ULSAN NATIONAL INSTITUTE OF SCIENCE AND TECHNOLOGY

Progress on Reactor Cross Sections Processing code--RXSP

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OUTLINES

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- **Features**
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  - **Fast Doppler broadening**
  - **S(a,b) Interpolation**
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  - **P-Table Interpolation**
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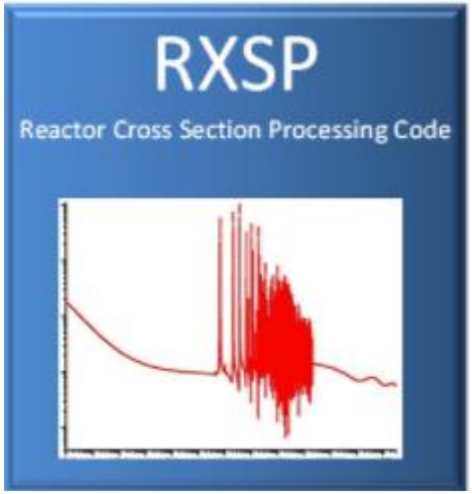
- **Conclusion**

Introduction

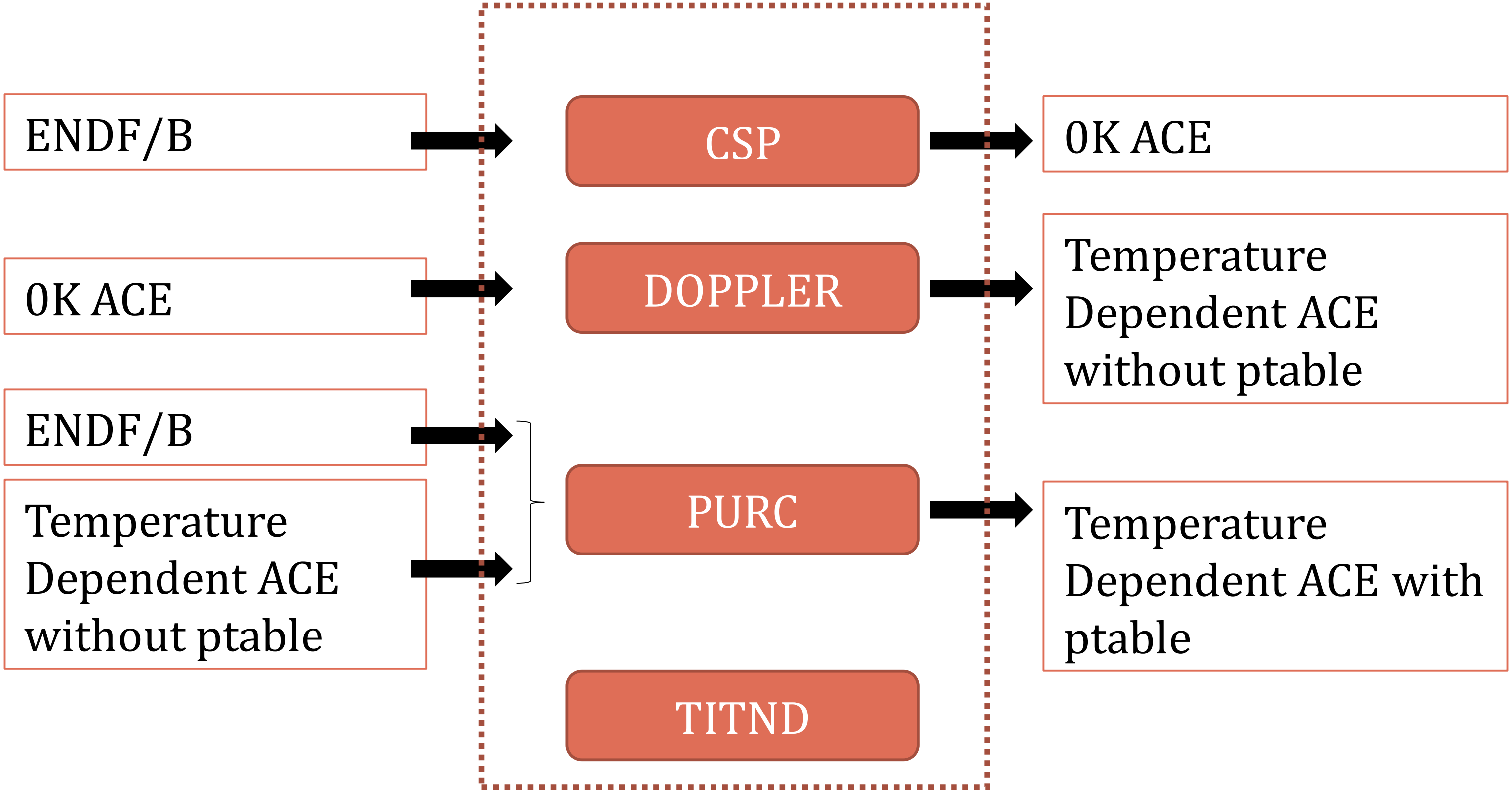
Introduction

- **Background**
  - **The accuracy of the nuclear cross section data is a prerequisite for the accuracy of reactor neutron transport calculations, i.e. MC method.**
  - **RXSP is a nuclear Cross Section Processing code being originally developed by REAL group, Department of Engineering Physics, Tsinghua University, which is mainly intended to reactor analysis.**
  - **The current version is RXSP-Beta 2.0 released in August,2013 domestically in China Mainland. The Beta3.0 version is being developed jointly by UNIST and Tsinghua University(per the agreement of Prof. Lee and Prof. WANG).**



Introduction

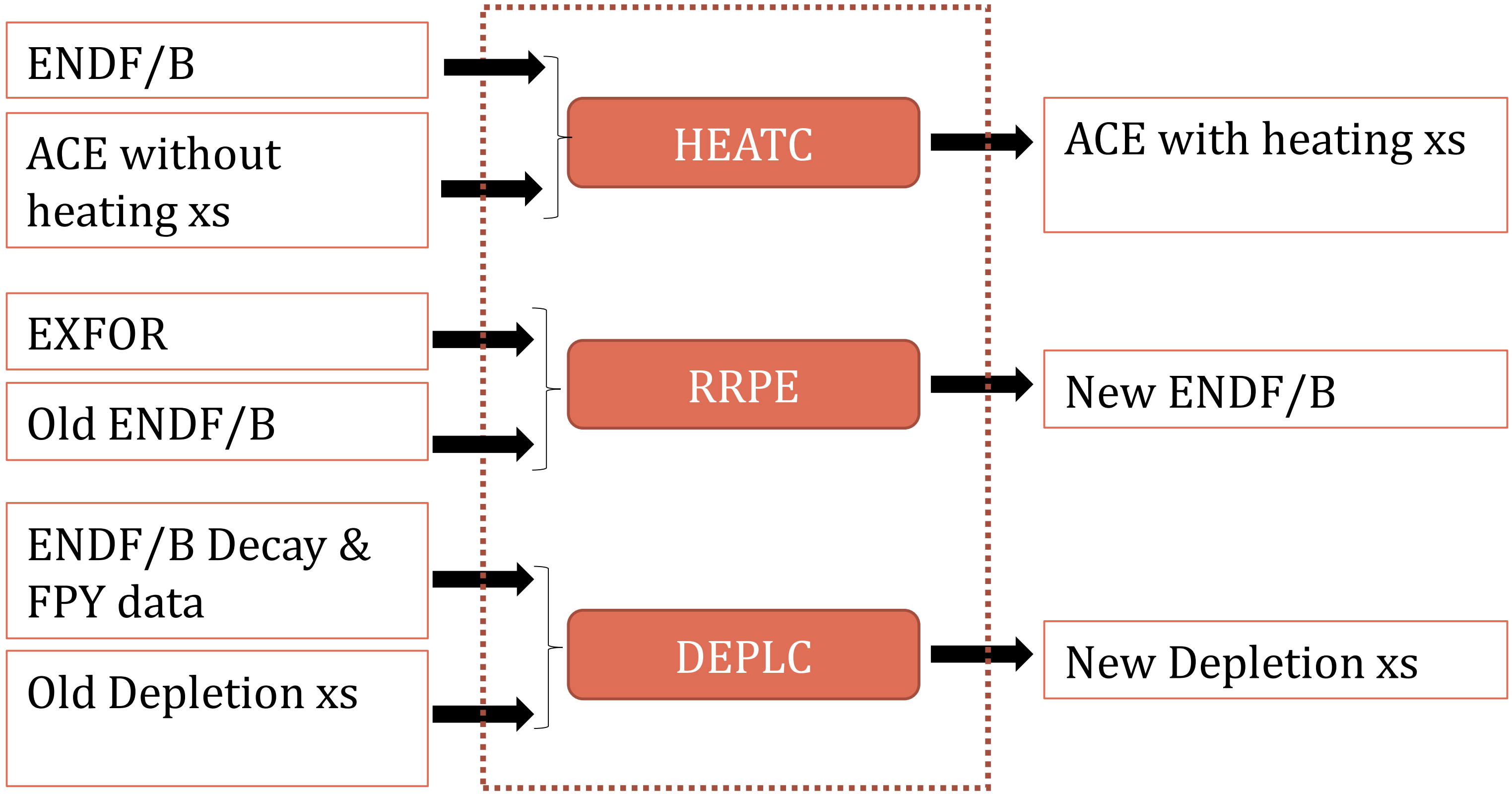
▪ Modules and Functions



CSP: module for resonance reconstruction and linearization
DOPPLER: module for Doppler Broadening
PURC: module for probabilistic table in unresolved resonance region
TITND: module for interpolation of thermal cross section

Introduction

▪ Modules and Functions



HEATC: module for Heating number calculation

RRPE: module for resolved resonance parameters evaluation

DEPLC: module for Depletion Library Updated Calculation

Introduction

▪ Modules and Functions

RXSP v.s. Others

CSP	RECONR+ACER /NJOY
DOPPLER	BROADR/NJOY
PURC	PURR/NJOY
TITND	MAKXSF/MCNP
HEATC	HEATR/NJOY
RRPE	SAMMY
DEPLC	AVEFPY/WLUP

Features

Features

- a. Support all resonance parameters
- b. Fast Doppler broadening
- c. Fast P-Table Generation
- d. P-Table Interpolation
- e. S(a,b) Interpolation

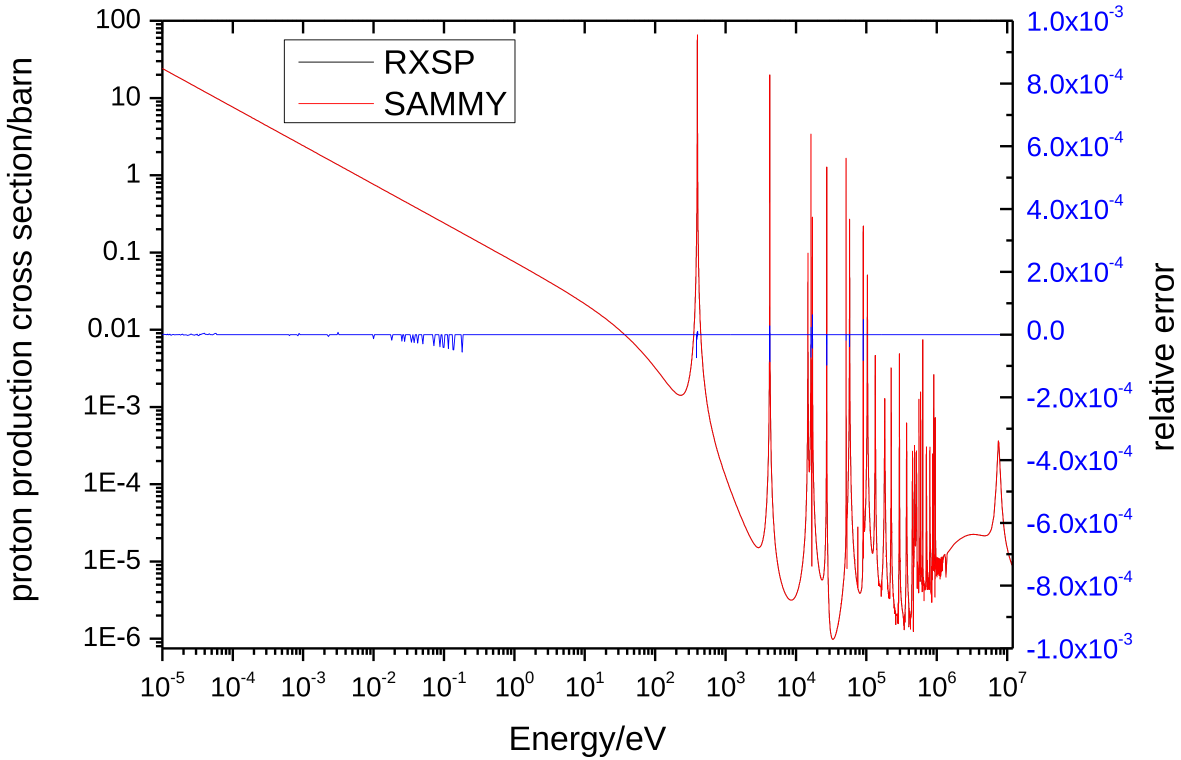
Features

a. Support all R-Matrix Resonance Parameters

Formula	approximation	application
SLBW	Ignores all interferences of all resonances of all cross sections	Narrow resonances only
MLBW	Ignores non-diagonal items of level matrix	Non-fission reactions only
Adler-Adler	No physical approximation, but make complex orthogonal transformation to level matrix	Widely Used in earlier engineering, but fall into disuse now
Reich-Moore (widely used)	Igonres interferrences of all but elastic scttering cross sections	Can handle interferences of multi-level elastic scattering reactions for fissile isotopes, widely used
R-Matrix Limited (latest)	Ignores only interferences of resonances of capture cross sections	To be used and developed, highly recommended by CSEWG
Full R-Matrix Not applied	No approximation	Too complicated

Features

Proton production cross section for ^{35}Cl

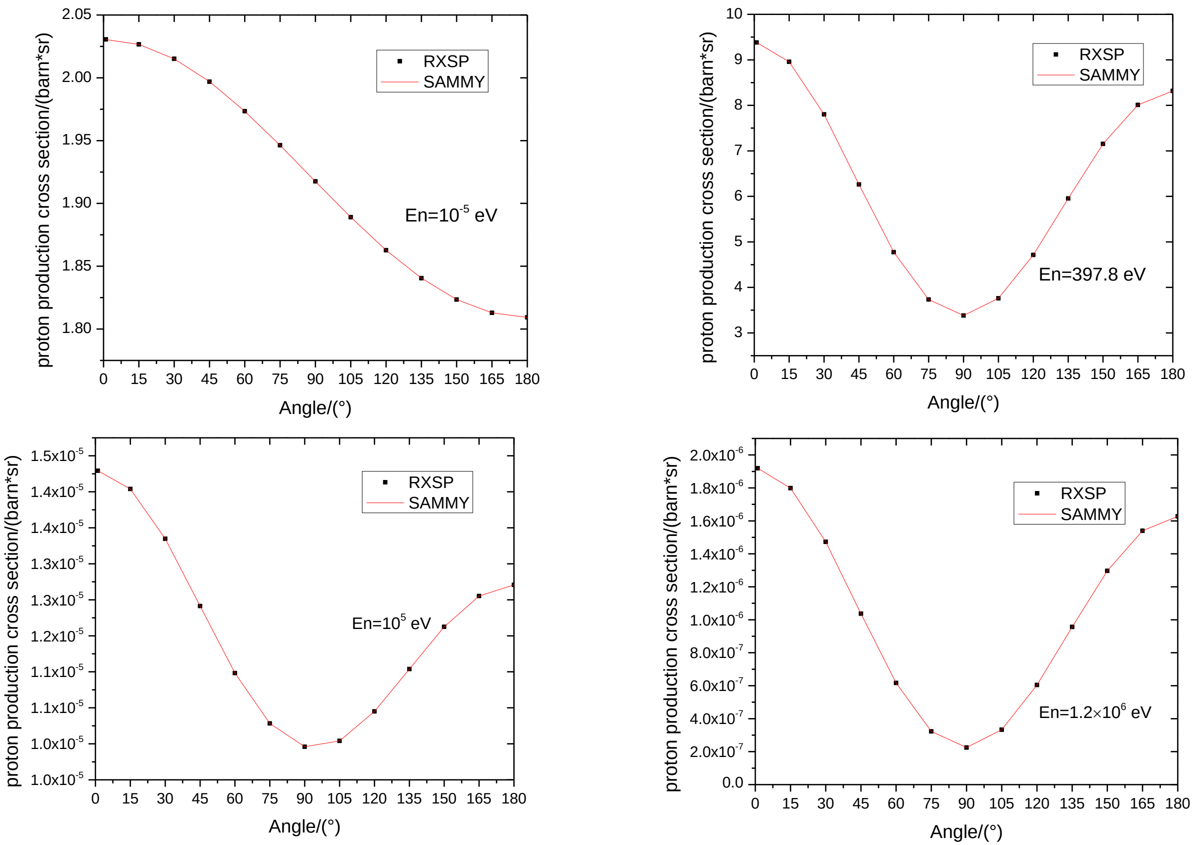


RRR:10^{-5}eV--1.2MeV

Only RML can express proton production cross sections by resonance parameters

Features

Angular-differential proton production cross section for ^{35}Cl



Only RML can express differential cross sections by resonance parameters

b. Fast Doppler broadening

- **Gauss-Legendre quadrature**
  - Reduce computational cost

$$\bar{\sigma}(v) = \frac{\alpha^{1/2}}{\pi^{1/2}} \int_0^\infty dV \sigma(V) V^2 \left\{ e^{-\alpha(V-v)^2} - e^{-\alpha(V+v)^2} \right\}$$

$$\sigma^*(y,T) = \frac{1}{\pi^{1/2} y^2} \sum_{i=0}^{N} \int_{x_i}^{x_{i+1}} \sigma(x) x^2 e^{-(x-y)^2} dx = \sum_i \left\{ A_i[\sigma_i - s_i x_i^2] + B_i s_i \right\}$$

$$s_i = (\sigma_{i+1} - \sigma_i) / (x_{i+1}^2 - x_i^2)$$

$$A_i = \frac{H_2}{y^2} + \frac{2H_1}{y} + H_0$$

$$B_i = \frac{H_4}{y^2} + \frac{4H_3}{y} + 6H_2 + 4yH_1 + y^2 H_0$$

$$H_n(a,b) = \frac{1}{\sqrt{\pi}} \int_a^b z^n e^{-z^2} dz$$

$$\int_{-1}^{+1} f(x)dx \approx \sum_{k=1}^{N} w_k f(r_k)$$

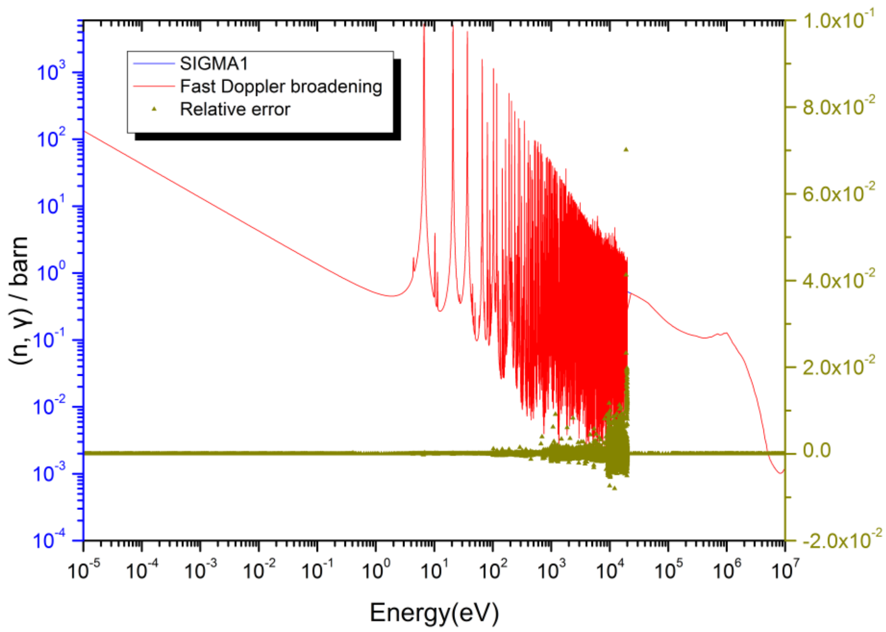
$$\sigma^*(y,T) = \frac{1}{\pi^{1/2} y^2} \cdot \sum_i \frac{x_{i+1} - x_i}{2} \sum_{k=1}^{N} w_k f\left(\frac{x_{i+1} - x_i}{2} r_k + \frac{x_i + x_{i+1}}{2}\right)$$

$$w_1 = w_2 = 1$$

$$x_1 = \frac{x_{i+1} + x_i}{2} - 0.5773502692 \times \left(\frac{x_{i+1} - x_i}{2}\right)$$

$$x_2 = \frac{x_{i+1} + x_i}{2} + 0.5773502692 \times \left(\frac{x_{i+1} - x_i}{2}\right)$$

- **Results**



Comparison of capture cross sections for ^{238}U at 600 K calculated from SIGMA1k kernel and Fast Doppler broadening method

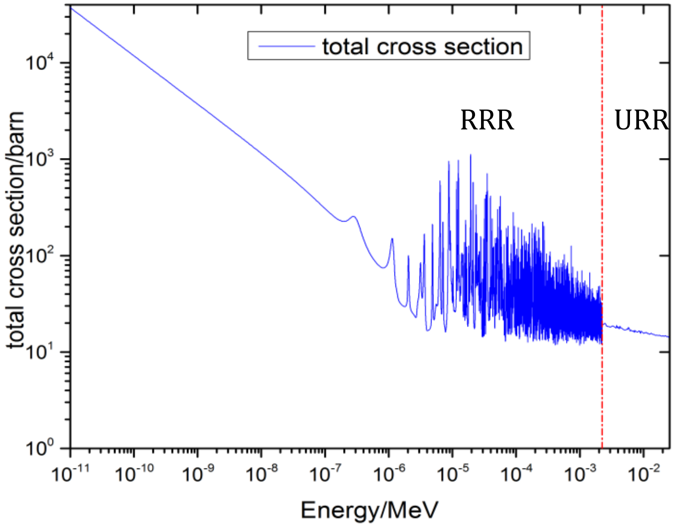
Features

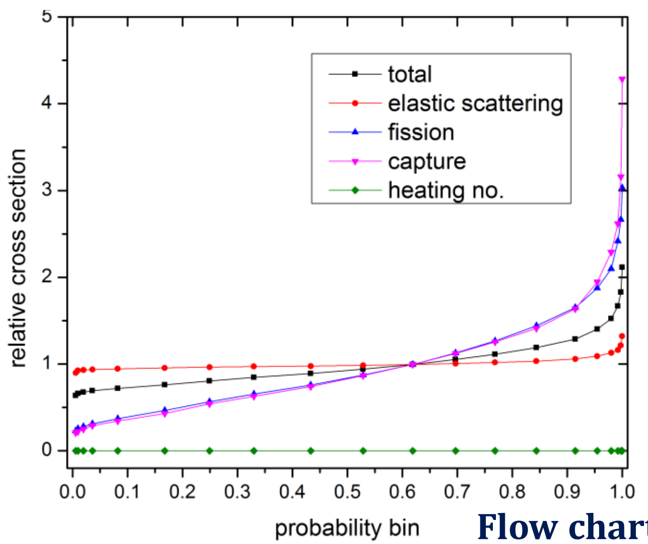
- **Results**

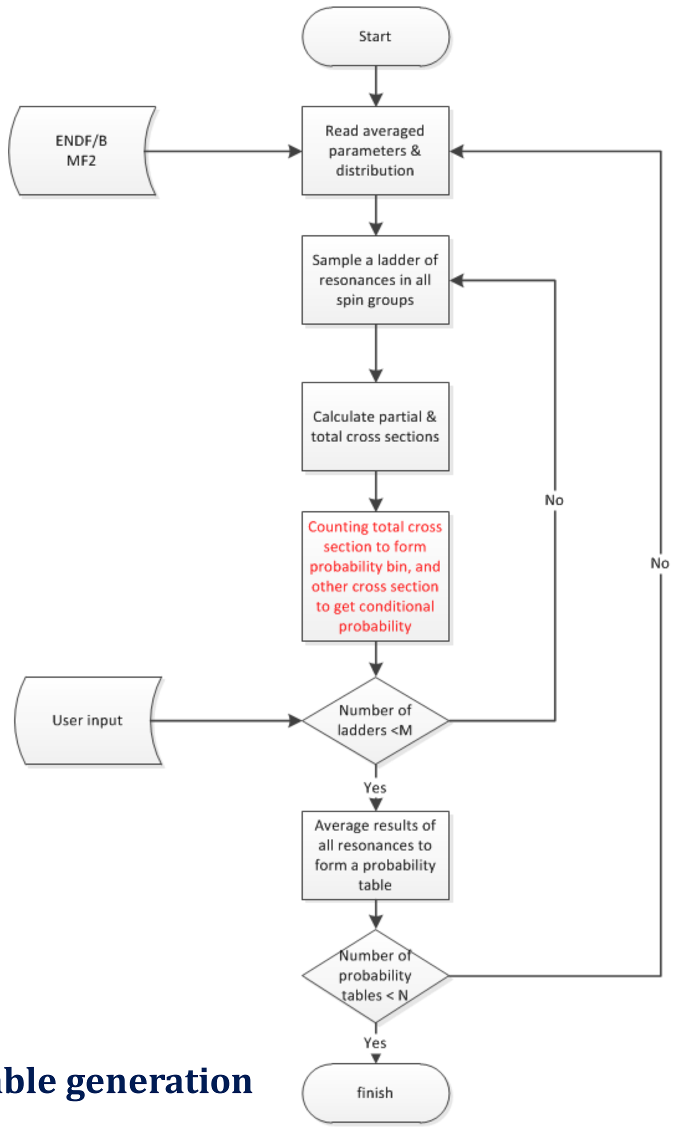
Isotope	t_{NJOY} / sec	t_{RXSP} / sec
^{238}U	35.0	13.88
^{235}U	21.7	9.594
^{233}U	3.2	1.482
^{239}Pu	16.9	6.099
^{232}Th	13.3	4.555

Comparison of CPU time for typical Isotope at 600K

c. Fast P-Table Generation

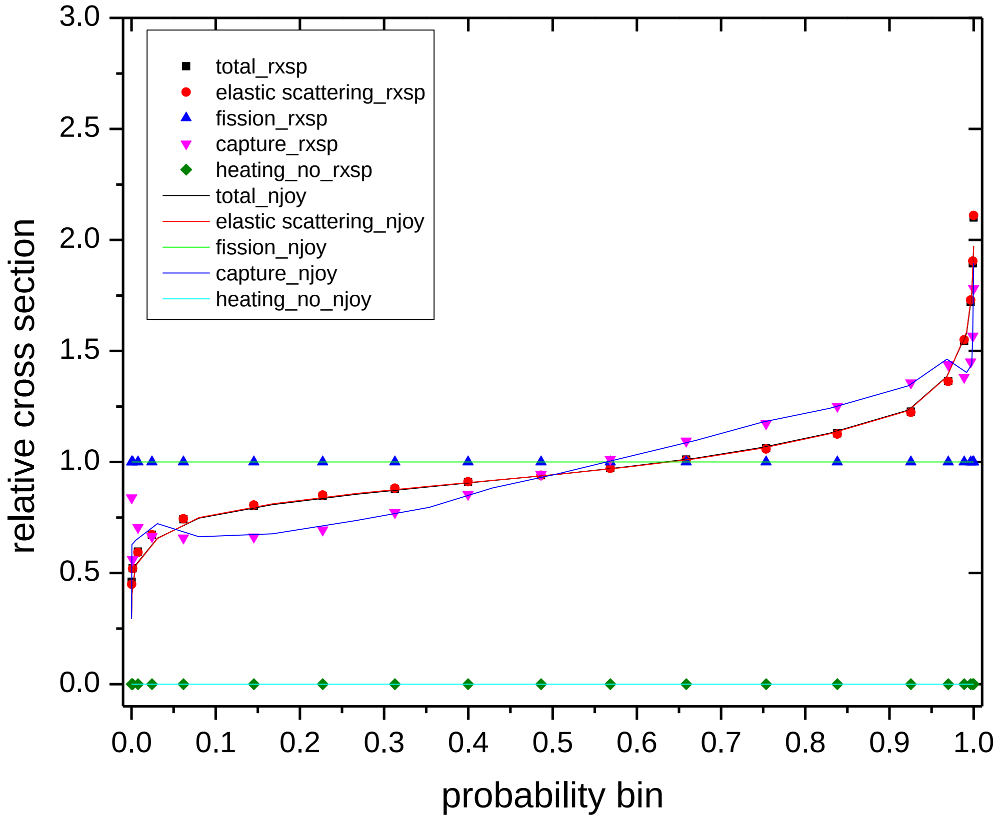






Flow chart of URR P-Table generation

Features

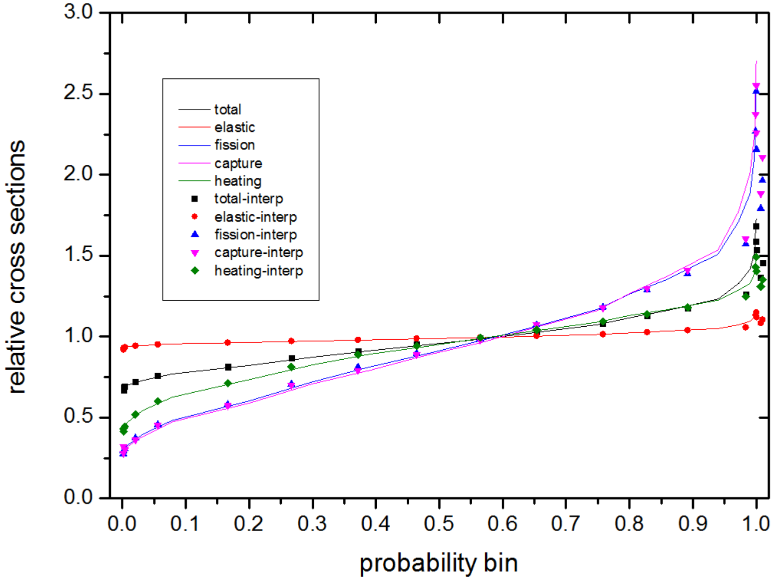


Probability table in 50keV of ^{232}Th in 293.6

d. P-Table Interpolation

- **Equi-probable interpolation**

$$\sigma(E,T)=\sigma(E,T_1)\cdot\exp\left(\frac{\ln T/T_1}{\ln T_2/T_1}\cdot\ln\left(\frac{\sigma(E,T_2)}{\sigma(E,T_1)}\right)\right)$$

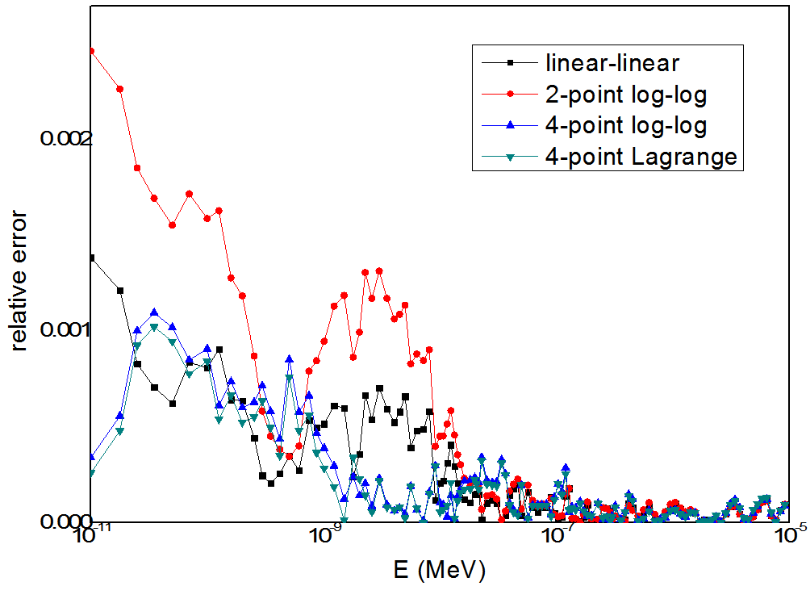


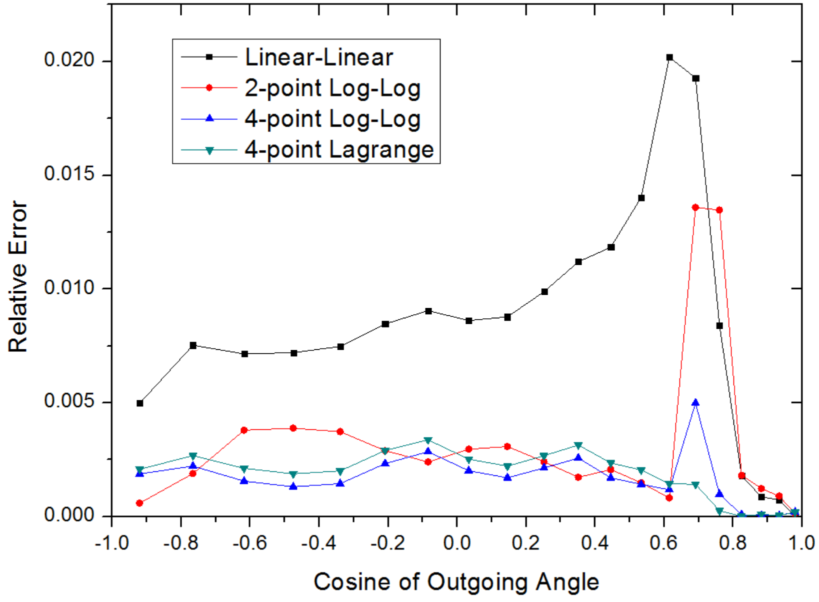
Comparison of probability tables calculated from NJOY and log-log interpolated (from 293.6K and 900 K) for ^{235}U (E_{in}=2.25keV) at 600 K.

e. S(a,b) Interpolation

- **4-point Lagrange interpolation**

$$\sigma(E,T)=\sigma(E,T_1)\cdot\frac{T-T_2}{T_1-T_2}\cdot\frac{T-T_3}{T_1-T_3}\cdot\frac{T-T_4}{T_1-T_4}+\sigma(E,T_2)\cdot\frac{T-T_1}{T_2-T_1}\cdot\frac{T-T_3}{T_2-T_3}\cdot\frac{T-T_4}{T_2-T_4}$$
$$+\sigma(E,T_3)\cdot\frac{T-T_1}{T_3-T_1}\cdot\frac{T-T_2}{T_3-T_2}\cdot\frac{T-T_4}{T_3-T_4}+\sigma(E,T_4)\cdot\frac{T-T_1}{T_4-T_1}\cdot\frac{T-T_2}{T_4-T_2}\cdot\frac{T-T_3}{T_4-T_3}$$

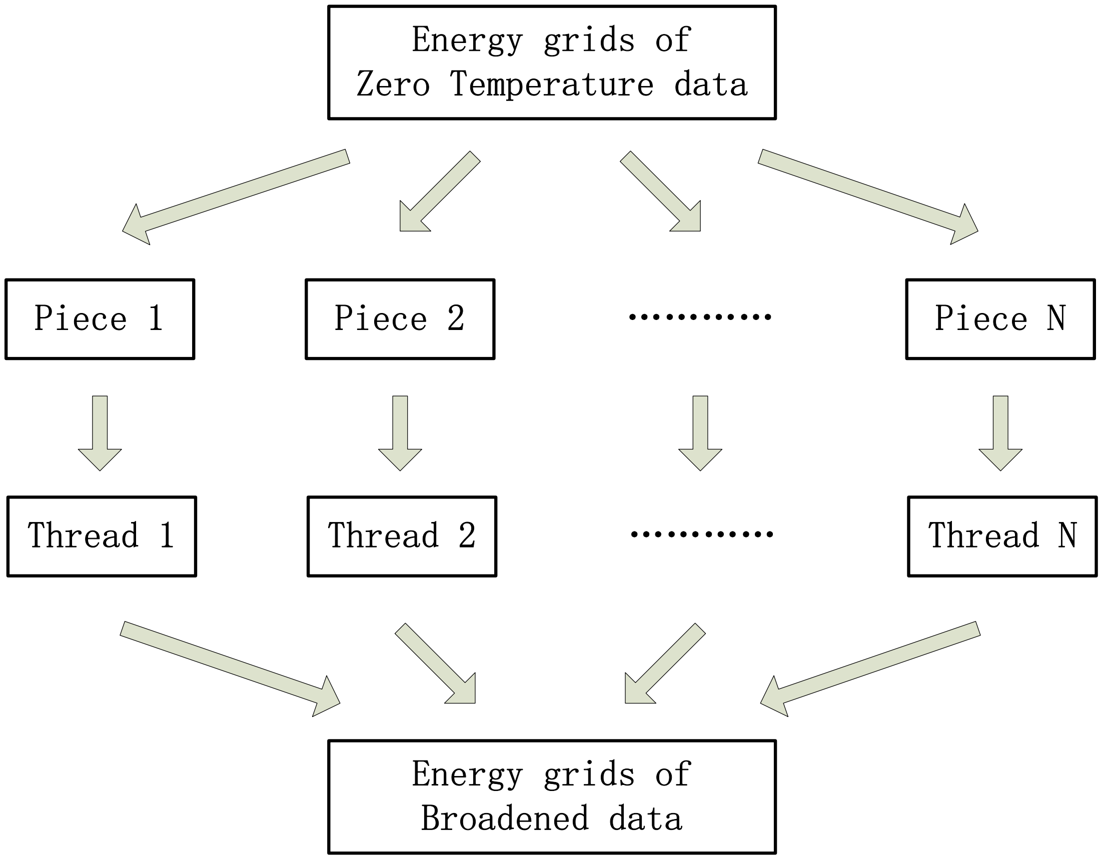




Comparison of different interpolation schemes for inelastic scattering(integral : left, differential : right) cross sections for light water

f. OpenMP parallel

- **Parallel in Doppler broadening**



f. OpenMP parallel

- **Parallel in Doppler broadening**

Condition of Computation:

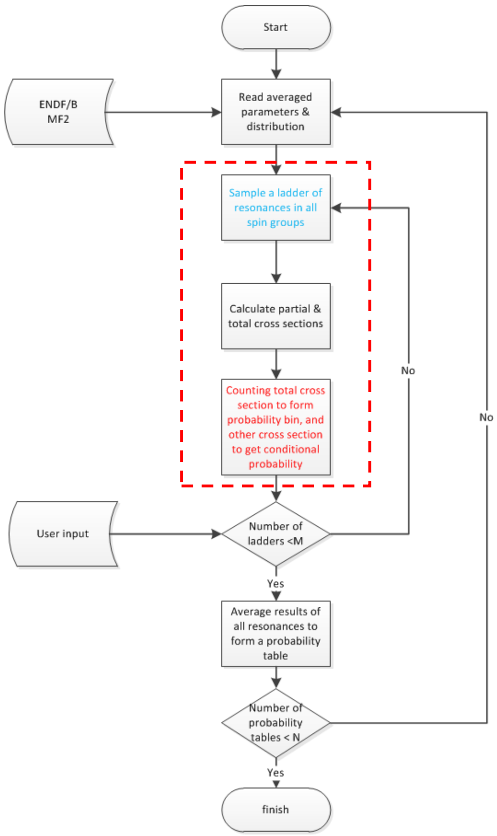
Intel X5670,12 CPUs,2.93 GHz.

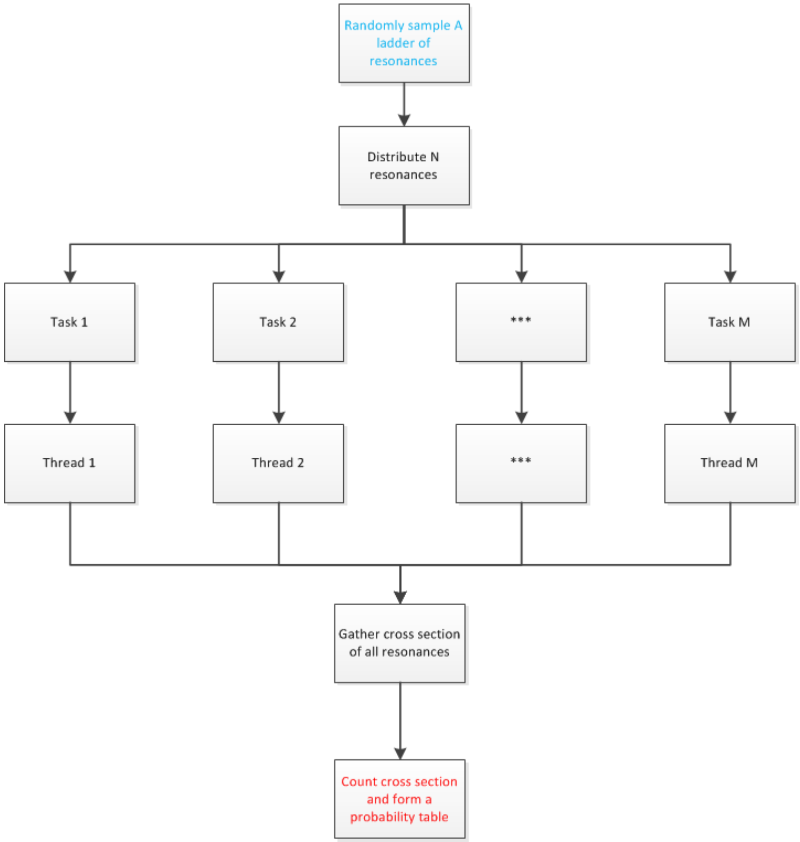
Isotopes	t_{RXSP} / sec	t_{NJOY} /sec
^{238}U	2.086	231.0
^{235}U	1.442	192.9
^{233}U	0.37	12.7
^{239}Pu	0.984	34.1
^{232}Th	1.102	60.2

Comparison of CPU time for typical isotopes at 600K by NJOY and RXSP

f. OpenMP parallel

- **Parallel in P-Table Generation**





f. OpenMP parallel

- **Parallel in P-Table Generation**

Condition of Computation:

Intel X5670,20 CPUs,2.93 GHz.

Isotopes	t_{NJOY}/sec	t_{RXSP}/sec	Ratio
^{233}U	436.4	32.8	13.3
^{238}U	111.9	2.75	40.7
^{232}Th	567.9	7.7	73.7
^{239}Pu	546.8	12.1	45.2

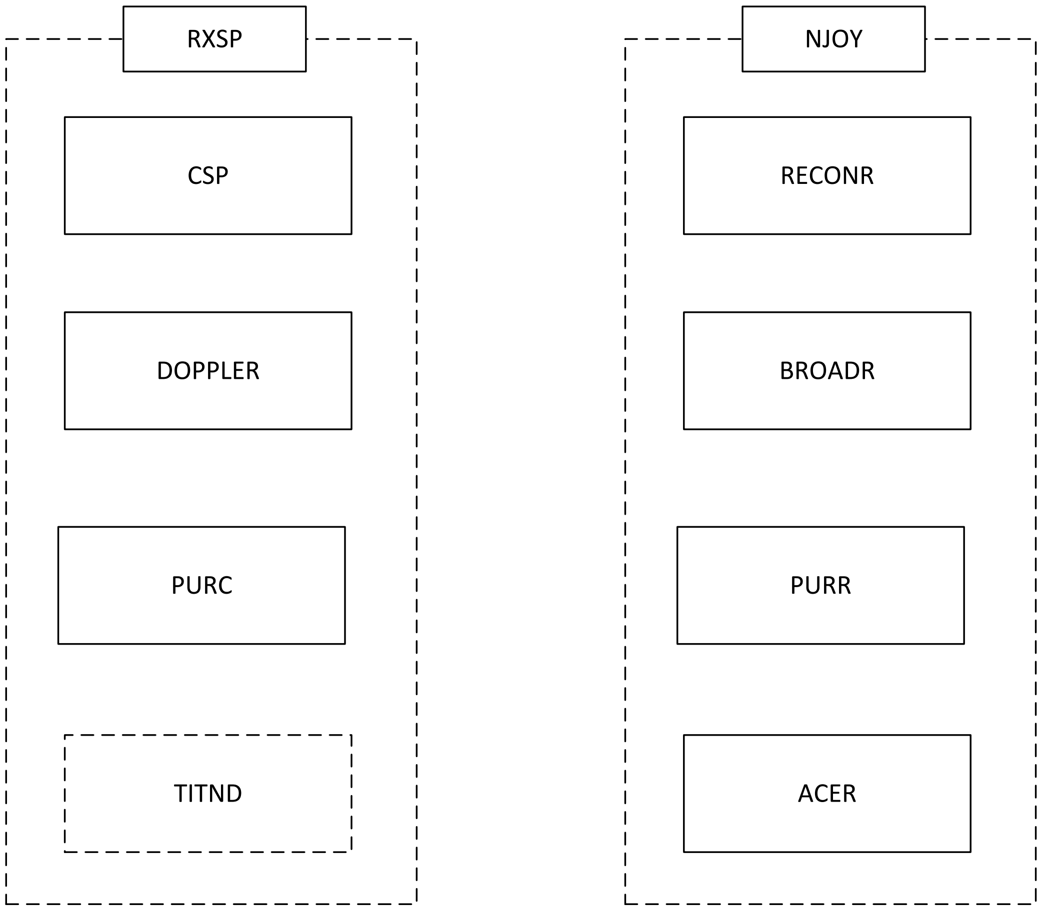
Comparison of CPU time for typical isotopes by NJOY and RXSP

Validation

Validation

Cross Sections Library Processing

- **Source**
  - ENDF/B-VII.0
- **Toolkit**
  - RXSP
  - NJOY
- **Libraries**
  - ENDFb7_r
  - ENDFb7_n
- **Resonance Reconstruction**
  - 0.001
- **Doppler Broadening**
  - 0.001
  - 293.6 K
  - 1.0 MeV
- **Probability Tables**
  - 20 bins
  - 16 ladders
  - 293.6 K



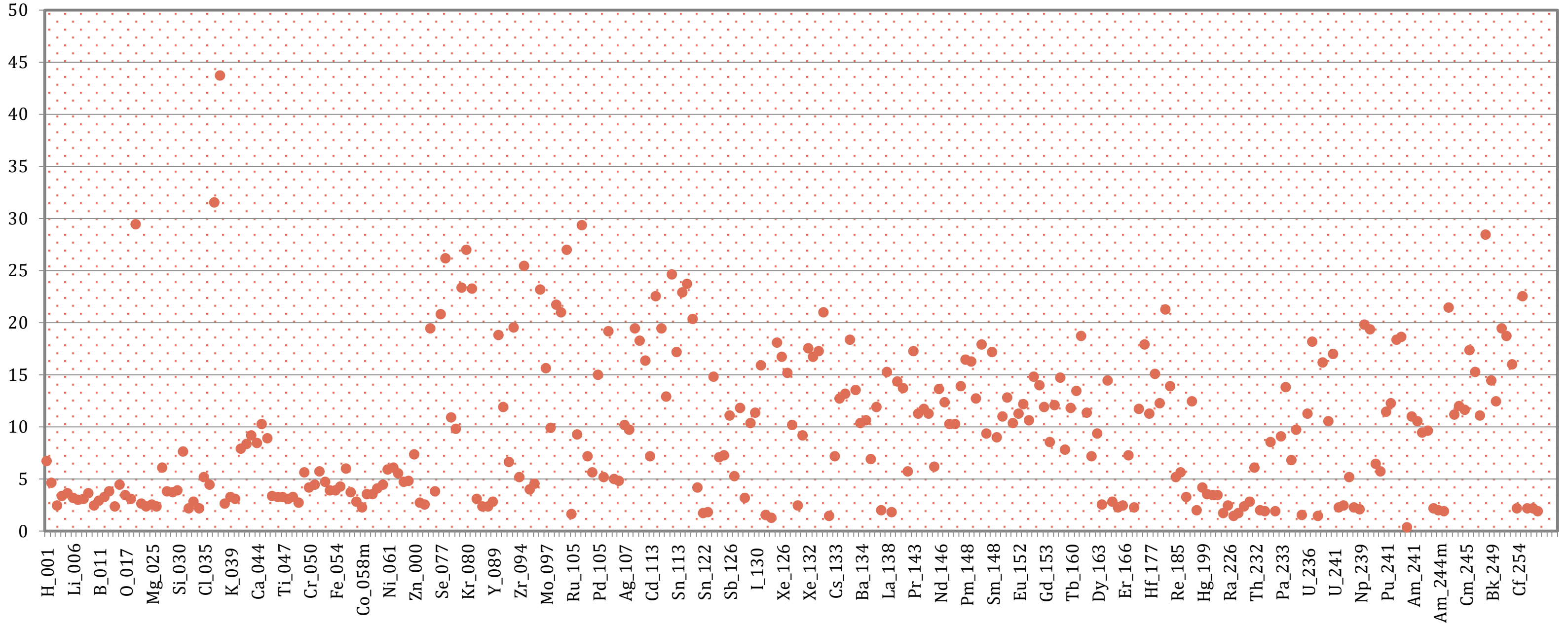
Validation

Isotopes List(285/393)

H-001	**H-002**	**H-003**	**He-003**	**He-004**	**Li-006**	**Li-007**	**Be-007**
Be-009	B-010	B-011	C-000	N-014	N-015	O-016	O-017
F-019	Na-022	Na-023	Mg-024	Mg-025	Mg-026	Al-027	Si-028
Si-029	Si-030	P-031	S-032	S-033	S-034	Cl-035	Cl-037
Ar-036	Ar-038	Ar-040	K-039	K-041	Ca-040	Ca-042	Ca-043
Ca-044	Ca-046	Ca-048	Sc-045	Ti-046	Ti-047	Ti-048	Ti-049
Ti-050	V-000	Cr-050	Cr-052	Cr-053	Cr-054	Mn-055	Fe-054
Fe-056	Fe-057	Fe-058	Co-058	Co-058m	Co-059	Ni-058	Ni-059
Ni-060	Ni-061	Ni-062	Ni-064	Cu-063	Cu-065	Zn-000	Ga-069
Ga-071	Ge-070	Ge-073	Se-077	Se-079	Br-079	Br-081	Kr-078
Kr-080	Kr-083	Kr-084	Kr-086	Sr-088	Y-089	Zr-090	Zr-091
Zr-092	Zr-093	Zr-094	Zr-095	Zr-096	Nb-093	Nb-094	Mo-097
Tc-099	Ru-099	Ru-101	Ru-103	Ru-105	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-106	Cd-111	Cd-113	Cd-115m	In-113	In-115	Sn-112
Sn-113	Sn-114	Sn-115	Sn-117	Sn-120	Sn-122	Sn-124	Sn-125
Sb-121	Sb-123	Sb-126	Te-122	Te-123	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
Ba-130	Ba-132	Ba-133	Ba-134	Ba-135	Ba-136	Ba-137	Ba-138
La-138	Ce-140	Ce-141	Ce-143	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-149	Pm-151	Sm-144	Sm-147	Sm-148	Sm-149	Sm-151	Sm-153
Eu-151	Eu-152	Eu-153	Eu-154	Eu-155	Eu-157	Gd-153	Gd-154
Gd-155	Gd-157	Tb-159	Tb-160	Dy-156	Dy-158	Dy-160	Dy-161
Dy-163	Ho-165	Ho-166m	Er-162	Er-164	Er-166	Er-167	Er-168
Lu-175	Lu-176	Hf-177	Hf-179	Ta-181	Ta-182	W-183	Re-185
Re-187	Ir-191	Ir-193	Au-197	Hg-199	Pb-204	Pb-207	Bi-209
Ra-223	Ra-226	Ac-226	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-236	U-237	U-238	U-239	U-240	U-241	Np-235	Np-236
Np-237	Np-238	Np-239	Pu-236	Pu-238	Pu-239	Pu-240	Pu-241
Pu-242	Pu-243	Pu-244	Pu-246	Am-241	Am-242	Am-242m	Am-243
Am-244	Am-244m	Cm-241	Cm-242	Cm-243	Cm-244	Cm-245	Cm-246
Cm-247	Cm-248	Cm-250	Bk-249	Cf-249	Cf-250	Cf-252	Cf-253
Cf-254	Es-253	Es-254	Es-255	Fm-255			

Comparison of Processing Time

Processing time ratio of NJOY to RXSP for all 285 isotopes



Platform: Intel(R) Xeon(R) cpu E5-2690 @ 2.90GHz(12 units)

Comparison of Processing Time

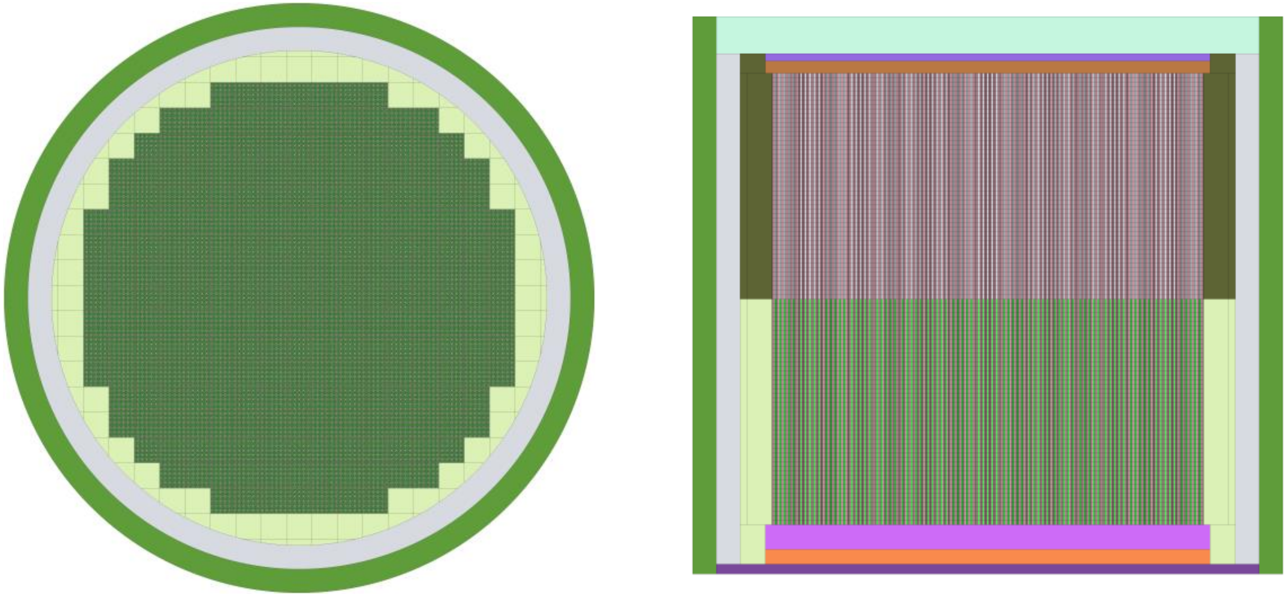
- **Processing Time(285 isotopes)**
  - **RXSP: 32.5 min**
  - **NJOY: 294.7 min**
- **The processing efficiency ratio of RXSP to NJOY for all 285 isotopes va ries from 1.4 to 43.6.**
- **The values for most isotopes are centered around 10.0, which is reaso nable for the process performed on the 12 threads computational pla tform.**
- **The averaged ratio of efficiency is 9.1, very close to the number of thr eads in it.**
- **It is concluded that the RXSP can achieve the increase of processing ef ficiency by over one order of magnitude compared with NJOY in the c urrent calculation condition.**

Case 1. Criticality Benchmark Suites

- **The suites of criticality validation used to verify the change of MCNP code and nuclear data libraries are expanded in early 2013 by Monte Carlo team in LANL**
  - **132 benchmarks**
  - **a wide representation of fissile materials, reflector materials, and spectra.**
  - **at least three fast, one intermediate, and two thermal benchmarks for U-233 system, highly enriched uranium system, intermediate enriched uranium systems, and plutonium systems**
- **Toolkit & ACE library**
  - **RMC / MCNP5**
  - **ENDFb7_r v.s. ENDFb7_n**

Case 2. Full Core Criticality Model

- **A typical PWR full-core criticality calculation is performed.**
  - J. Eduard Hoogenboom
  - M&C 2011
  - 34 isotopes

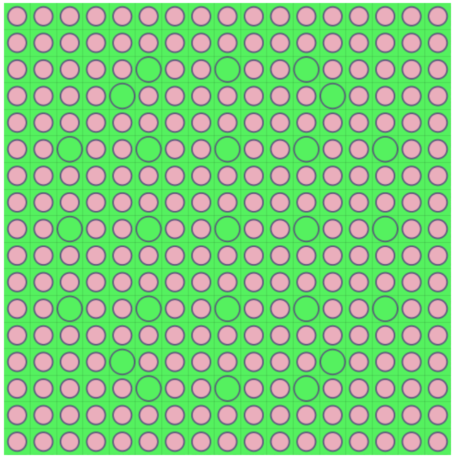


Top and front view of PWR full-core model

Case 3. Assembly Depletion Model

- **Here is a fuel assembly configuration shown in Figure to validate the depletion using ENDFb7_r library.**
  - **same dimension with the assembly in case 2**
  - **J. Eduard Hoogenboom**

Materials	Mass Density /(g·cm^{-3})	Isotopes	Atomic Density /(barn·cm^{-1})
Fuel	10.1960	U-235 U-238 O-16	6.91000E-03 2.20620E-01 4.55100E-01
Moderator （Coolant）	0.99977	H-1 O-16	6.66430E-02 3.33340E-02
Gap	0.00100	O-16	3.76622E-05
Cladding	6.55000	Zr-Nat	4.32411E-02

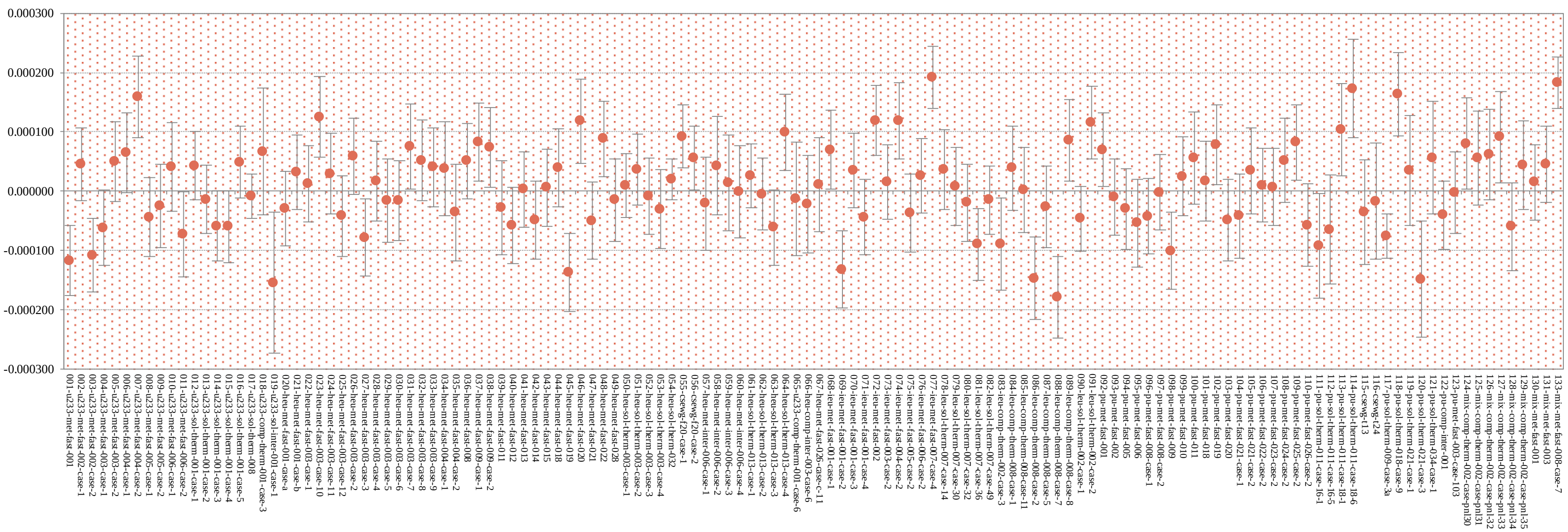


Material compositions & Configuration of a PWR fuel assembly

Validation

Results of Case 1： keff

- **20,000 histories/cycle**
- **100 inactive cycles/ 1,000 active cycles**

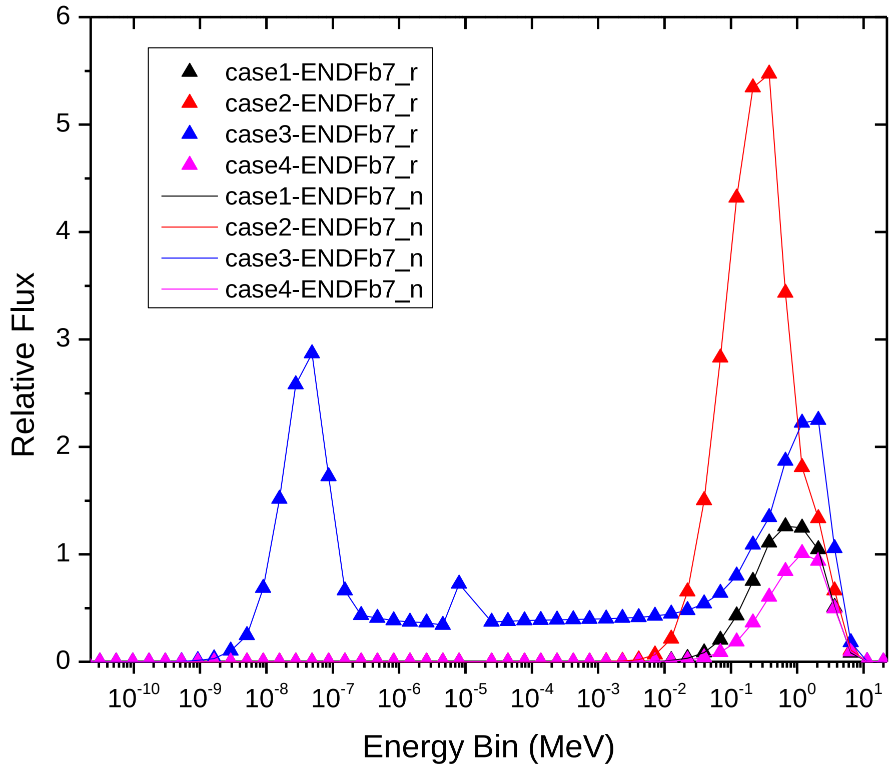


Total view of differences of k-effective of 132 benchmarks

Validation

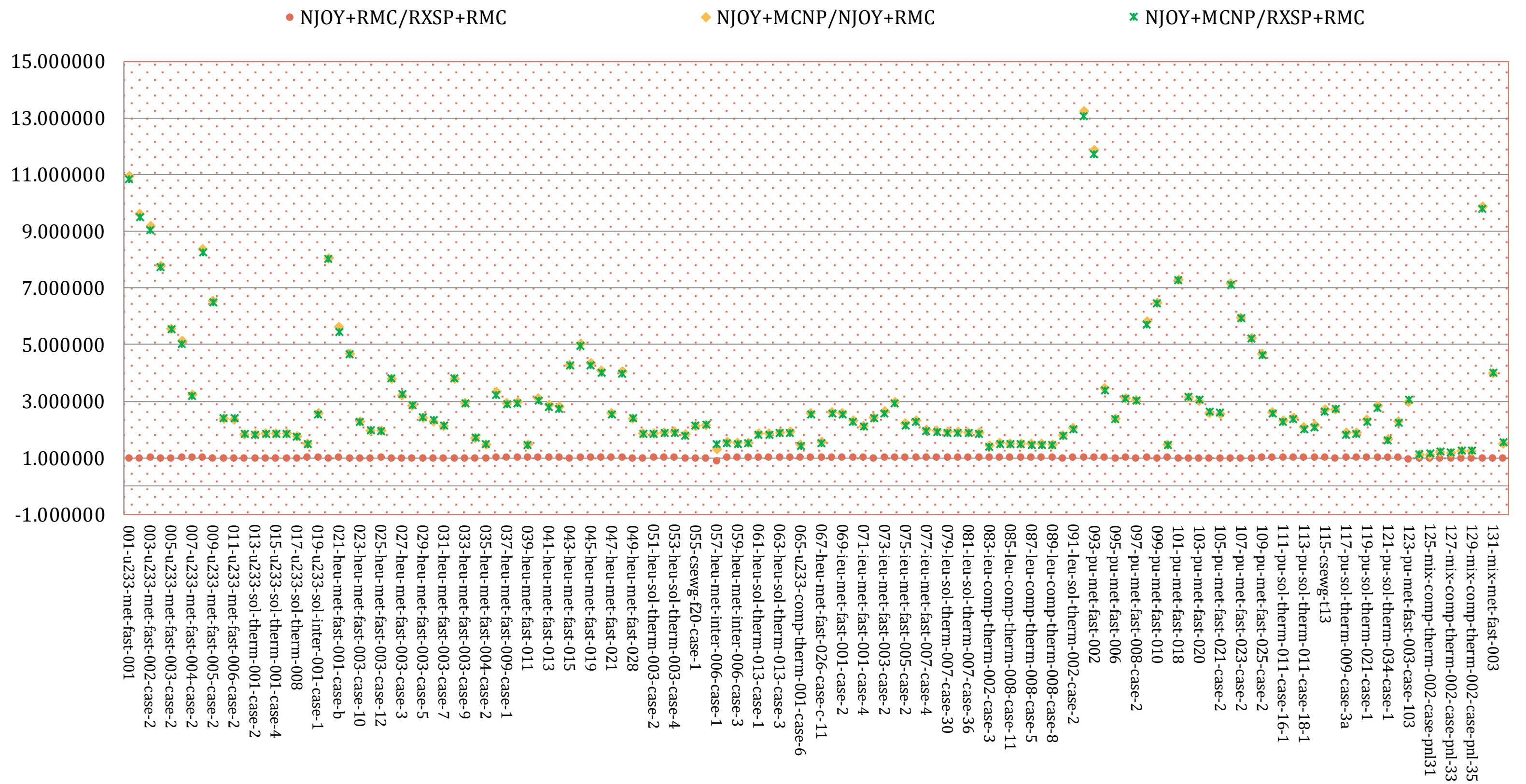
Results of Case 1: neutron spectrum

- Case 1: heu-met-fast-001-case-a
- Case 2: ieu-met-fast-002
- Case 3 : leu-sol-therm-007-case-14
- Case 4 : pu-met-fast-001



Validation

Results of Case 1: Simulation time



Results of Case 2

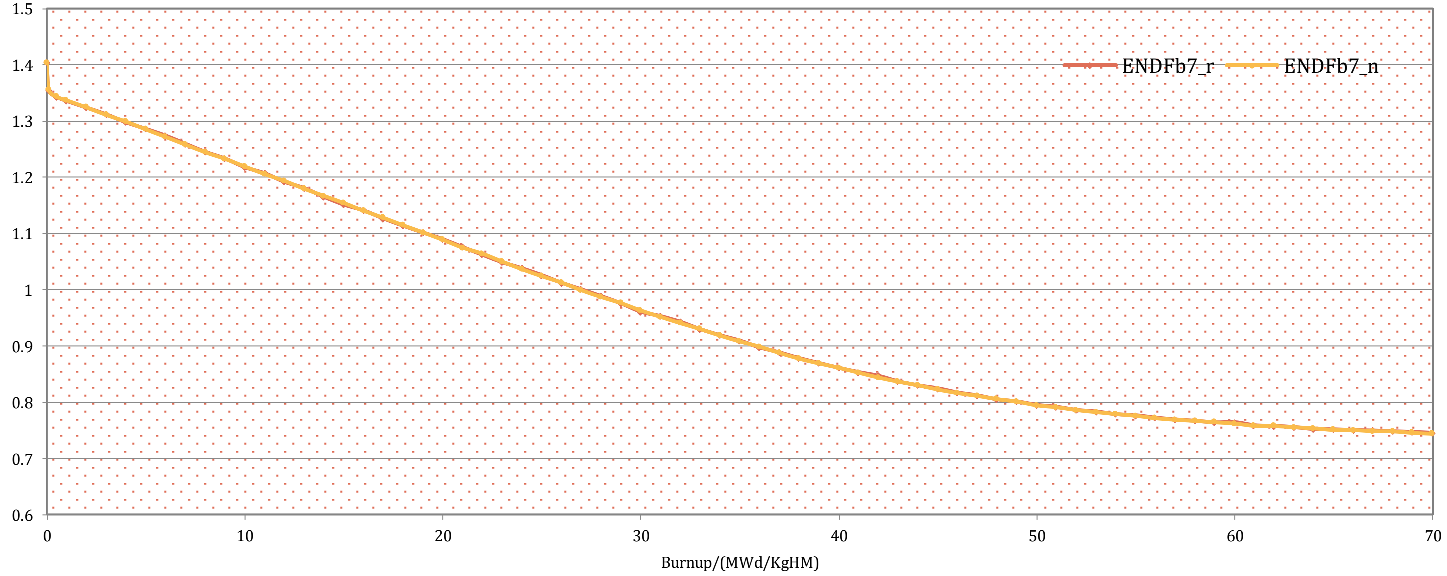
- 10,000 histories/cycle
- 250 inactive cycles/1000 active cycles

Library	k-effective
ENDFb7_n	1.001739 ± 0.000065
ENDFb7_r	1.001798 ± 0.000066

Validation

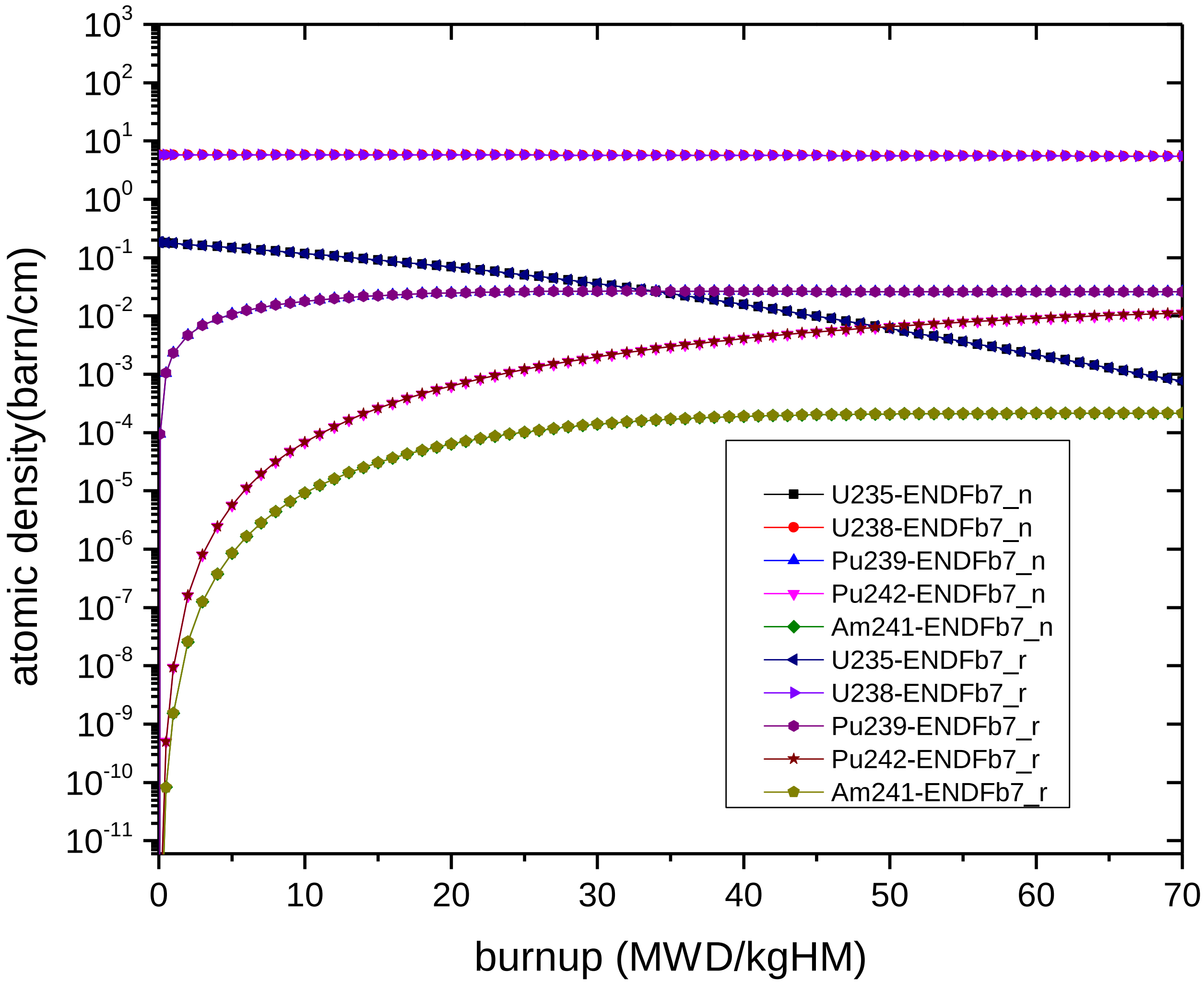
Results of Case 3: keff

- 10,000 histories/cycle
- 250 inactive cycles/1000 active cycles
- 72 major step(10 minor steps/major)
  - 3.3, 13.3, 16.6, 69 × 33.3 days



Validation

Results of Case 3: isotopic concentration

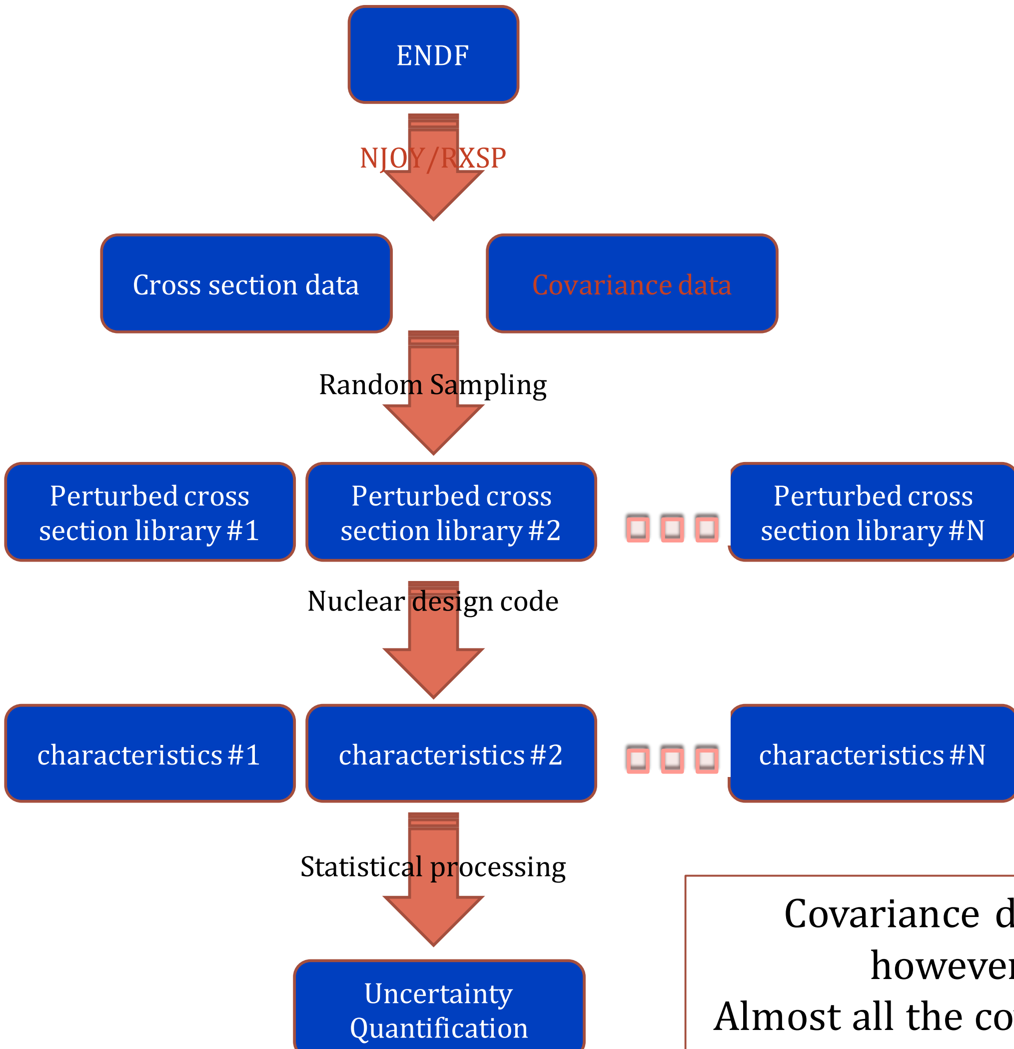


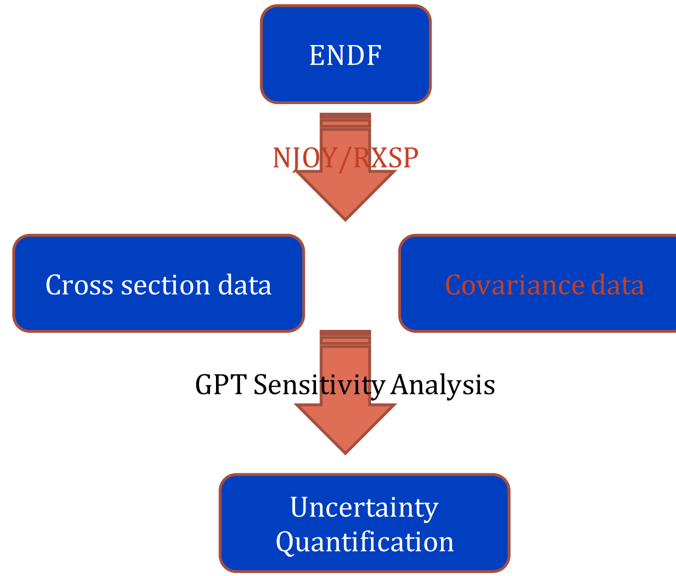
Extension

Extension

- **Covariance data processing**
  - **Multi-group covariance**
  - **Continuous-energy covariance**
  - **Implicit uncertainty from resonance parameters**
- **Automation sequence for random sampling UQ**
  - **Random sampling/ Latin Hypercube Sampling**
  - **Automatic generation of perturbed cross section libraries**

- **Flow chart of uncertainty quantification**





Covariance data processing code is very important,
however too few researcher is interested;
Almost all the covariance data libraries are borrowed from
SCALE package(44groupcov/56groupcov);

▪ Flow chart of covariance data processing

Input parameters

Construct union grid

Generate erg structure

Calculate weight flux/spectrum

Compute group-averaged covariance

Group collapse

Transfer to COVERX

Validation

Complicated :
All data in MF31+MF32+MF33 should be processed.
Different data treated by different method
Treatment of MF32 is very time consuming

Conclusion

Conclusion

- A comprehensive nuclear cross section processing code RXSP has been developed, which has the validated capability for generating temperature dependent point-wise cross section libraries used in nuclear reactor neutron transport.
- Some advanced features i.e. R-Matrix Limited, Fast Doppler broadening, S(a,b) Interpolation, Fast P-Table generation, P-Table Interpolation ,OpenMP parallel are shown.
- The extension of RXSP code for covariance data library processing is undergoing.

Thanks!

UNIST CORE