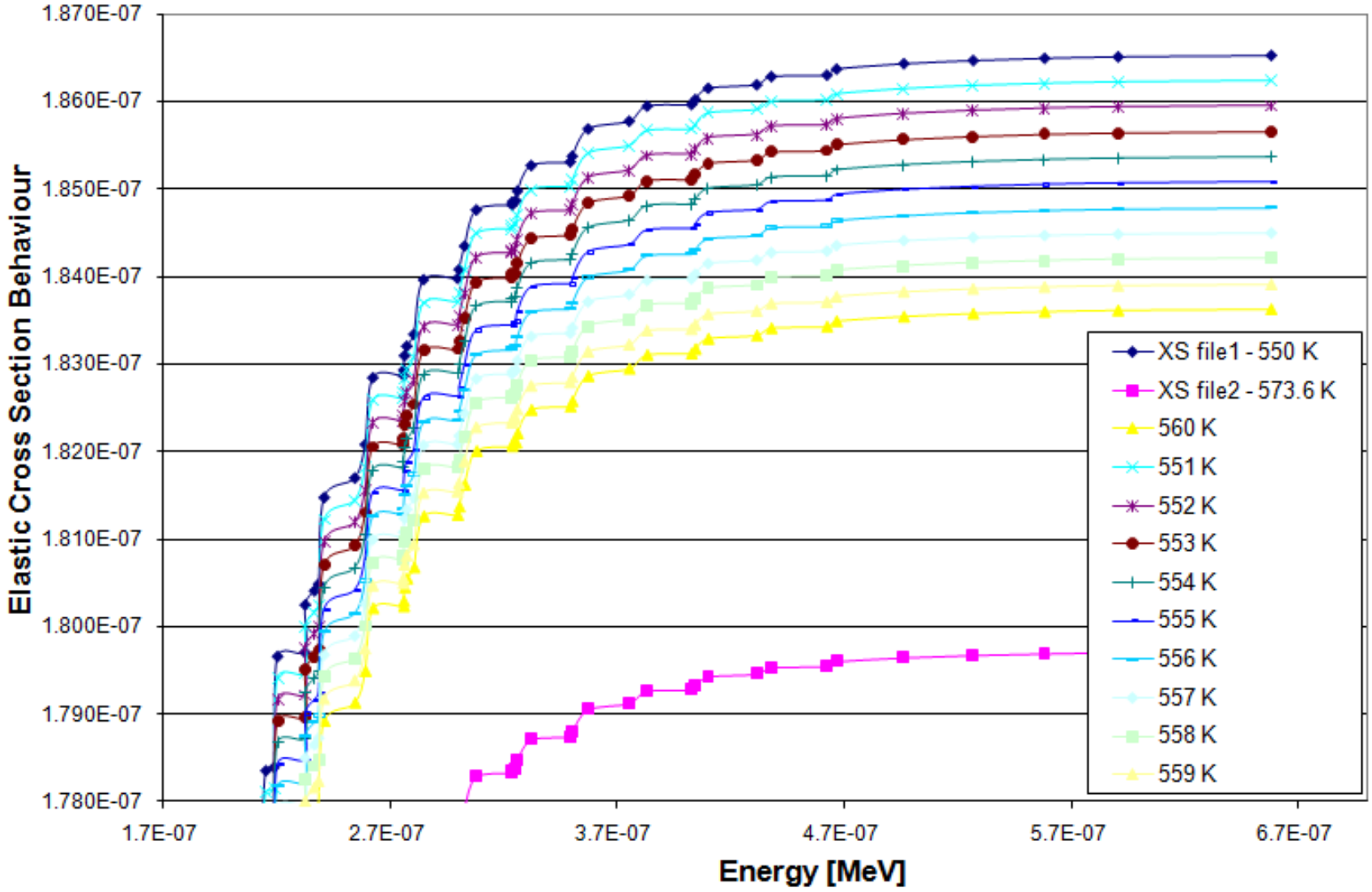
Thermal Scattering XS

- *IKE model: rho-energy distributions for different temperatures*



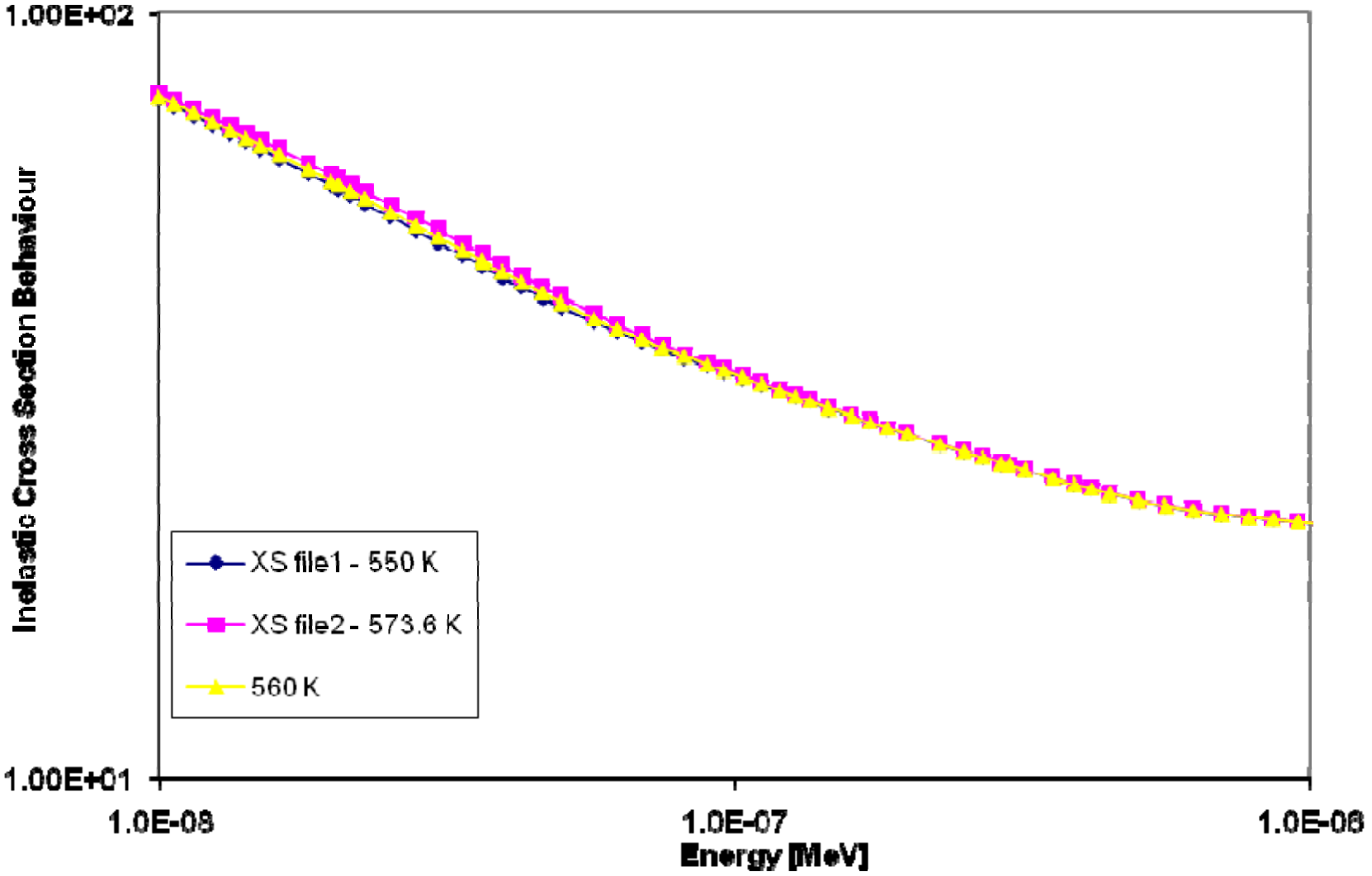
Thermal Scattering XS

- *Interpolation methodology applied to the elastic cross section of H_2O*



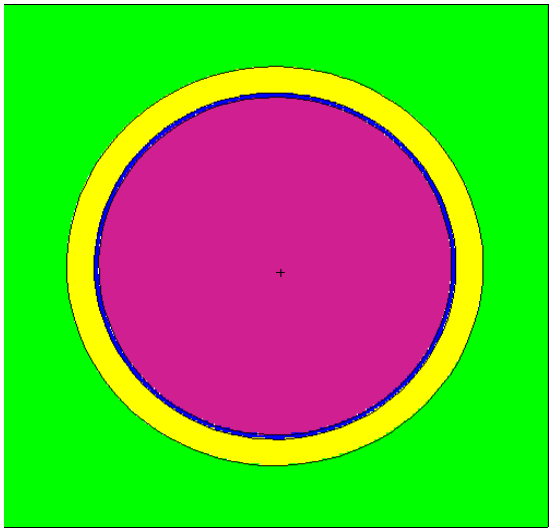
Thermal Scattering XS

- *Interpolation methodology applied to the inelastic cross section of H_2O*



Thermal Scattering XS

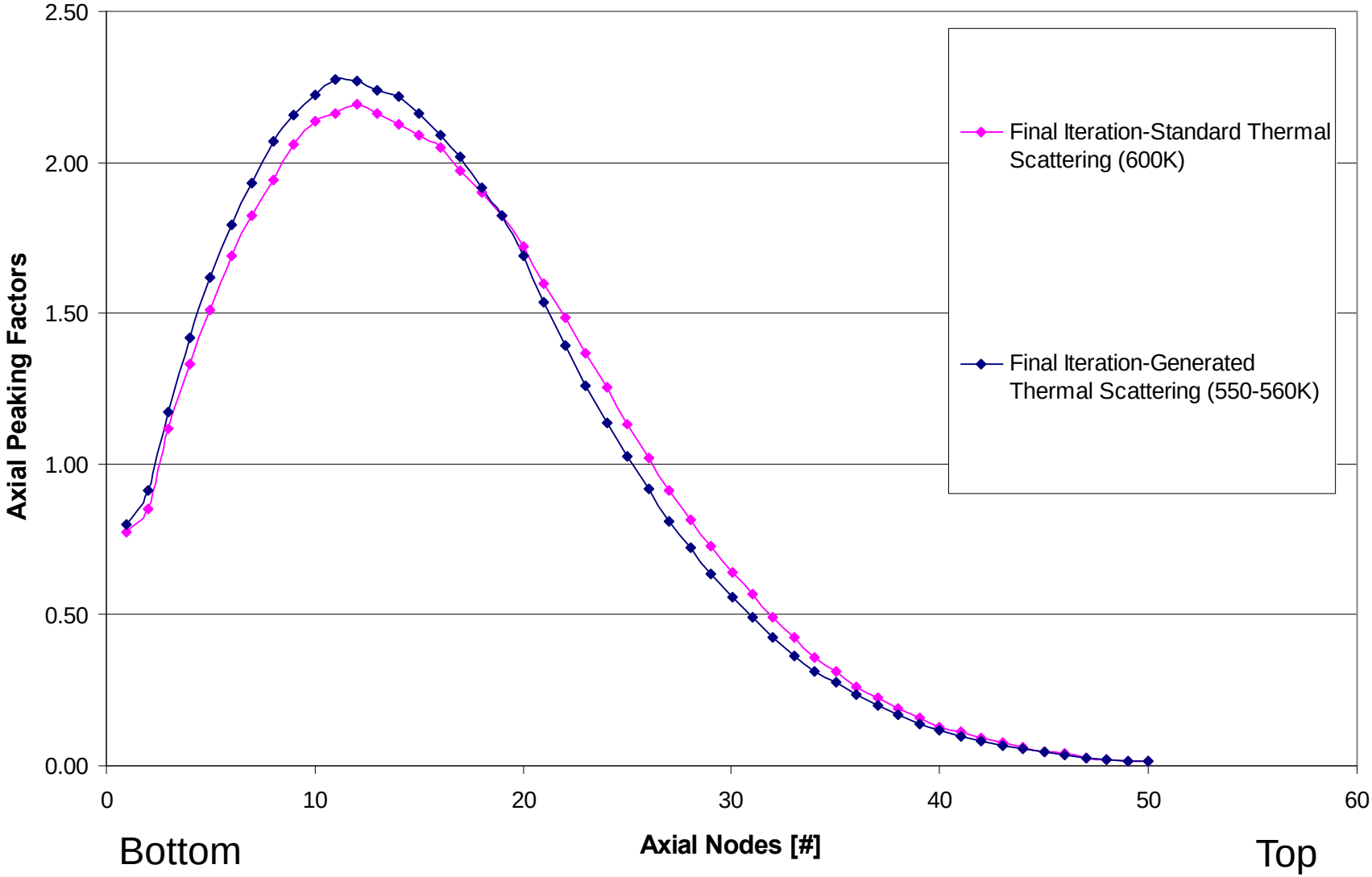
- *MCNP5 k_{eff} results using thermal scattering libraries at different temperatures*



Thermal Library Temperature [K]	k_{eff}	Standard Deviation
550	1.36617	0.00026
560	1.36571	0.00025
573	1.36553	0.00025
600	1.36489	0.00026

Simplified 3-D 2x2 BWR fuel-pin array

➢ *Comparison between the Standard and Generated Thermal Scattering XS*



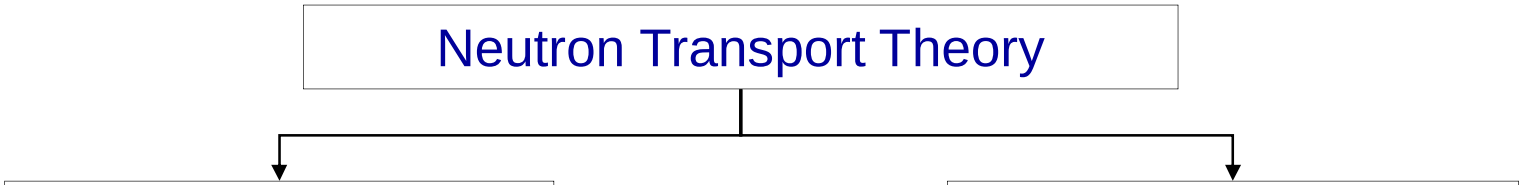
Simplified 3-D 2x2 BWR fuel-pin array

- *Comparison between the Standard and Generated Thermal Scattering XS*

- *k_{eff} comparison*

Coupled Iteration	Rod Centered TH		Rod Centered No TH		k_{eff} Difference
#	k_{eff}	Std-Dev	k_{eff}	Std-Dev	Diff.
1	1.35039	0.00037	1.34914	0.00034	0.00125
2	1.33470	0.00038	1.33161	0.00037	0.00309
3	1.33502	0.00039	1.33266	0.00036	0.00236
4	1.33619	0.00034	1.33283	0.00038	0.00336
5	1.33574	0.00037	1.33298	0.00038	0.00276

Monte Carlo Modeling



Monte Carlo Methods

- ✓ Continuous Energy Treatment
- ✓ Exact 3D geometry modeling
- ✓ Solves the exact model statistically

Deterministic Methods

- ✓ Energy discretization
- ✓ Spatial discretization
- ✓ Angular discretization
- ✓ Solutions of the approximated representation of the model

For our purposes

- ✓ **Core environments that present increased geometry complexity and material heterogeneity are well modeled in MCNP5.**

- ✓ **The Monte Carlo method can be considered a numerical experiment that represents a high quality reference solution for validation of deterministic codes.**

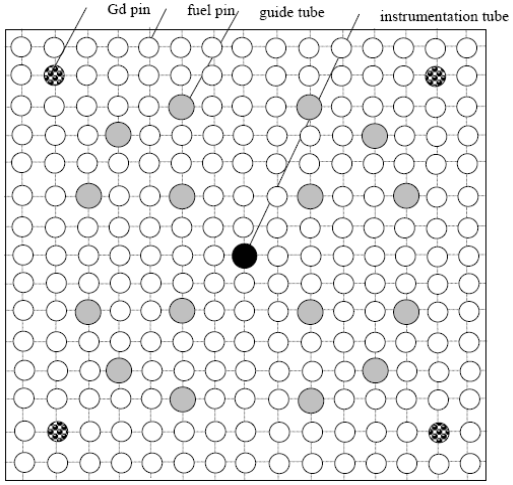
Monte Carlo Modeling

- ✓ **The MCNP5 version (1.40 release) is used for the studies of mainly two effects:**
  - ❖ **The effect of temperatures**
  - ❖ **The effect of the NDLs on the example of the latest released versions such as ENDF/B-VI.8, ENDF/B-VII.0, JEFF-3.1, and JENDL-3.3.**

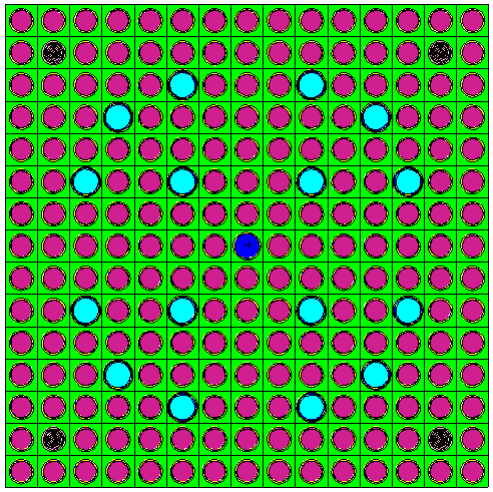
Automated tool for generation of MCNP cont. energy XS

- ✓ The automated tool is used to generate temperature dependant cross-section libraries using NDLs.
- ✓ Then, the differences in the effective multiplication factor (k_{eff}) and other parameters, calculated by MCNP5 using the different libraries, are compared.

MCNP Calculations



TMI Assembly Design

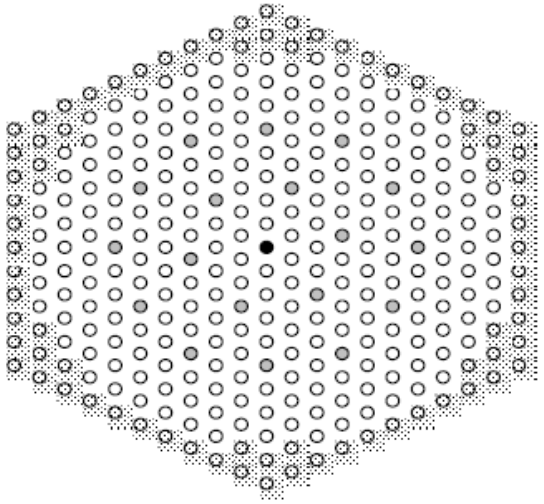


TMI MCNP5 Assembly Model

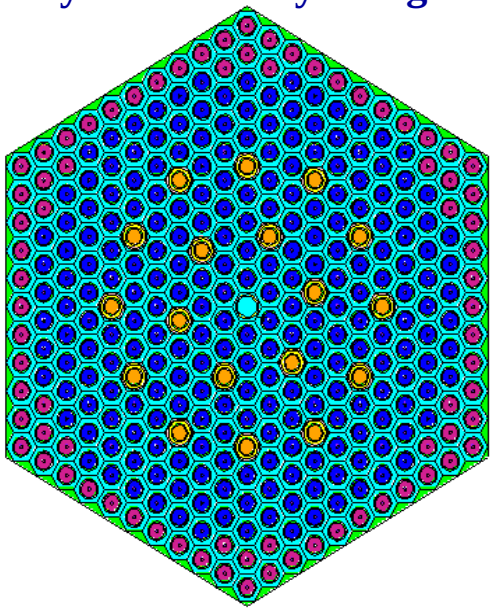
Description of Benchmark

Parameter	Value
No. of Fuel rods per FA	208
No of guide tubes per FA	16
Number of Gd pins per FA	4
Fuel rod pitch, cm	1.4427
Fuel rod outside diameter, cm	1.0922
Fuel pellet diameter, cm	0.9390
Cladding thickness, cm	.0673
Guide tube outside diameter, cm	1.3462
Guide tube inside diameter, cm	1.2649
Instrumentation tube outside	1.2522
diameter, cm	1.1201
Instrumentation tube inside diameter,	21.8110
mm	0.1702
Fuel assembly pitch, cm	
Gap between fuel assemblies, cm	

MCNP Calculations



Kozloduy –6 Assembly Design

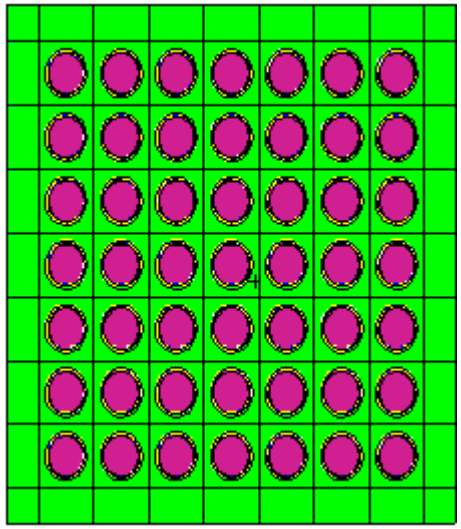


Kozloduy –6 MCNP Assembly Model

Description of Benchmark

Parameter	Value
Number of fuel rods	312
Number of fuel rods with 3.0 w/o enrichment	78
Number of fuel rods with 3.3 w/o enrichment	234
Number of water rods per FA	1
Number of guide tubes	18
Pellet diameter, mm	7.56
Central void diameter, mm	1.4
Cladding outside diameter, mm	9.1
Cladding thickness, mm	0.69
Fuel rods pitch, mm	12.75
Guide tube outside diameter, mm	12.6
Guide tube inside diameter, mm	11.0
Absorber (control rods) pellet diameter, mm	7.0
Absorber cladding outside diameter, mm	8.2
Water rod outside diameter, mm	11.2
Water rod inside diameter, mm	9.5

MCNP Calculations



MCNP5 2D model of PB-2 BWR Fuel Assembly

Description of Benchmark

Parameter	Value
Fuel assembly dimensions	7 x 7
Number of fuel rods per FA	49
Fuel rod pitch, mm	18.75
Cladding outside diameter, mm	14.3002
Fuel pellet diameter, mm	12.1158
Cladding thickness, mm	0.9398
Fuel assembly pitch, mm	152.4

MCNP Calculations

Test calculations are studied at Hot Zero Power (HZP) conditions, as summarized in the following table

HZP conditions for UAM test problems

HZP Conditions / Reactor	BWR PB-2	PWR TMI-1	Kozloduy-6 VVER-1000
Fuel and Moderator (coolant) Temperatures [K]	552.830	551.000	552.150
Moderator (coolant) density [kg/m^3]	753.978	766.000	767.100
Reactor Power [MW]	3.293	2.772	3.000

MCNP Calculations

Effect of NDLs

- The assembly tests were simulated using cross-section libraries based on ENDF/B-VII.0 and JEFF – 3.1.1 for the first test.

- The objective of this first section were to run the assemblies using three different thermal scattering libraries (the two provided in MCNP5 : lwtr.62t, lwtr.04t, ant the new generated at PSU: th552.68t)

- The comparisons between the three thermal cross section libraries will serve as a base to assess the accuracy of the newly developed thermal library (th552.68t)

- Therefore, for subsequent runs only the latest libraries were used (lwtr62.t and th552.68t) to provide reference calculations using ENDF/B-VII.0, JEFF3.1.1 and JENDL3.1

MCNP Calculations

Effect of NDLs

- Both of the MCNP5 built in thermal scattering libraries (lwtr.04t and lwtr.62t) are at 600 K, a much higher temperature than the desired at 552 K.

- The intermediate point of interest for the thermal scattering grid are obtained by using a novel interpolation automated tool, based on the square root of temperature interpolation method developed at PSU.

- This gives the possibility of performing MCNP5 criticality calculations at the correct moderator temperature and improving the accuracy of the calculation.

MCNP Calculations

Effect of NJOY Modules

- Two possible approaches to generate temperature dependent continuous energy MCNP5 cross sections in NJOY

1). Probability Tables (PURR module);

Produces probability tables to treat unresolved-resonance self-shielded for the continuous-energy MCNP5 code (most appropriate methodology for MCNP5 calculations)

2). Bondarenko (GROUPR module)

UNRESR module generates unresolved self-shielding data suitable for multi-group methods after being processed by the GROUPR module. The method used by this module (Bondarenko method) is not the best aproach for continuous-energy Monte Carlo methods

MCNP Calculations

Effect of NJOY Modules

- The correct and natural approach for treating unresolved resonance self-shielding for Monte Carlo codes is to use the Probability Table method.

- This method creates probability tables of the elastic, fission, capture and total cross sections.

- The Monte Carlo code would sample a random number between 0 and 1 to determine the corresponding cross section in the appropriate probability table.

Effect of Nuclear Data Libraries

Assembly	Nuclear Data Library	Thermal Scattering Library	PURR k_{inf}/Std.		GROUPR k_{inf}/Std.	
TMI	ENDF/B-VII.0	lwtr.62t	1.05899	0.00016	1.05826	0.00015
		lwtr.04t	1.05737	0.00016	1.05718	0.00016
		th552.68t	1.06239	0.00025	1.06212	0.00025
	JEFF3.1.1	lwtr.62t	1.05490	0.00015	1.05409	0.00015
		lwtr.04t	1.05359	0.00015	1.05253	0.00016
		th552.68t	1.05851	0.00023	1.05746	0.00025
	JENDL3.1	lwtr.62t	1.05544	0.00025	1.05511	0.00023
		th552.68t	1.05924	0.00026	1.05849	0.00024
VVER	ENDF/B-VII.0	lwtr.62t	0.95752	0.00022	0.95692	0.00021
		lwtr.04t	0.95619	0.00021	0.95548	0.00021
		th552.68t	0.96192	0.00024	0.96087	0.00023
	JEFF3.1.1	lwtr.62t	0.97187	0.00022	0.97174	0.00021
		lwtr.04t	0.97048	0.00021	0.97033	0.00022
		th552.68t	0.97574	0.00024	0.97565	0.00024
	JENDL3.1	lwtr.62t	0.97246	0.00023	0.97131	0.00024
		th552.68t	0.97655	0.00023	0.97574	0.00025
PB-2	ENDF/B-VII.0	lwtr.62t	1.05940	0.00009	1.05918	0.00009
		lwtr.04t	1.05982	0.00009	1.05927	0.00009
		th552.68t	1.06038	0..00006	1.06028	0.00014
	JEFF3.1.1	lwtr.62t	1.06277	0.00009	1.06235	0.00009
		lwtr.04t	1.06280	0.00009	1.06255	0.00009
		th552.68t	1.06328	0.00014	1.06326	0.00014
	JENDL3.1	lwtr.62t	1.05951	0.00014	1.05907	0.00015
		th552.68t	1.06025	0.00014	1.05962	0.00015

Summary and Conclusion

- Calculations with cross sections derived from, ENDF/B-VII.0 and JEFF-3.1.1 have been performed for all LWR type test problems.
- When comparing the calculations, the PURR calculations produce higher kinf value than GROUPR
- The largest differences in values for the results presented are the TMI-1 test problem when comparing the th522.68t cross section of the JEFF-3.1.1, 121 pcm.
- The choice of NDL used to perform the criticality calculation is of great relevance

Few-group structures

- Previous studies have shown that VHTR analyses require more energy groups than conventional LWR analysis because the spectral interactions between fuels and fuel and reflector are significant due to a much longer neutron mean free path.
- In this work, the number of energy groups versus accuracy has been studied using the PBMR-400 benchmark model
- It is used as a basis for energy group optimization as mentioned in Lecture 1
- As a reference continuous energy Monte Carlo core calculation is used
- The accuracy is sensitive not only to the number of groups but also to the energy group boundaries.

Few-group structures

(Unit: eV)

23	14(a)	14(b)	8(a)	8(b)	7	4(a)	4(b)
3.679E+06	3.679E+06						
1.353E+06	1.353E+06					1.353E+06	
5.000E+05	4.979E+05	5.000E+05		5.000E+05	5.000E+05		
	1.832E+05						
1.110E+05		1.110E+05					
6.738E+04	6.738E+04	6.738E+04					
	2.479E+04						
9.118E+03	9.119E+03	9.118E+03		9.118E+03	9.118E+03	9.118E+03	9.118E+03
	4.540E+02			4.540E+02			
3.673E+02		3.673E+02	3.120E+02				
4.000E+00	4.000E+00	4.000E+00		4.000E+00	4.000E+00		
	2.380E+00						
1.500E+00							
	1.300E+00						
1.097E+00		1.097E+00	1.072E+00	1.097E+00	1.097E+00		
1.045E+00							
9.720E-01		9.720E-01					
8.500E-01		8.500E-01				8.500E-01	8.500E-01
	6.250E-01						
5.000E-01		5.000E-01	5.300E-01	5.000E-01	5.000E-01		
4.000E-01							
3.500E-01		3.500E-01	3.577E-01				
3.000E-01							
2.500E-01							
1.800E-01							
1.400E-01		1.400E-01					
	1.200E-01						
1.000E-01			1.116E-01	1.000E-01	1.000E-01		1.000E-01
5.000E-02		5.000E-02	5.692E-02				
			2.049E-02				

Few-group structures

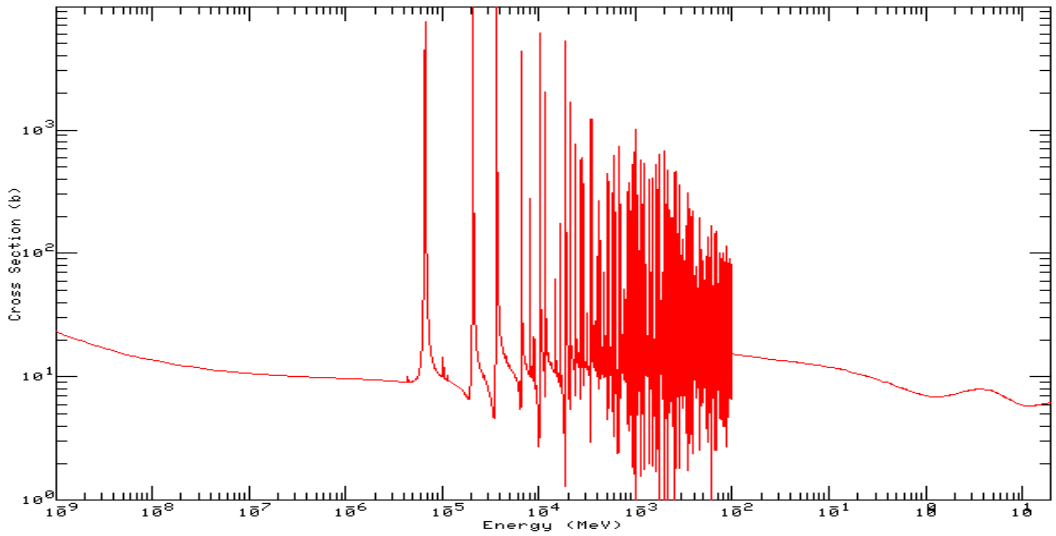
Energy boundaries (eV)				
upper	lower	9 groups	7 groups	4 groups
1.5×10^7	1.83×10^5	1	1	1
1.83×10^5	961	2	2	2
961	17.6	3		
17.6	3.93	4	3	3
3.93	2.38	5		
2.38	0.414	6	4	4
0.414	0.10	7	5	
0.10	0.04	8	6	
0.04	0.0	9	7	

The Fort Saint Vrain 4, 7, and 9 Group Structures

Few-group structures

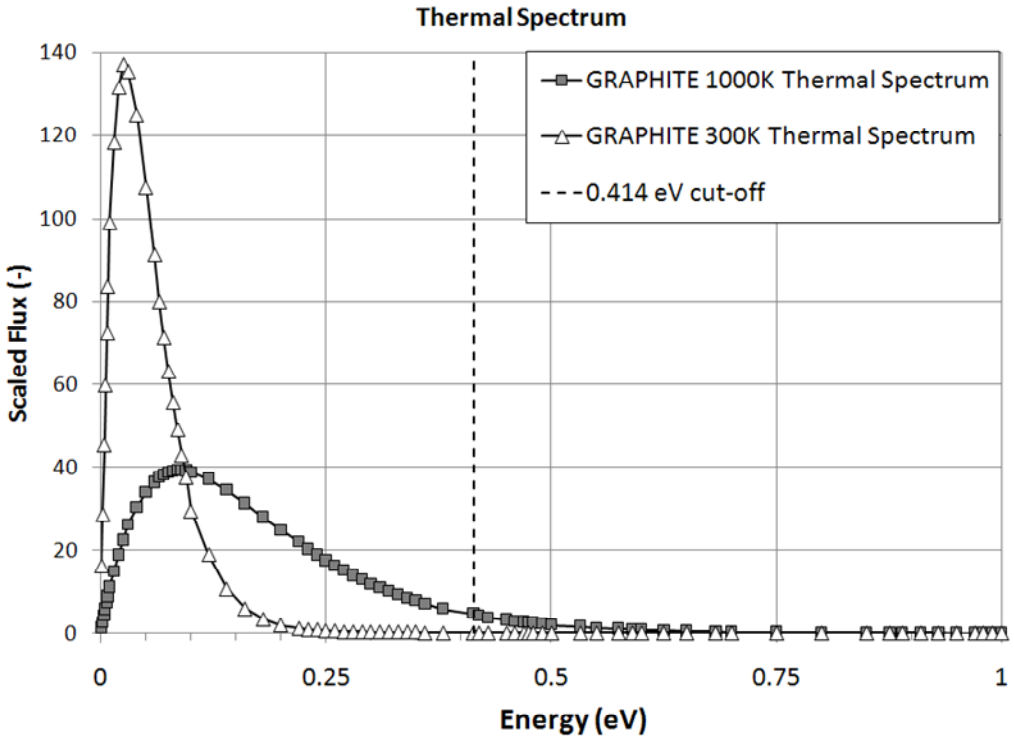
	Fast Group Structure				
Upper Energy	*3.93 eV*	*17.6 eV*	*961 eV*	*183 keV*	*15 MeV*
Group Number	**5**	**4**	**3**	**2**	**1**
Selection Basis	Up-scatter		Resonances of Th-232		Source Containment
	Buildup of U-233, 234, 235		Depletion of Th-232		
	Downscatter To Thermal				

Group Number	Energy Range	Purpose
1	183 keV to 15 MeV	To contain nearly all of the **fission source.**
2 & 3	17.6 keV to 183 keV	To group the unresolved and resolved resonance cross section ranges for **thorium**, which is principal resonance absorber.
5	2.38 eV to 3.93 eV	To provide restriction of **up-scatter** from thermal groups to a physically realistic range.
2 – 5	2.38 eV to 183 keV	Groups of energies between fission spectrum and thermal cutoff serve to **follow the spectral hardening** that occurs with **burn-up** and help improve downscattering.



U-238 Total Cross Section

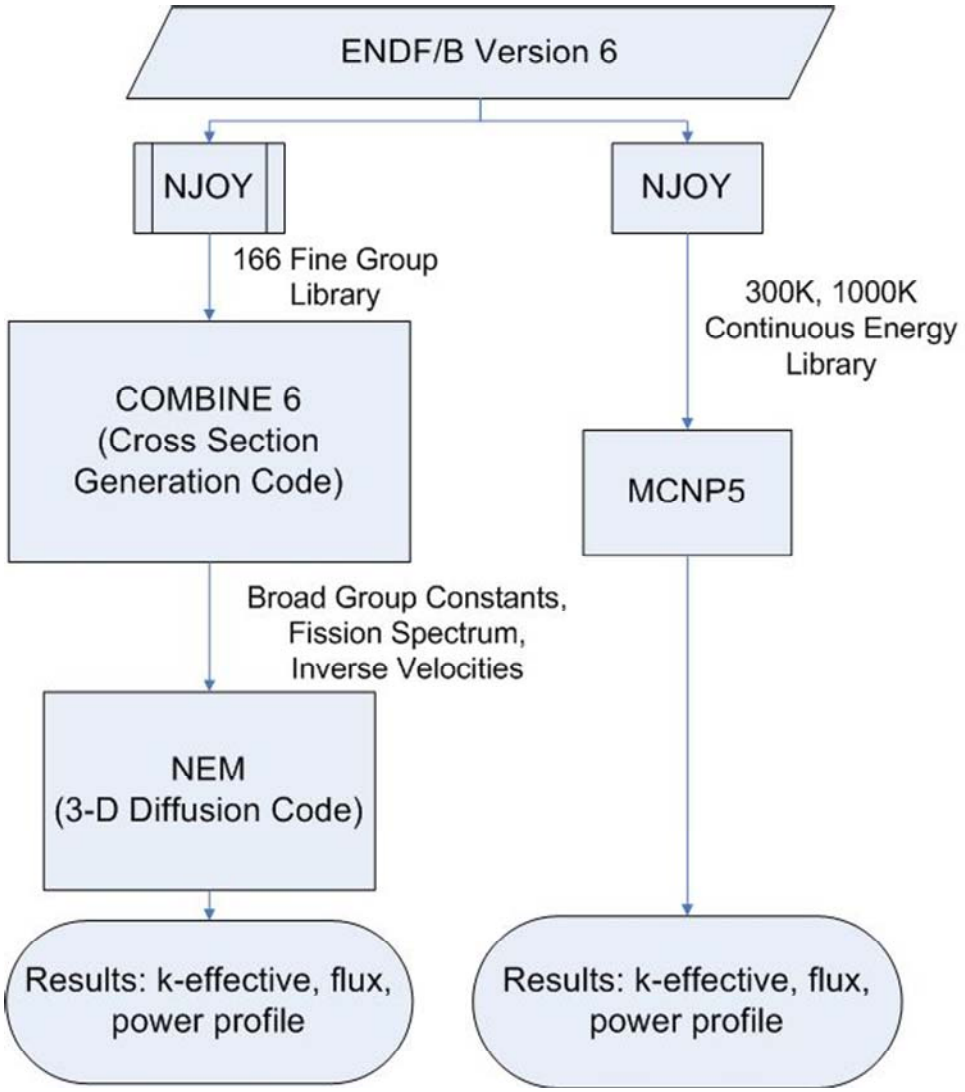
Few-group structures



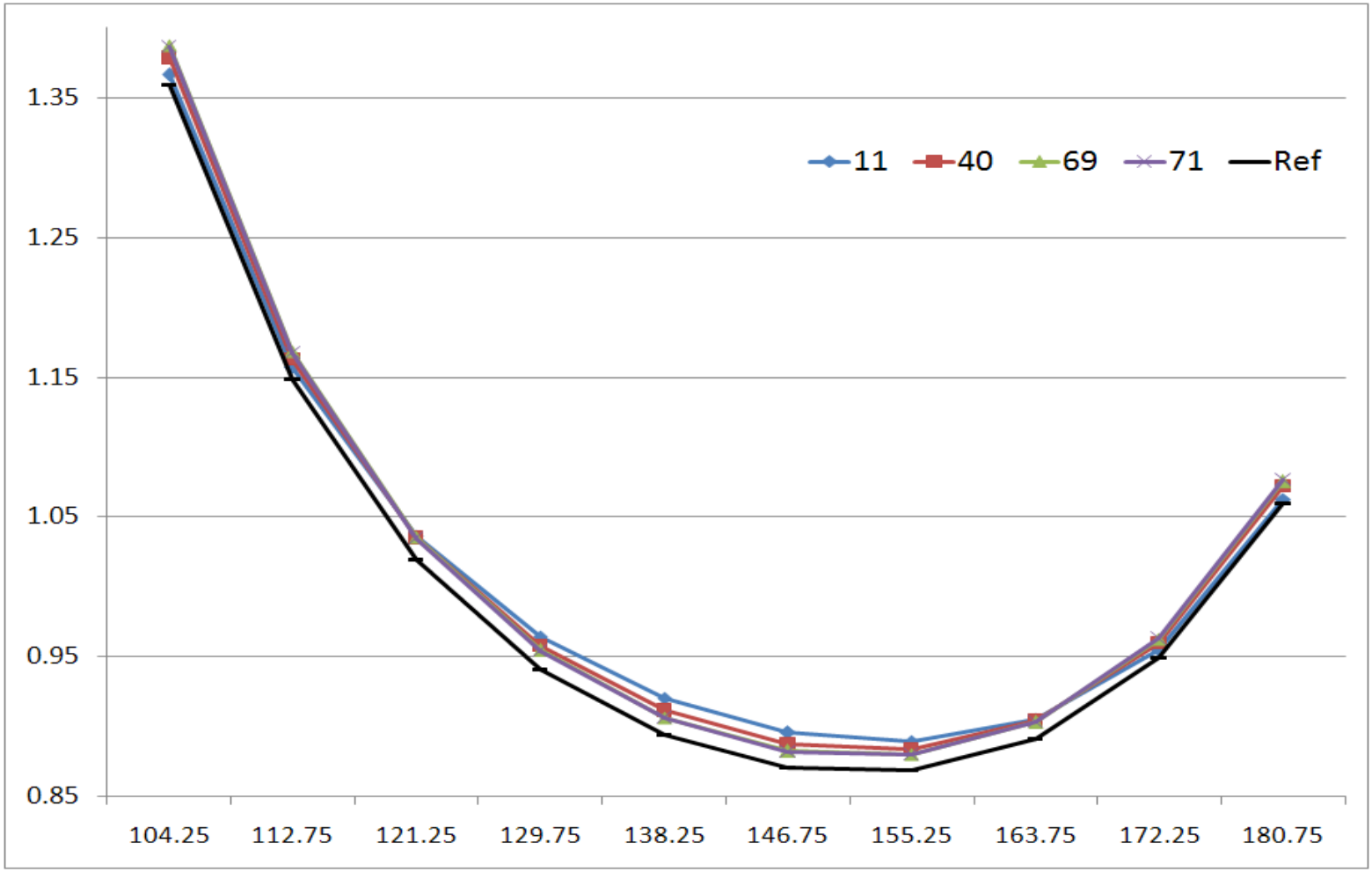
The up-scattering application has been helpful in showing the magnitude of up-scattering present at different cut-off's.

At *1000K* up-scattering seems to be negligible only at cut-off energies of 1.86 eV and above.

Few-group structures



Few-group structures



Radial Power Profile Comparison of Selected Group Numbers

Few-group structures

- ✓ Numerical studies of energy group structures have been performed to obtain optimal candidate group structures for PBMR analysis.
- ✓ These tests were performed using a nodal diffusion code (NEM) and a cross section generation code (COMBINE6).
- ✓ The results of the energy dependent nodal method were compared with results of energy independent Monte Carlo method code, MCNP5.
- ✓ An optimal 5, 6, 7, 8, and 9 Group structure has been determined.
- ✓ These group structures have been selected based on numerical tests but are also supported by physical basis.

Few-group structures

The following summarizes the group structure selection method (*in order of importance*):

- ✓ **Thermal spectrum and up-scatter containment.**
- ✓ **Fission source containment.**
- ✓ **Isolation of low lying resonances in thermal region (at least 2 thermal groups)**
- ✓ **Separation of continuum (smooth) resonances from the unresolved resonances for the most important fissile isotope.**
- ✓ **Separation of continuum (smooth) resonances from the unresolved resonances for the most important capture isotope.**
- ✓ **(Optional) Fast fission improvement for the fissionable isotope.**
- ✓ **(Optional) Improvement of the isolated resonance region by partition below or above this energy region.**

Few-group structures

Upper Energy Boundary	5 Group	6 Group	7 Group	8 Group	10 Group
16.9MeV	16.9MeV	16.9MeV	16.9MeV	16.9MeV	16.9MeV
821keV					821keV
183keV		183keV	183keV	183keV	
52.5 keV	52.5keV				52.5keV
9.12keV				9.12keV	9.12keV
2.04keV			2.04keV	2.04keV	2.04keV
454.0eV	454.0eV				
3.93eV					3.93eV
2.38eV	2.38eV	2.38eV	2.38eV	2.38eV	2.38eV
1.6eV		1.6eV	1.6eV	1.6eV	1.6eV
0.43eV	0.43eV	0.43eV	0.43eV	0.43eV	0.43eV
0.12eV		0.12eV	0.12eV	0.12eV	
0.04eV					0.04eV

Upper Energy Boundary	5 Group	Group Selection Cause	6 Group	Group Selection Cause	7 Group	Group Selection Cause
16.9MeV	16.9MeV	fission source containment	16.9MeV	fission source containment	16.9MeV	fission source containment
821keV						
183keV			183keV		183keV	
52.5 keV	52.5keV					
9.12keV						U-238 Smooth & Unresolved Resonances
2.04keV		U-238 Unresolved & Separated Resonances Containment			2.04keV	
454.0eV	454.0eV					
3.93eV						
2.38eV	2.38eV	Upscattering Containment	2.38eV	Upscattering Containment	2.38eV	Upscattering Containment
1.6eV		Thermal Energy Low Lying Resonances Pu-240, Pu-241, Pu-239 U-235, Np isotopes	1.6eV	Thermal Energy Low Lying Resonances Pu-240, Pu-241, Pu-239 U-235, Np isotopes	1.6eV	Thermal Energy Low Lying Resonances Pu-240, Pu-241, Pu-239 U-235, Np isotopes
0.43eV	0.43eV		0.43eV		0.43eV	
0.12eV			0.12eV		0.12eV	
0.04eV						

Few-group structures

8 Group	*Group Selection Cause*	*10 Group*	*Group Selection Cause*
16.9MeV	fission source	16.9MeV	fission source containment+
	containment	821keV	U-238 Fast Fission Threhold
183keV			
		52.5keV	
9.12keV	U-238 &	9.12keV	U-238 &
2.04keV	U-235	2.04keV	U-235
	Smooth & Unresolved		Smooth & Unresolved
	Resonance Containment	3.93eV	Resonance Containment
2.38eV	Upscattering Containment	2.38eV	Upscattering Containment
1.6eV	Thermal Energy	1.6eV	Thermal Energy
0.43eV	Low Lying Resonances	0.43eV	Low Lying Resonances
0.12eV	Pu-240, Pu-241, Pu-239		Pu-240, Pu-241, Pu-239
	U-235, Np isotopes	0.04eV	U-235, Np isotopes

- ✓**The first phase of the study of energy group structure performed by the Pennsylvania State University Department of Mechanical and Nuclear Engineering (PSU) for the Idaho National Laboratory (INL) addressed the coarse group structure used in analyzing graphite-moderated high-temperature gas-cooled reactors.**

- ✓**It is likely that one of the largest sources of error encountered in the Phase-1 study stems from the method through which nodal leakage is incorporated into the spectrum calculation.**

Few-group structures

- ✓Tables of cross sections are generated for a few selected values of fast and thermal buckling.
- ✓Cross sections for the core simulation are interpolated from these tables using two-group inter-nodal currents, omitting much of the information contained in the fine-group energy spectrum.
- ✓Furthermore, the fine group structure hardwired within INL's COMBINE-6 code that is used to generate broad group constants is fixed and has not been optimized for HTR analyses.
- ✓ If the fine group structure is not sufficiently refined in energy regions of importance, such a structure may prevent the flexibility needed for more accurate cell-level energy collapsing.
- ✓Development by examining a new fine group structure that is optimized for the compositions expected in the NGNP as described in Lecture 1
- ✓Then development of new optimized few-group structure for AGCR applications

Cross-section uncertainty propagation

- ✓ Phase I of the OECD LWR Uncertainty Analysis in Modeling (UAM) benchmark addresses cross-section uncertainties propagation in a manner consistent with current calculation scheme for reactor core analysis
- ✓ Similar activity will be started this year under IAEA Research Coordinated Program (RCP) for AGCRs
- ✓ In the major NDLs standards and formats are in place to permit the communication of estimated uncertainties in the evaluated cross-section data.
- ✓ The evaluation of nuclear data induced uncertainty is possible by the use of nuclear covariance data.
- ✓ By including the uncertainty or covariance information, the analyst can propagate cross-section data uncertainties through sensitivity studies to the final calculated quantities of interest.
- ✓ The covariance data files provide the estimated variance for the individual data as well as any correlation that may exists.
- ✓ To propagate nuclear data uncertainties in reactor core calculations files MF31, MF32, and MF33 are the only data currently available within ENDF/B and other NDL's.

Cross-section uncertainty propagation

- ✓ For example, for each isotope and type of reaction, quantities in MF33 are the covariances of the expected cross-section values, providing a measure of the accuracy and correlations of the evaluated cross-sections.
- ✓ Stored quantities in MF3 (or MF 10) - expected value of a physical quantity, where is the density function averaged over all variables other that *x*.
- ✓ Stored quantities in MF33 - relative and absolute covariances of the 2nd degree moments of the joint density function, where is the density function averaged over all variables other than *x* and *y* .
- ✓ In this way the uncertainties are presented in terms of variances and covariances (variance-covariance matrices).
- ✓ The total covariance matrix for a given energy-dependent cross-section (by isotope and type of reaction) is made up of the contribution of single covariance matrices, each one defining a type of correlation (between energy intervals or correlation with a different cross-section).

$$\langle x \rangle = \int x\, f(x)\, dx$$

$$\mathrm{Cov}(x, y) = \iint \left(x - \langle x \rangle\right)\left(y - \langle y \rangle\right) f(x, y)\, dx\, dy$$

$$x = y$$

$$\mathrm{Cov}(x, y) = \mathrm{Cov}(x, x) = \mathrm{Var}(x)$$

Overview

Phase I (Neutronics Phase)

Exercise I-1: "Cell Physics" - focused on the derivation of the multi-group microscopic cross-section libraries & their uncertainties

Exercise I-2: "Lattice Physics" - focused on the derivation of the few-group macroscopic cross-section libraries & their uncertainties

Exercise I-3: "Core Physics" - focused on the core steady state stand-alone neutronics calculations & their uncertainties

Phase II (Core Phase)

Exercise II-1: Fuel thermal properties relevant for transient performance

Exercise II-2: Neutron kinetics stand-alone performance (kinetics data, space-time dependence treatment, etc.)

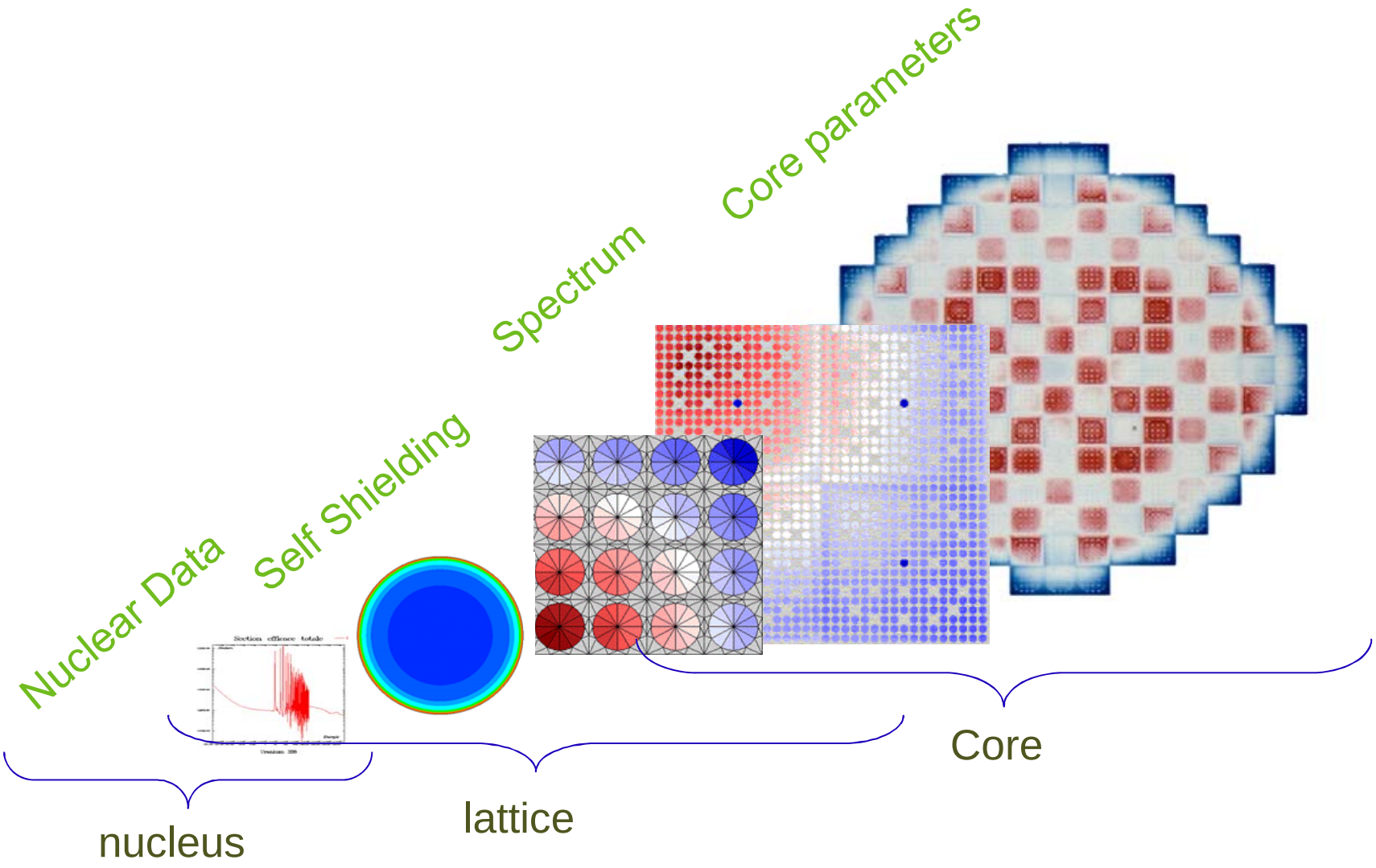
Exercise II-3: Thermal-hydraulic fuel bundle performance

Phase III (System Phase)

Exercise III-1: Coupled neutronics/thermal-hydraulics core performance (coupled steady state, coupled depletion, and coupled core transient with boundary conditions)

Exercise III-2: Thermal-hydraulics system performance

Exercise III-3: Coupled neutron kinetics thermal-hydraulic core/thermal-hydraulic system performance



Source CEA-DEN

Exercise I-1

Exercise I-1, Cell Physics, is focused on the derivation of the multi-group microscopic cross-section libraries

- **Exercise I-1 propagates the uncertainties in evaluated Nuclear Data Libraries - NDL - (microscopic point-wise cross sections) into multi-group microscopic cross-sections used as an input by lattice physics codes**
- **The participants can use any of the major NDLs such as ENDF, JEFF, and JENDL**
- **The development of nuclear data covariance files is in progress in major NDLs**

Exercise I-1

Number of materials and cross-sections with covariances of neutron cross-sections

Data files	*Number of materials*	*Number of cross-sections*
ENDF/B-VI.8	44	400
JEFF-3.1	34	350
JENDL-3.3	20	160
TENDL-2008	from F-19-Po-209	all

Number of nuclides and energy groups in the available multi-group covariance matrices

Name	*Number of nuclides*	*Number of energy groups*
ANL	42	17
NEA/OECD	31	15
SCALE5.1/ORNL SCALE6.0/ORNL	299 401	44 44

Exercise I-1

- The current status of the evaluated cross-section NDLs is such that the most comprehensive covariance library is available with SCALE-5.1 and now with the extension / improvement in SCALE-6

- For this reason initially it was decided to utilize the nuclide dependent multi-group covariance data from SCALE-5.1 for the purposes of Exercise I-1 (44GROUPV6REC was the recommended library) – now the new SCALE-6 covariance library will be used for Phase I

- It is based on a 44-group structure. For other group structures, NEA/OECD has provided the tools for handling and transforming the cross-section covariance in a consistent way (ANGELO and LAMBDA)

- Covariance data are relative values and can be used with different NDLs

Exercise I-1

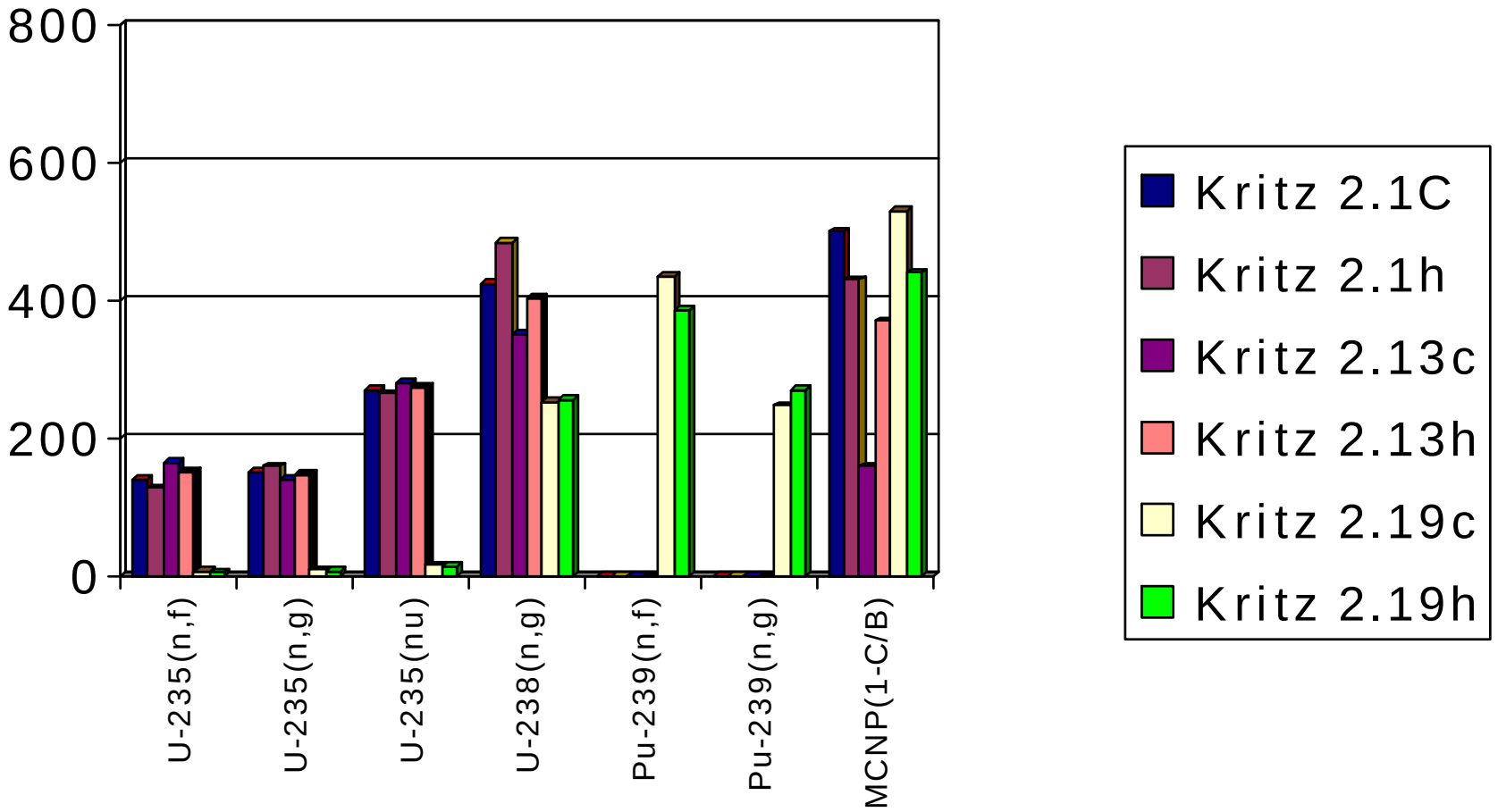
H-1, H-ZrH, H-poly, H-freegas, H-2, H2-freegas, H-3, He-3, He-4, Li-6, Li-7, Be-7, Be-9, Be-bound, B-10, B-11, C-0, C-graphite, N-14, N-15, O-16, O-17, F-19, Na-23, Mg-0, Mg-24, Mg-25, Mg-26, Al-27, Si-0, Si-28, Si-29, Si-30, P-31, S-0, S-32, S-34, S-36, Cl-0, Cl-35, Cl-37, Ar-36, Ar-38, Ar-40, K-0, K-39, K-40, K-41, Ca-0, Ca-40, Ca-42, Ca-43, Ca-44, Ca-46, Ca-48, Sc-45, Ti-0, Ti-46, Ti-47, Ti-48, Ti-49, Ti-50, V-0, Cr-50, Cr-52, Cr-53, Cr-54, Mn-55, Fe-0, Fe-54, Fe-56, Fe-57, Fe-58, Co-58, Co-58(m), Co-59, Ni-58, Ni-59, Ni-60, Ni-61, Ni-62, Ni-64, Cu-63, Cu-65, Ga-0, Ga-69, Ga-71, Ge-70, Ge-72, Ge-73, Ge-74, Ge-76, As-74, As-75, Se-74, Se-76, Se-77, Se-78, Se-79. Se-80, Se-82, Br-79, Br-81, Kr-78, Kr-80, Kr-82, Kr-83, Kr-84, Kr-85, Kr-86, Rb-85, Rb-86, Rb-87, Sr-84, Sr-86, Sr-87, Sr-88, Sr-89, Sr-90, Y-89, Y-89, Y-90, Y-91, Zr-0, Zr-90, Zr-91, Zr-92, Zr-93, Zr-94, Zr-95, Zr-96, Nb-93, Nb-94, Nb-95, Mo-0, Mo-92, Mo-94, Mo-95, Mo-96, Mo-97, Mo-98, Mo-99, Mo-100, Tc-99, Ru-96, Ru-98, Ru-99, Ru-100, Ru-101, Ru-102, Ru-103, Ru-104, Ru-105, Ru-106, Rh-103, Rh-105, Pd-102, Pd-104, Pd-105, Pd-106, Pd-107, Pd-108, Pd-110, Ag-107, Ag-109, Ag-111, Cd-0, Cd-106, Cd-108, Cd-110, Cd-111, Cd-112, Cd-113, Cd-114, Cd-115(m), Cd-116, In-0, In-113, In-115, Sn-112, Sn-113, Sn-114, Sn-115, Sn-116, Sn-117, Sn-118, Sn-119, Sn-120, Sn-122, Sn-123, Sn-124, Sn-125, Sb-121, Sb-123, Sb-124, Sb-125, Sb-126, Te-120, Te-122, Te-123, Te-124, Te-125, Te-126, Te-127(m), Te-128, Te-129(m), Te-130, I-127, I-129, I-130, I-131, I-135, Xe-123, Xe-124, Xe-126, Xe-128, Xe-129, Xe-130, Xe-131, Xe-132, Xe-133, Xe-134, Xe-135, Xe-136, Cs-133, Cs-134, Cs-135, Cs-136, Cs-137, Ba-130, Ba-132, Ba-133, Ba-135, Ba-136, Ba-137, Ba-138, Ba-140, La-138, La-139, La-140, Ce-136, Ce-138, Ce-139, Ce-140, Ce-141, Ce-142, Ce-143, Ce-144, Pr-141, Pr-142, Pr-143, Nd-142, Nd-143, Nd-144, Nd-145, Nd-146, Nd-147, Nd-148, Nd-150, Pm-147, Pm-148, Pm-148(m), Pm-149, Pm-151, Sm-144, Sm-147, Sm-148, Sm-149, Sm-150, Sm-151, Sm-152, Sm-153, Sm-154, Eu-151, Eu-152, Eu-153, Eu-154, Eu-155, Eu-156, Eu-157, Gd-152, Gd-153, Gd-154, Gd-155, Gd-156, Gd-157, Gd-158, Gd-160, Tb-159, Tb-160, Dy-156, Dy-158, Dy-160, Dy-161, Dy-162, Dy-163, Dy-164, Ho-165, Er-162, Er-164, Er-166, Er-167, Er-168, Er-170, Lu-175, Lu-176, Hf-0, Hf-174, Hf-176, Hf-177, Hf-178, Hf-179, Hf-180, Ta-181, Ta-182, W-0, W-182, W-183, W-184, W-186, Re-185, Re-187, Ir-191, Ir-193, Au-197, Hg-196, Hg-198, Hg-199, Hg-200, Hg-201, Hg-202, Hg-204, Pb-204, Pb-206, Pb-207, Pb-208, Bi-209, Ac-225, Ac-226, Ac-227, Th-227, Th-228, Th-229, Th-230, Th-232, Th-233, Th-234, Pa-231, Pa-232, Pa-233, U-232, U-233, U-234, U-235, U-235, U-236, U-237, U-238, U-239, U-240, U-241, Np-235, Np-236, Np-237, Np-238, Pu-236, Pu-237, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Pu-243, Pu-244, Pu-246, Am-241, Am-242, Am-242(m), Am-243, Am-244, Cm-241, Cm-242, Cm-243, Cm-244, Cm-245, Cm-246, Cm-247, Cm-248, Cm-249, Cm-250, Bk-249, Bk-250, Cf-249, Cf-250, Cf-251, Cf-252, Cf-253, Cf-254, Es-253, Es-254, Es-255, Fm-255

In red : added nuclides / materials

Kritz experiments

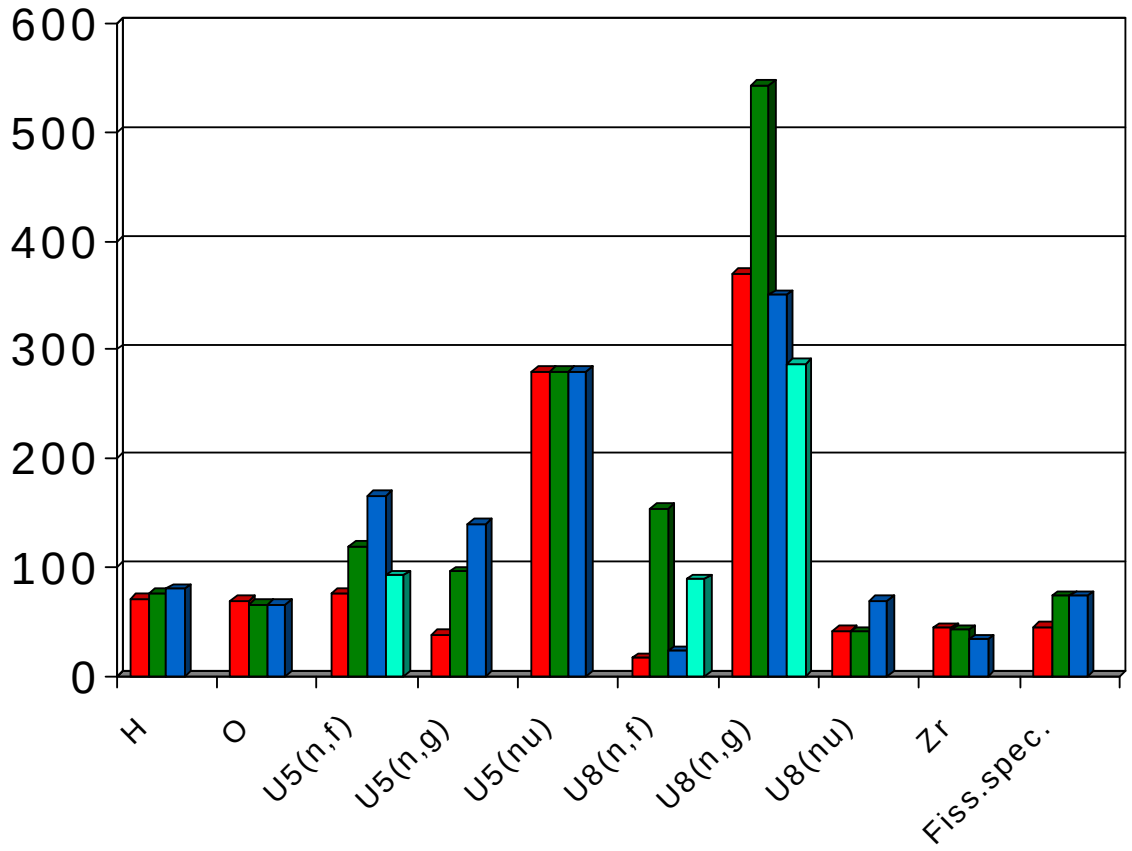
Data uuncertainties (in pcm) vs. (1-C_{MCNP}/B)

Covariances from SCALE-6



Kritz experiments

Kritz 2.13c: Uncertainties (in pcm) based on various covariance data



Total:

JENDL-3.3: 491 pcm

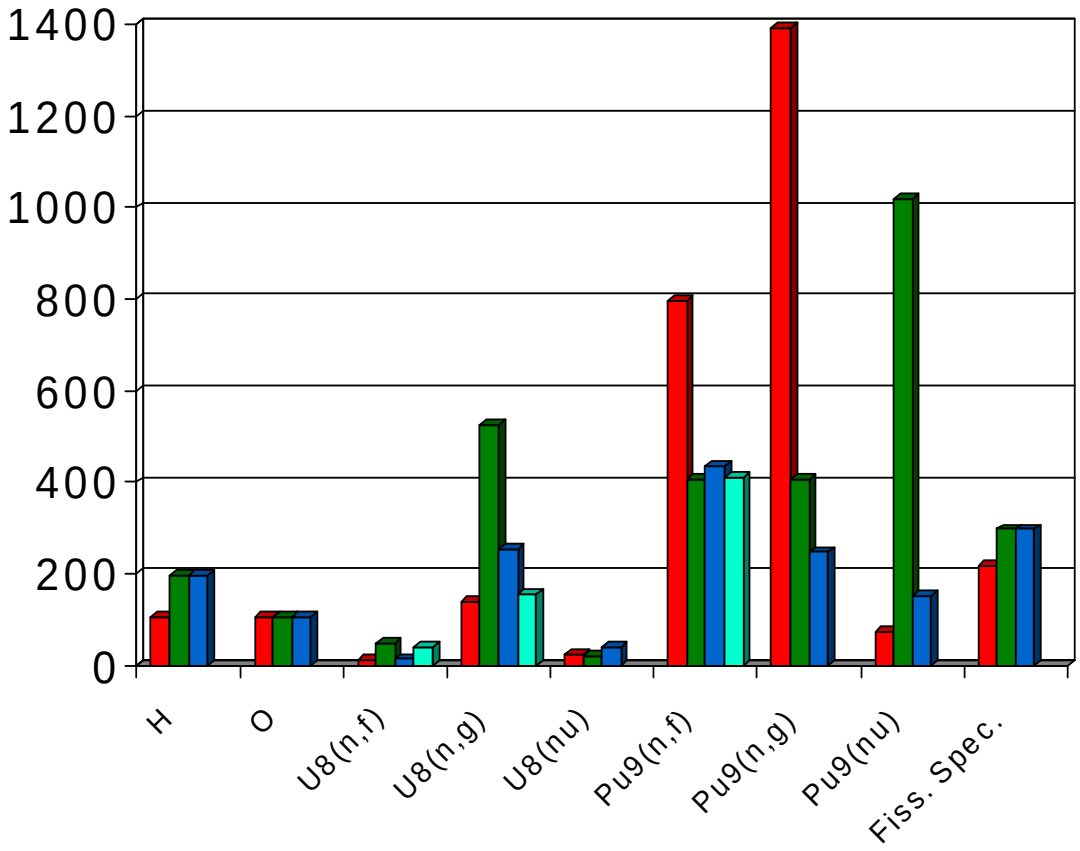
SCALE-5.1: 657 pcm

SCALE6: 559 pcm

IRDF-2002+J33: 711 pcm

Kritz experiments

Kritz 2.19c: Uncertainties (in pcm) based on various covariance data



Total:

JENDL-3.3: 1650 pcm

SCALE-5.1: 1300 pcm

SCALE6: 790 pcm

IRDF-2002+J33: 454 pcm

Uncertainty and Sensitivity Analysis

Models are developed to approximate systems and processes in the real world

Applying models in such domains involves uncertainty.

Uncertainty and sensitivity analysis techniques can be applied to study uncertainty in model predictions arising from imprecisely-known processes and input data.

Global Sensitivity Analysis

- ✓ Global sensitivity analysis deals with uncertainty sources spanning over finite or infinite ranges of uncertainties and with the simultaneous variation of such sources.

- ✓ This in turn enables the identification of high-order interactions among inputs in determining the uncertainty in the output of interest.

- ✓ This exercise applies global sensitivity analysis to the modeling of nuclear reactor applications using the Monte Carlo method.

Global Sensitivity Analysis

- ✓ **Uncertainty Analysis (UA) focuses on quantifying uncertainty in a model output.**

- ✓ **Sensitivity Analysis (SA) studies how this output uncertainty of a model can be apportioned to different sources of uncertainty in the model input. SA can be classified in two categories:**
  - ❖ **Local Sensitivity Analysis (LSA)**
    - ❖ **The LSA is based on derivatives and is efficient in computer time**
    - ❖ **The derivatives are only informative at the base point where they are computed, and do not provide for an exploration of the rest of the space of the input factors**
  - ❖ **Global Sensitivity Analysis (GSA)**
    - ❖ **Explores the full space of input factors**

- ✓ **UA and SA should be run in tandem, usually in an iterative fashion.**

Sensitivity Analysis

- ✓ **The uncertainty within the nuclear data files:**
  - ❖ **The development of uncertainty data is in progress in the major NDLs.**
  - ❖ **The uncertainty within the nuclear data files is difficult to assess.**
  - ❖ **The uncertainty data is expressed in percentage with respect to the nominal value of a given cross section for a given energy.**
  - ❖ **The uncertainty data is available for few isotopes and not all of the nuclear data files include uncertainties.**

Sensitivity Analysis

- ✓ The current exercise focuses on the application of global sensitivity analysis to particular uncertainties found in cross-sections.
- ✓ It does not considered the engineering uncertainties found in geometrical models and material descriptions.
- ✓ It is important to note that the isotopes used in this exercise were limited by the available uncertainty data.
- ✓ The isotopes contained in the fuel do not correspond to the ones listed in the OECD UAM Benchmark for Exercise 1 and certain important isotopes like U-238 could not be used because of the lack of uncertainty data.
- ✓ The main objective of this exercise is to apply global sensitivity analysis to cross section data using Monte Carlo continuous energy calculations in an innovative manner.

Sensitivity Analysis

- ✓ **In order to conduct the sensitivity test**
  - ❖ **The reactions that have cross section larger than 100 barns have been identified (considering that the uncertainty effect of less probable reactions have no effect on k_{eff}).**
  - ❖ **Ideally, the uncertainties of the cross sections should be modified within the nuclear data file.**
  - ❖ **The cross section values are assumed to be normally distributed with a mean value given by the nominal value and a standard deviation that is given by the product of the nominal cross section and the uncertainty value expressed in percentage points.**

Sensitivity Analysis

- ✓ In order to apply global sensitivity analysis to the modeling of nuclear reactor applications using the Monte Carlo method:
  - ❖ The cross section values of several important isotopes of different regions were treated as uncertain quantities.
  - ❖ For each of these regions, the most important isotopes, for which the uncertainty values exist, are selected and adjusted.
  - ❖ The cross section values of the three regions are modified simultaneously (20 cross section values in total: 6 for the fuel, 3 for the absorber and 11 for the moderator) as summarized in the following tables =>

Application of Global Sensitivity: Sensitivity Analysis

- ***Fuel region: cross sections and uncertainty values as a function of energy***

Isotope	Energy (MeV)	Fission XS (barns)	Uncertainty (%)	Capture XS (barns)	Uncertainty (%)
U-235	2.53E-08	584.25	0.19	98.96	0.75
Pu-239	2.53E-08	747.99	0.25	271.43	0.79
Pu-241	2.53E-08	1012.68	0.65	361.29	1.37

Application of Global Sensitivity: Sensitivity Analysis

- ***Absorber region: cross sections and uncertainty values as a function of energy***

Isotope	Energy (MeV)	Absorption XS (barns)	Sigma XS (barns)	Uncertainty (%)
B-10	2.53E-08	10B(n,a0)	241.2677	0.21
		10B(n,a1)	3598.228	0.16
	9.40E-06	10B(n,a1)	186.435	0.16

Application of Global Sensitivity: Sensitivity Analysis

- ***Moderator region: cross sections and uncertainty values as a function of energy***

H-1		
Energy (MeV)	**Uncertainty (%)**	**Elastic Scattering XS (barns)**
2.53E-08	0.20	20.436330
2.0	0.22	2.903645
4.0	0.30	1.894349
6.0	0.36	1.418157
8.0	0.44	1.129564
10.0	0.50	0.934397
12.0	0.49	0.793504
14.0	0.46	0.687114
16.0	0.40	0.604026
18.0	0.35	0.537384
20.0	0.30	0.482746

Application of Global Sensitivity: Sensitivity Analysis

- ***Summary of modified cross sections***

Values/Column	Cross Section Modified
1	Fission U-235 Thermal
2	Fission Pu-239 Thermal
3	Fission Pu-241 Thermal
4	Capture U-235 Thermal
5	Capture Pu-239 Thermal
6	Capture Pu-241 Thermal
7	Absorption B-10 (n,a0) Thermal
8	Absorption B-10 (n,a1) Thermal
9	Absorption B-10 (n,a1) Fast
10 to 20	Elastic Scattering H-1 from 0 to 20 MeV

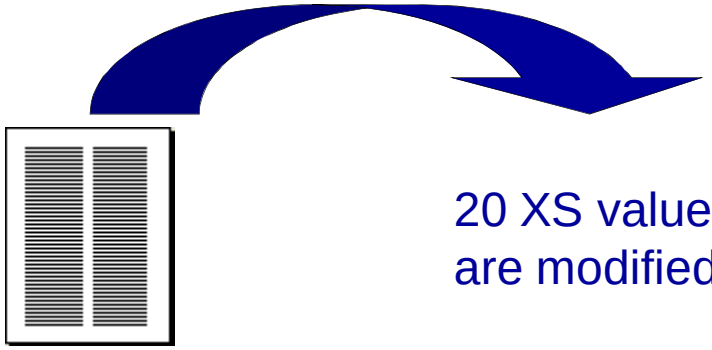
Sensitivity Analysis

- ✓ Only the uncertainties of the 20 cross sections mentioned previously are considered.
- ✓ A 20-column sample matrix with 2816 rows (cases) was generated to represent such uncertainties. The sample matrix was later expanded to 5110 cases to check convergence.
- ✓ Each row represents 20 cross section values that are used to simulate continuous energy MCNP5 criticality calculation.
- ✓ A code was prepared to automate the flow of all calculations and to directly modify the cross section files of each isotope.

Sensitivity Analysis

1st analysis:
2816 calcs.

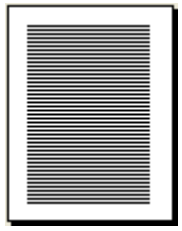
2nd analysis:
5110 calcs.



20 XS values
are modified

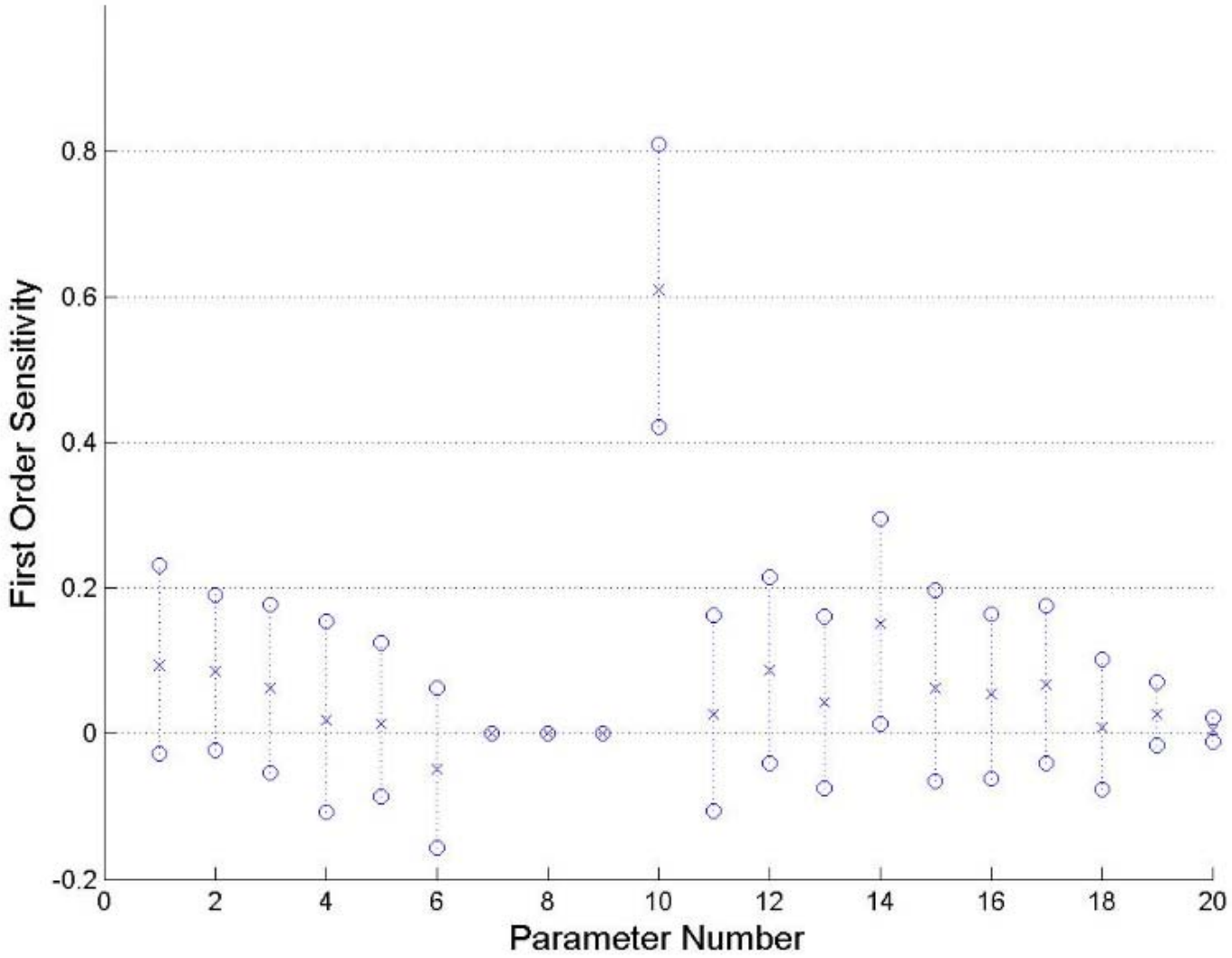
MCNP5 continuous
energy calculations

k_{eff}



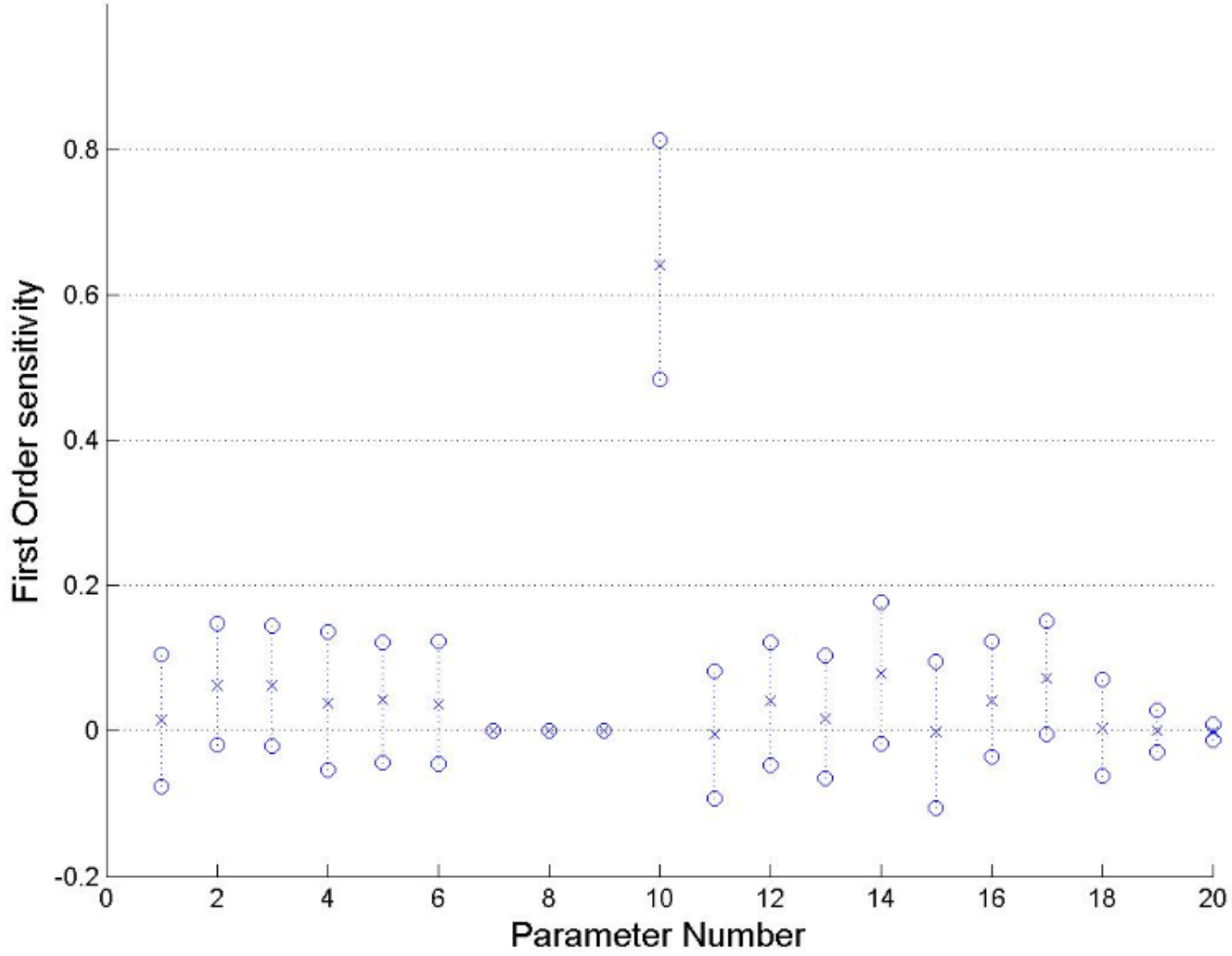
Application of Global Sensitivity: Sensitivity Analysis

- ***First Order 2816 Sensitivity Indices***



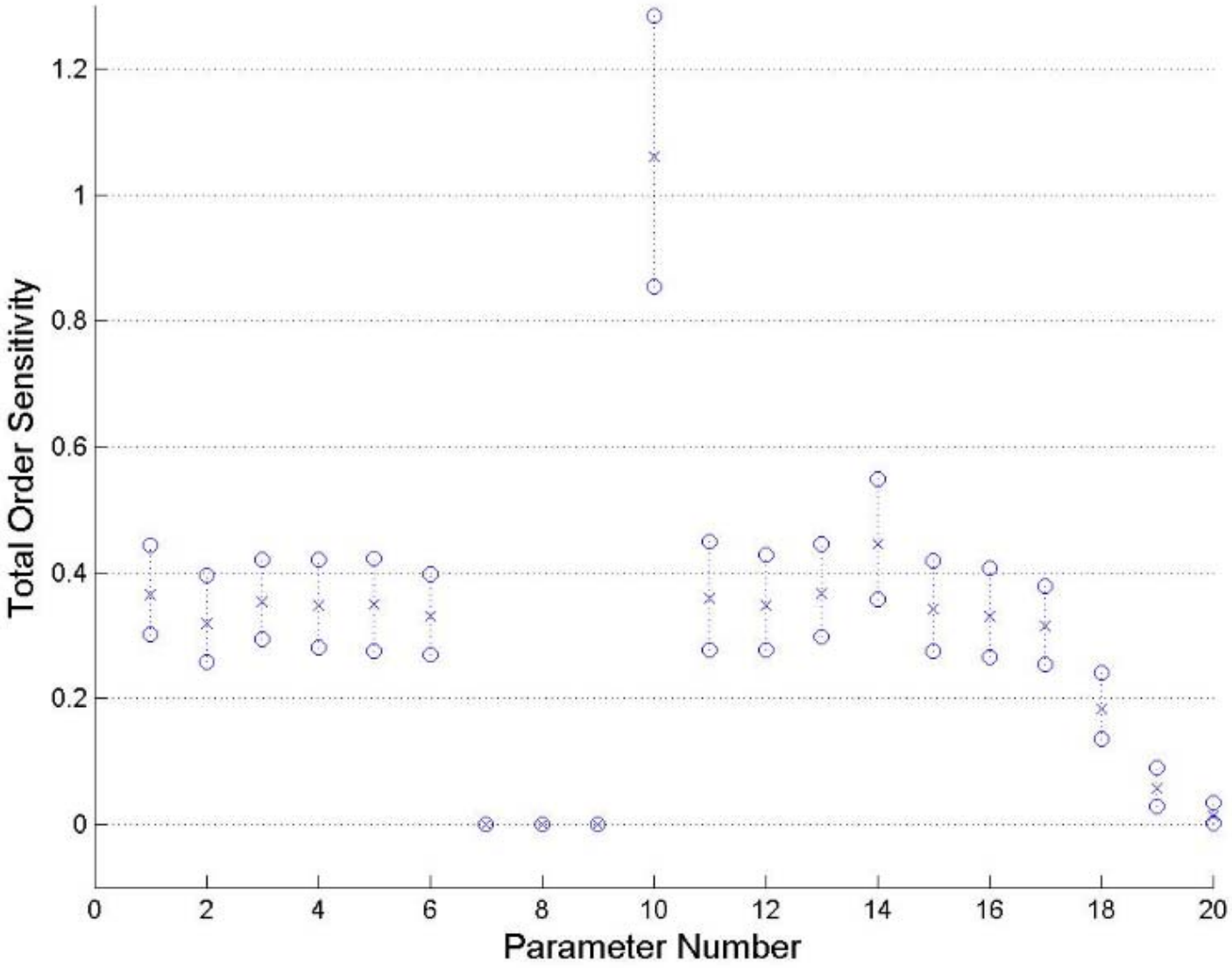
Application of Global Sensitivity: Sensitivity Analysis

- ***First Order 5110 Sensitivity Indices***



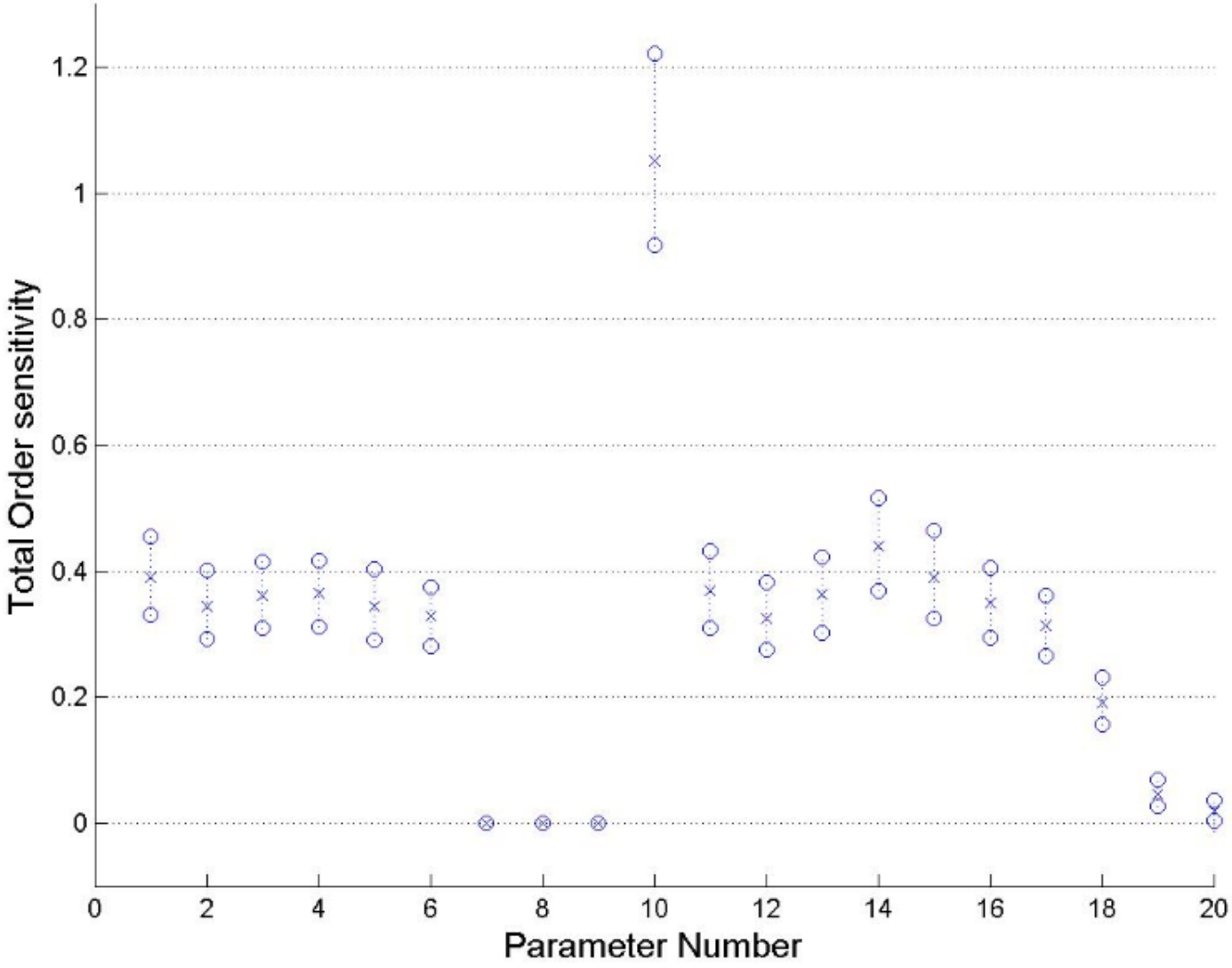
Application of Global Sensitivity: Sensitivity Analysis

- ***Total Order 2816 Sensitivity Indices***



Application of Global Sensitivity: Sensitivity Analysis

- ***Total Order 5110 Sensitivity Indices***



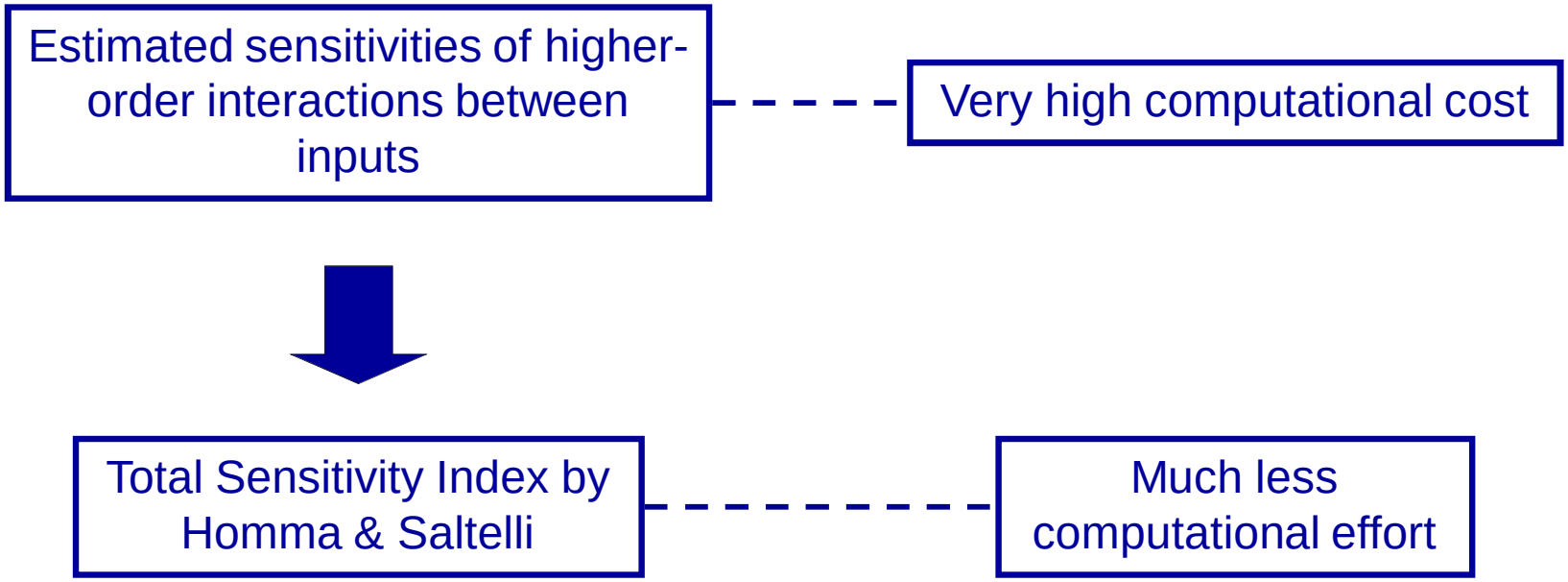
Sensitivity Analysis

- ✓ The sensitivity analysis methodology applied in this test, originally due to Sobol, has been ameliorated by Saltelli.

- ✓ The method of Sobol is variance-based, meaning that the variance of the model output can be decomposed into terms of increasing dimension, called partial variances, that represent the contribution of each single input to the overall uncertainty of the model output.

- ✓ This method allows the simultaneous exploration of the space of the uncertain inputs, which is carried out via Monte Carlo.

Sensitivity Analysis



- ✓ **The total sensitivity index provides an indication of the overall effect of a given input, taking into account all possible interaction of that input with all the others.**

Sensitivity Analysis

- ✓ The results show,
  - ✓ The first order indices, measuring the importance of individual parameters, illustrate that parameter 10 (thermal scattering cross section of H-1) is the most important (with the highest variation in the output).
  - ✓ The second highest indices were found for the elastic scattering of H-1 at a middle energy point (8 MeV).
  - ✓ The next higher indices were for the fission cross sections (U-235, Pu-239 and Pu-241, for which the highest is for U-235, as expected) and the capture cross sections. These parameters present an equivalent influence on the output.

Sensitivity Analysis

- ✓ The results show,
  - ✓ The total sensitivity indices, which measure the importance of one parameter considering all the interactions with the rest, help to identify the parameters that are not important and can be fixed; like parameters 7, 8, 9 and 20.
  - ✓ The bootstrap analysis is very similar for both studies (for the 2816 and 5110 cases).
  - ✓ The small variation on the bound's amplitude illustrate the certain convergence has been reached. The results are stable and no unexpected changes should appear.

Conclusions

- ✓ Global sensitivity analysis is applied to the modeling of nuclear reactor physics for better model understanding.
- ✓ In particular, it is investigated how much criticality conditions are affected by uncertainties in nuclear cross-sections, at different energies, from several isotopes in the fuel, the absorber and the moderator.