

Introduction of the Resonance dependent scattering kernel in SERPENT

In the Memory of John Rowlands

Institute for Neutron Physics and Reactor Technology

R. Dagan

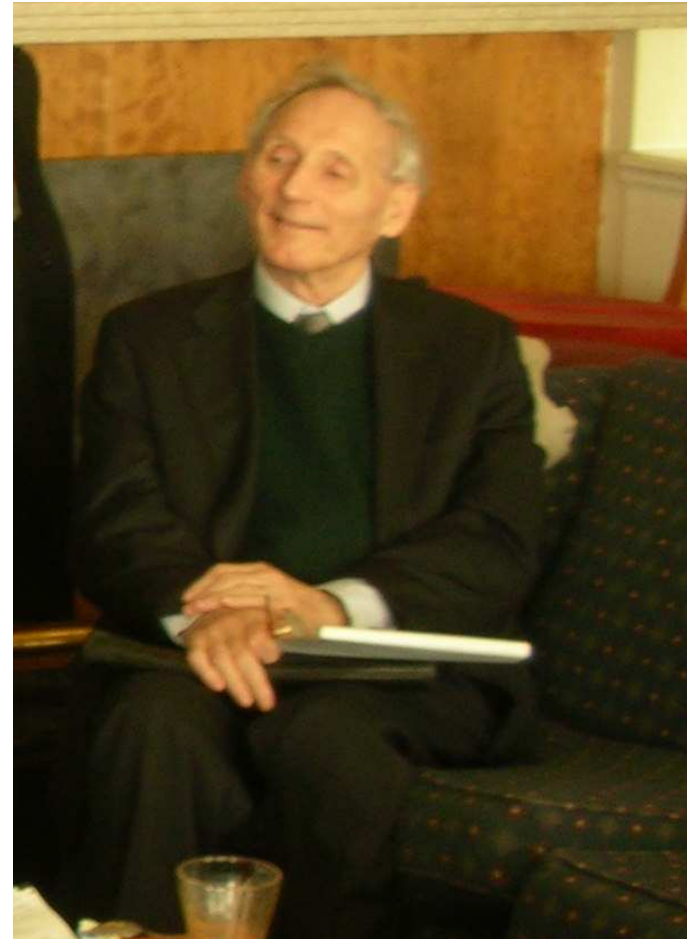
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outline

- John Rowlands
- Introduction to the resonance dependent double differential cross section.
- The analytic and the stochastic solutions.
- The implementation new scattering kernel MC codes, in particular in SERPENT.
- Future challenges with SERPENT.

In the Memory of John Rowlands

- The scientific founder and the Spirit of the JEFF project (Libraries)
- The World Expert on XS and scattering kernels
- The initiator of the development of the Double Differential Cross Section in the 1990's for heavy nuclides
- Etc, etc ,,,,,,



The transport equation and the scattering kernel term

$$\frac{1}{v} \frac{\partial f(E, r, \Omega, t)}{\partial t} + \Omega \cdot \nabla f(E, r, \Omega, t) + [\Sigma_s(E) + \Sigma_a(E)] f(E, r, \Omega, t) =$$

$$= \int_{\Omega'} \int_0^{\infty} \Sigma(E' \rightarrow E; \Omega' \rightarrow \Omega) f(E', r, \Omega', t) d\Omega' dE' + S(E, r, \Omega, t)$$

How good can we calculate the scattering kernel term for heavy isotopes?

- The scattering cross section is temperature and energy dependent

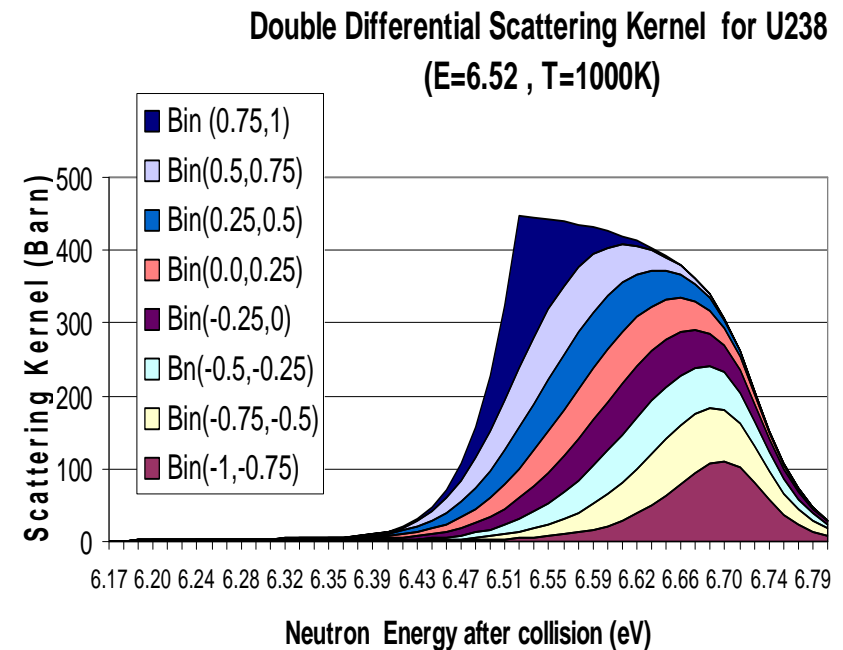
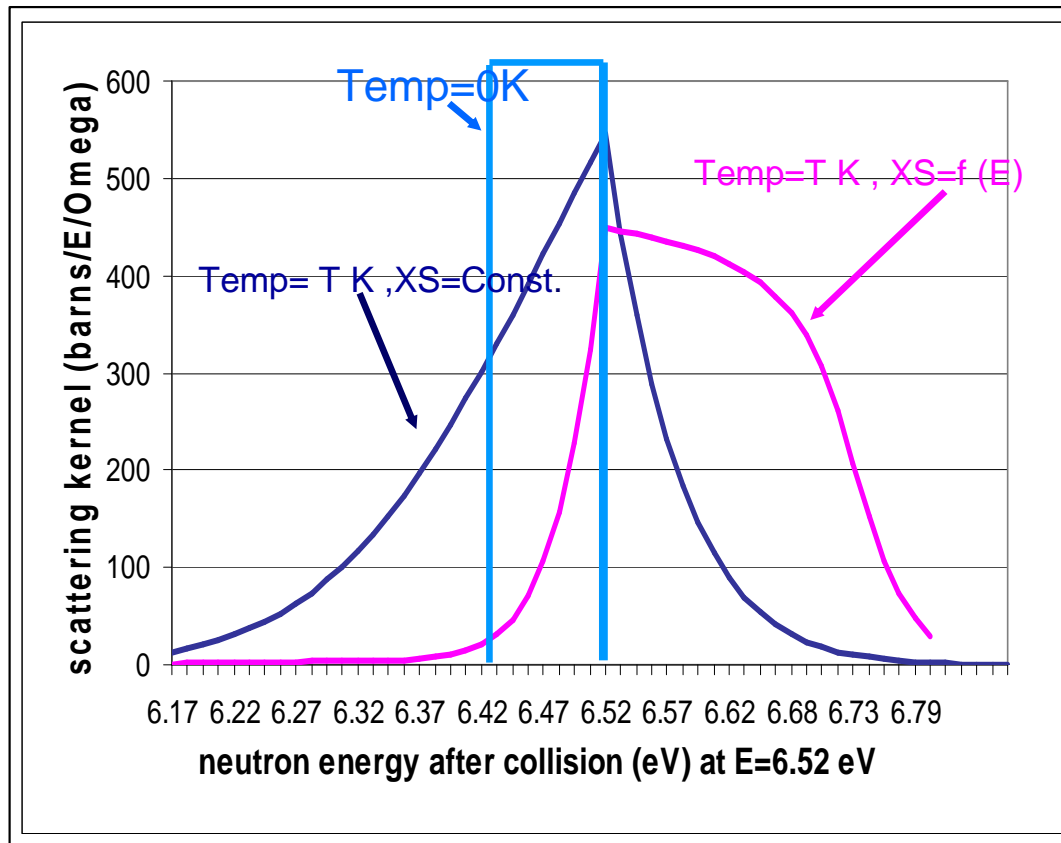
BUT → The scattering kernel is (mostly) used at 0K and is energy independent.

What are the consequences of this approximation?

~1920-1998: Different types of scattering kernels for a 6.52 eV neutron interacting with U238

- MCNP Manual:**

“If the energy of the neutron is greater than $400KT$ and the target is not Hydrogen the velocity of the target is set to Zero” (**Asymptotic kernel**)



The double differential resonant scattering kernel

$$\sigma_s^T(E \rightarrow E', \Omega \rightarrow \Omega') ; \sigma_s = \sigma_s(E)$$

- Ann. Nucl. Energy. 1998 25 p 209
- Ann. Nucl. Energy. 2004 31 p 9
- This kernel can be solved numerically in reasonable time and was implemented in THERMR.
- The new kernel is mathematically consistent and in accordance with the BROADR module (Doppler broadening) of NJOY
- Formatted probability tables can be prepared for MCNP calculations as it is done for light isotopes.

IDEAL GAS KERNEL: ENERGY DEPENDENT $\sigma_s(E_\tau)$

$$\sigma_s^T(E \rightarrow E', \Omega \rightarrow \Omega') =$$

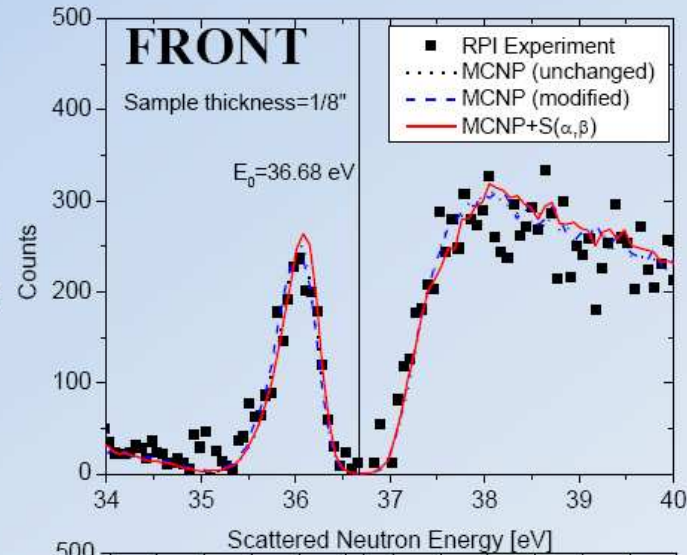
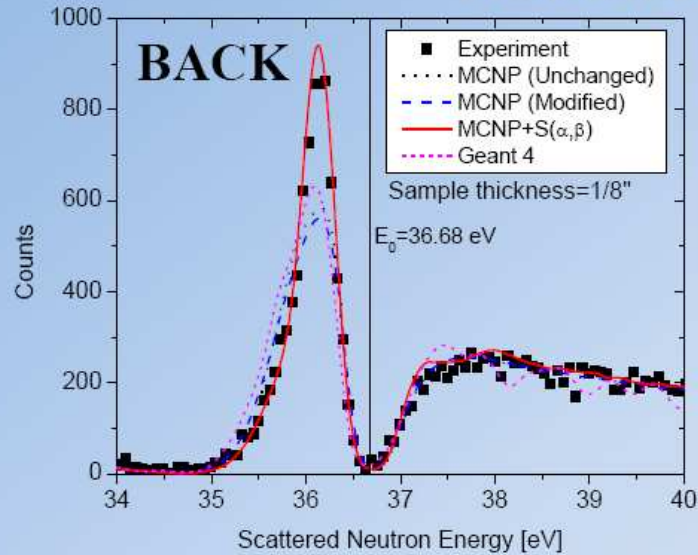
$$\frac{1}{4\pi E'} \sqrt{\frac{A+1}{A\pi}} \int_{\epsilon_{max}}^{\infty} d\xi \int_{\tau_0(\xi)}^{\tau(\xi)} d\tau$$

$$\left[\frac{(\xi + \tau)}{2} \right] \left(\frac{A+1}{A} \right)^2 \sigma_s \left[\left(\frac{A+1}{A^2} \right) \frac{(\xi + \tau)^2}{4} k_B T \right]$$

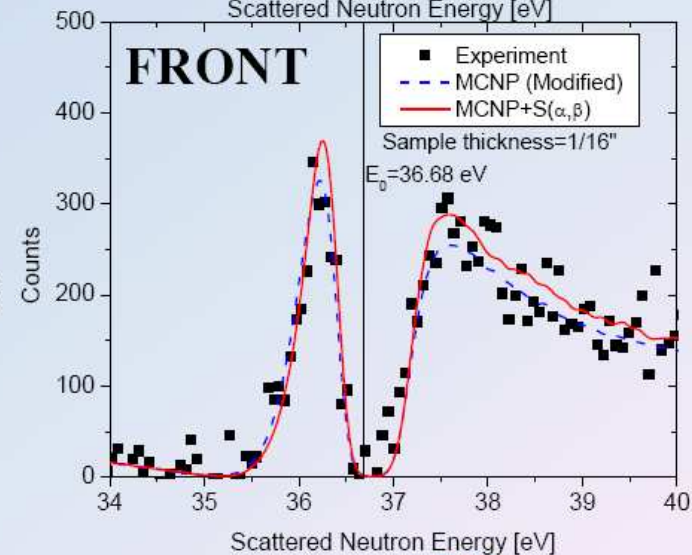
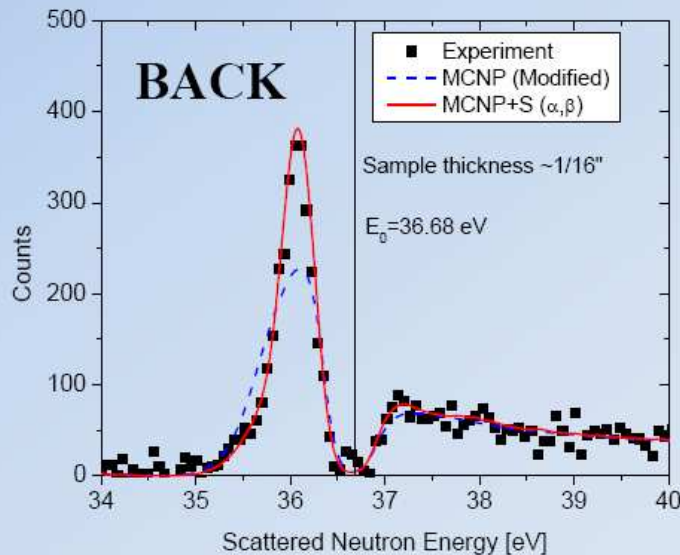
$$\exp \left\{ v^2 - \left[\frac{(\xi + \tau)^2}{4A} + \frac{(\xi - \tau)^2}{4} \right] \right\} \left[\frac{\epsilon_{max} \epsilon_{min} (\xi - \tau)^2}{B_0 \sin^2 \hat{\phi}} \right]$$

Results - ^{238}U Scattering

Thick
Sample



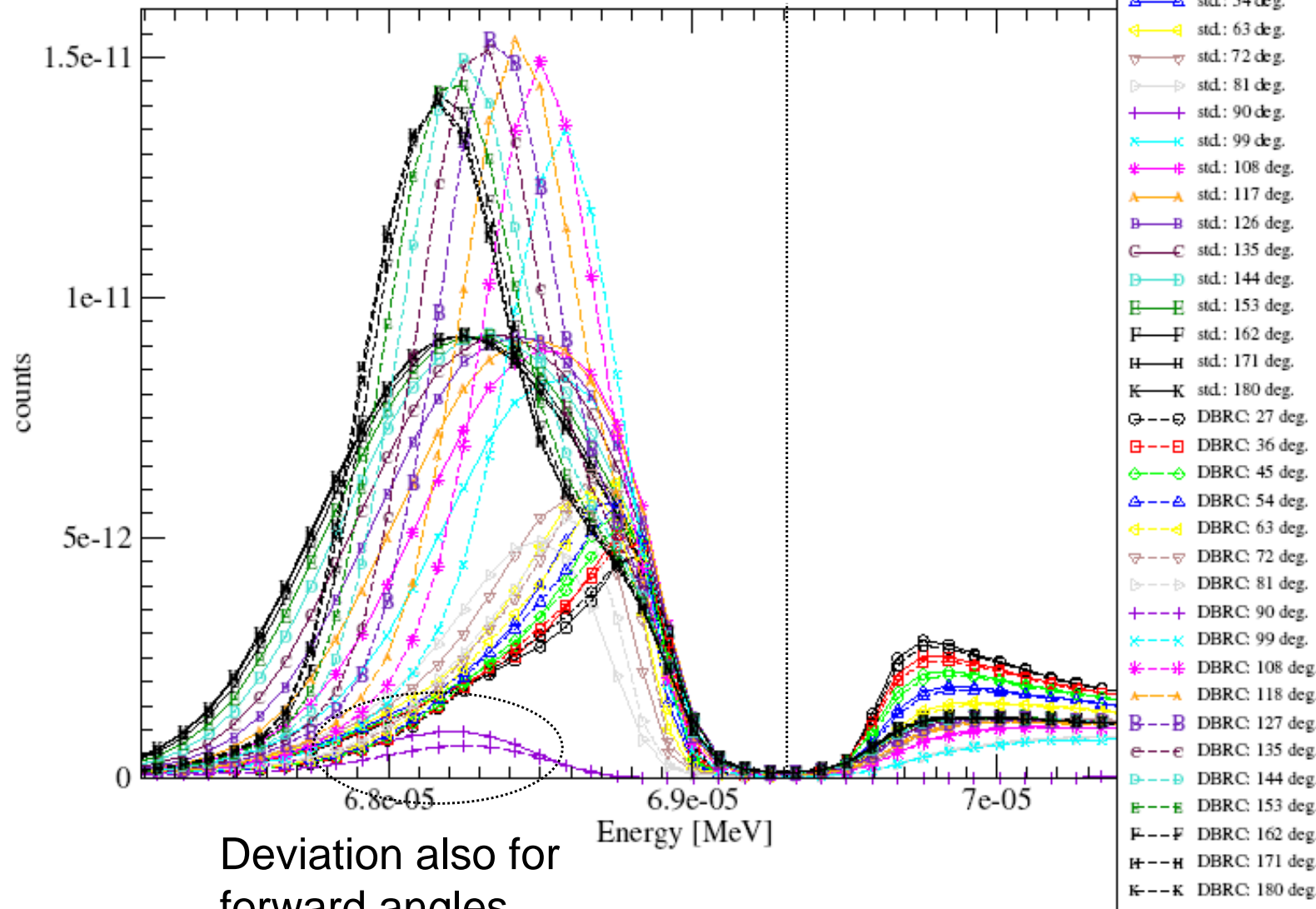
Thin
Sample



Simulation of ^{232}Th Scattering

Th232 Resonance Scattering

Detector Counts for Different Angles



MC Scattering Kernel Treatment:

“Sampling the target velocity”

The Doppler Broadening formula for the scattering cross section

$$\sigma_s(v', T) = \frac{1}{v'} \int \int v'_r \sigma_s(v'_r, 0) p(V) dV \left(\frac{d\mu}{2}\right) \quad (1)$$

where $\vec{v}' = (v', \vec{\Omega}') is the neutron velocity, $\mu = (\vec{\Omega}' \cdot \vec{\Omega}_V)$, and the relative speed is given by$

$$|\vec{v}'_r| = |(\vec{v}' - \vec{V})| = (v'^2 + V^2 - 2v'V\mu)^{1/2} \quad (2)$$

In order to sample V and μ the probability density function

$$P(V, \mu) = \frac{v'_r \sigma_s(v'_r, 0) p(V)}{2v' \sigma_s(v', T)} \quad (3)$$

is used in accordance with equation (2).

Subroutine COLIDN in MCNP uses for $p(V)$ the Maxwell-Boltzmann distribution of the speed V of the target nucleus of mass Am at temperature T

$$p(V) = (4/\sqrt{\pi}) \beta^3 V^2 e^{-\beta^2 V^2}, \beta = \left(\frac{Am}{2kT}\right)^{1/2} \quad (4)$$

In order to take an initial sample of V from $P(V, \mu)$, the following form is used:

$$P(V, \mu) = C' \left\{ \frac{\sigma_s(E'_T, 0)}{\sigma_s^{max}(E'_\xi, 0)} \right\} = 1 ??$$

Rejection technique

$$\left\{ \frac{v'_r}{v' + V} \right\} \left\{ \frac{(2\beta^4)V^3 e^{-\beta^2 V^2} + (\beta v' \sqrt{\pi}/2)(4\beta^3/\sqrt{\pi})V^2 e^{-\beta^2 V^2}}{1 + \beta v' \sqrt{\pi}/2} \right\}$$

where

$$C' = \frac{\sigma_s^{max}(E'_\xi, 0)(1 + \beta v' \sqrt{\pi}/2)}{2v' \sigma_s(v', T)\beta \sqrt{\pi}/2}$$

is a normalisation constant.

The term in the first brackets is approximated to be one in MCNP. Consequently the influence of resonances on the probability density function is practically neglected.

DBRC -Doppler Broadening Rejection Correction

for the MCNP Scattering Kernel Treatment:
within “Sampling the target velocity”

In order to take an initial sample of V from $P(V, \mu)$, the following form is used:

$$P(V, \mu) = C' \left\{ \frac{\sigma_s(E'_T, 0)}{\sigma_s^{max}(E'_\xi, 0)} \right\} \left\{ \frac{v'_T}{v' + V} \right\}$$

Rejection technique

$$\left\{ \frac{(2\beta^4)V^3 e^{-\beta^2 V^2} + (\beta v' \sqrt{\pi}/2)(4\beta^3/\sqrt{\pi})V^2 e^{-\beta^2 V^2}}{1 + \beta v' \sqrt{\pi}/2} \right\}$$

where

$$C' = \frac{\sigma_s^{max}(E'_\xi, 0)(1 + \beta v' \sqrt{\pi}/2)}{2v' \sigma_s(v', T) \beta \sqrt{\pi}/2}$$

is a normalisation constant.

General Implementation of DBRC

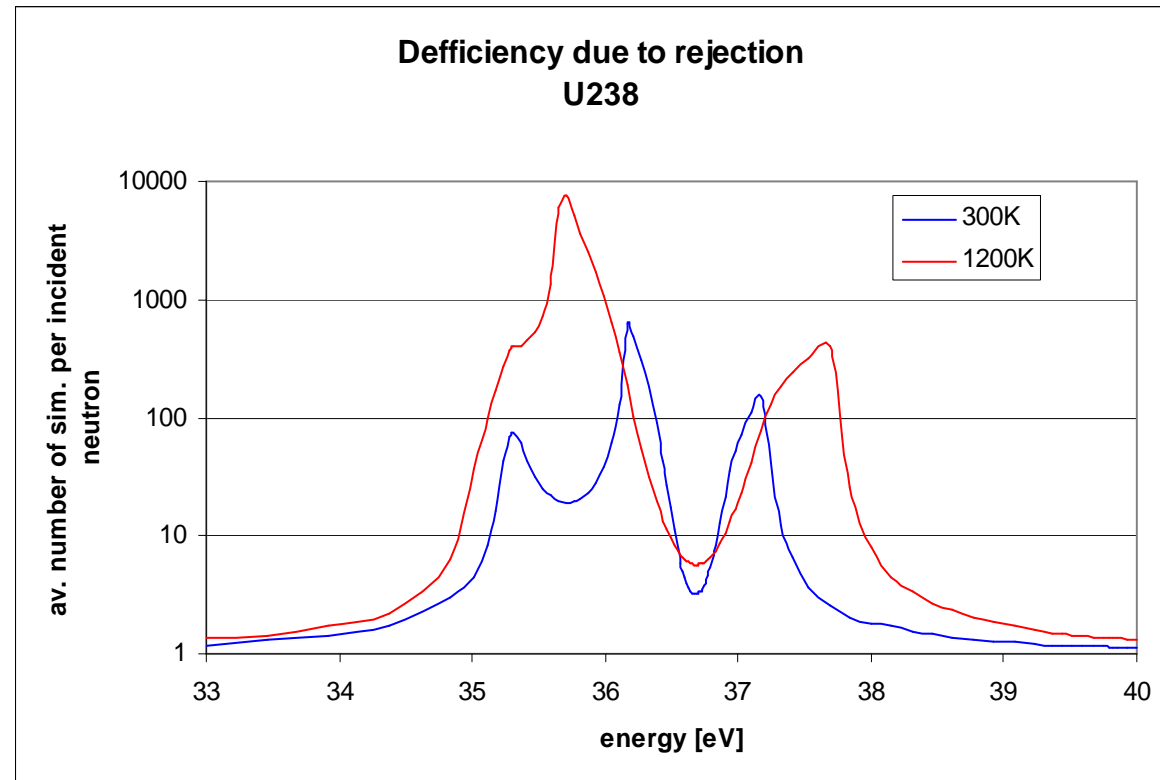
$$P(V, \mu) \rightarrow \left\{ \frac{(2\beta^4)V^3 e^{-\beta^2 V^2} + (\beta v \sqrt{\pi}/2)(4\beta^3/\sqrt{\pi})V^2 e^{-\beta^2 V^2}}{1 + \beta v \sqrt{\pi}/2} \right\}$$

<p>2</p> $\left\{ \frac{v_r}{v+V} \right\}$	<p>new: 3</p> $\left\{ \frac{\sigma_s(v_r, 0)}{\sigma_s^{\max}(v_\xi, 0)} \right\}$
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- Add the 0 degree cross sections of the resonant nuclide
- 1) Sample V and μ
- 2) Existing Velocity Rejection
- 3) introduce **DBRC**-Doppler Broadening Rejection Correction. (Seek for the max XS based on Weisbin-Cullen approach NSE 1976)

http://www.oecd-nea.org/dbforms/data/eva/evatapes/jeff_31/Resonant-Scattering-Kernel-Dagan/

Validation of the “sampling of the target velocity” approach



Rothenstein ANE1996: Does the stochastic solver in MCNP “sampling of the target velocity” lead to a mathematical “violation” and to a bias of the integral parameters (criticality etc.)?

Comparison of different calculations approaches

- Criticality k_{∞} of a LWR pin cell at TF=1200K and computer time (ctm) applying different scattering models

	Method	k_{∞}	ctm [min]
(1)	standard MCNP: k_1	1.31137 +/-6E-5	1052
(2)	standard MCNP ($E_n < 210\text{eV}$): k_2	1.31153 +/-6E-5	1076
(3)	S(α,β) (8 bins): k_3	1.30775 +/-6E-5	1092
(4)	S(α,β) (16 bins): k_4	1.30772 +/-6E-5	1028
(5)	DBRC: k_5	1.30791 +/-6E-5	1240
Differences	$k_2 - k_1$	-16 pcm	
	$k_3 - k_1$	-362 pcm	
	$k_4 - k_1$	-365 pcm	
	$k_5 - k_1$	-346 pcm	
	$k_5 - k_4$	19 pcm	

Implementation in SERPENT

- Similarly to “tgtvel” (“sampling the target velocity module in MC codes) the DBRC was implemented, namely adding a rejection test.
- Advantage of SERPENT : the calling of the zero data XS is simpler based on the data structure in SERPENT.
- Sampling procedure much quicker than by other MC codes. Ideal for parameter testing (known advantage of SERPENT)
- $S(\alpha, \beta)$ tables could accelerate the process with a “penalty” on the higher data storage. Should be pre-prepared
- Zero XS still have to be generated. (for the beginning could be optionally given for U238)

Use of the resonant dependent DDXS in SERPENT

- Zero XS still have to be generated. (for the beginning could be optionally given for U238)
- The $S(\alpha, \beta)$ Serpent format should be prepared.

Challenges of SERPENT: The applicability of Mubar

FJOH 2011

Topic 3 Neutronics & Core Physics

Homogenization

Serpent uses two fundamentally different techniques for calculating the neutron diffusion coefficient:

1) Diffusion coefficient from migration area:

$$D_g = L_g^2 \times \Sigma_{r,g}$$

2) Diffusion coefficient from transport cross section: $D_g(\mathbf{r}) = \frac{1}{3\Sigma_{tr,g}(\mathbf{r})}$

$$\Sigma_{tr,g}(\mathbf{r}) = \Sigma_{t,g}(\mathbf{r}) - \bar{\mu}_g \Sigma_{s,g}(\mathbf{r})$$

Both definitions are derived from transport theory and diffusion approximation, but the results can differ by tens of per cent within the same calculation case.

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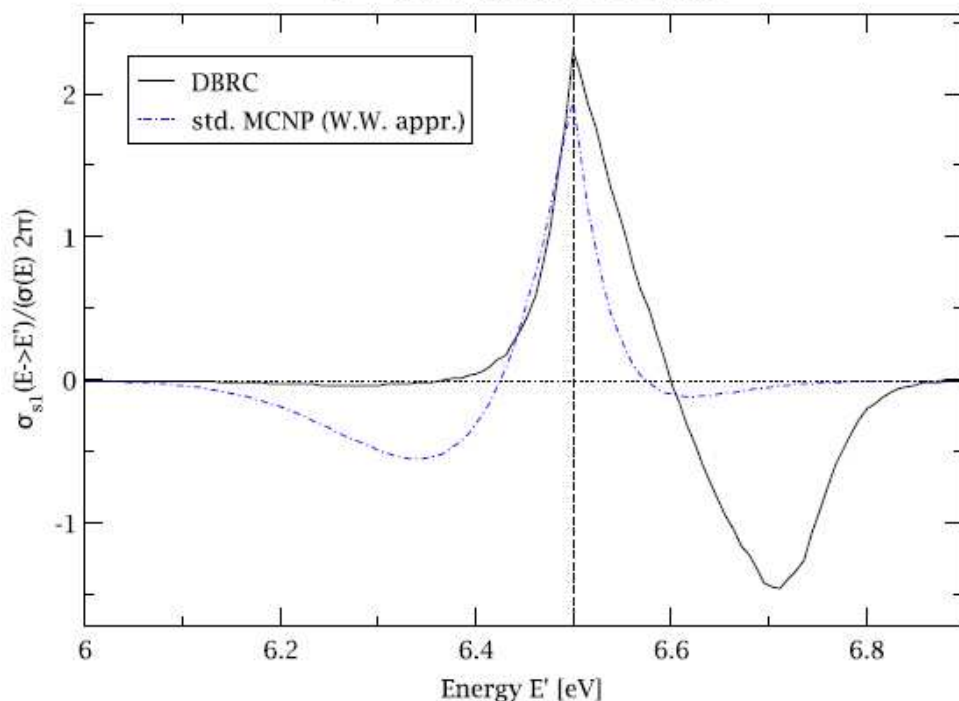
Dr. Jaakko Leppänen, VTT

1st and 2nd Angular Moment (PhD work of B. Becker)

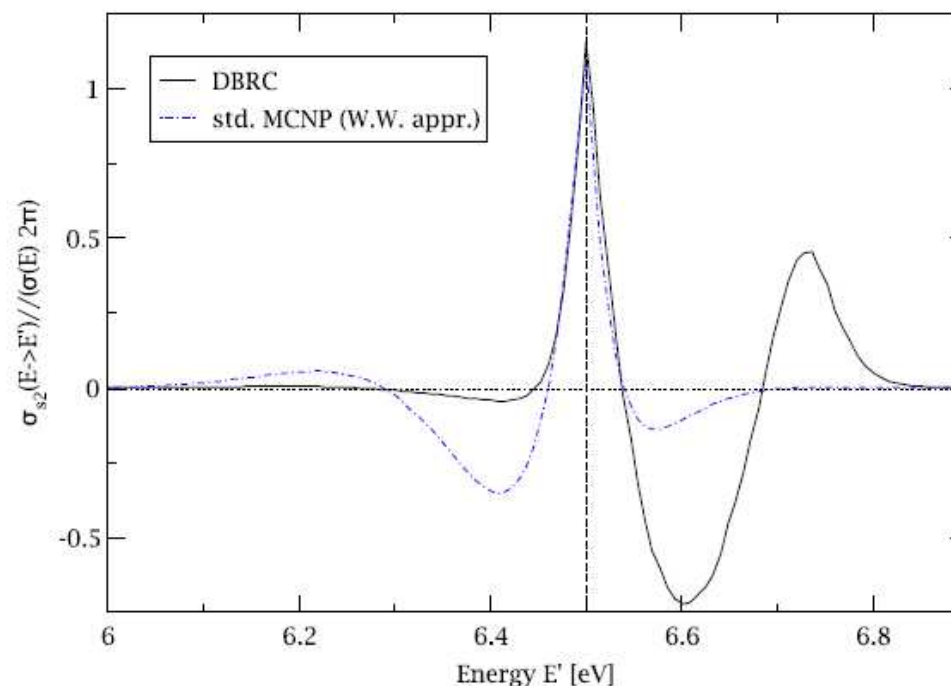
- Commonly used in deterministic codes and not in MC codes
- Illustrates the angular discrepancy between the std. MCNP and DBRC kernels

$$\sigma_{sn}(E \rightarrow E') = \int_{-1}^1 2\pi P_n(\mu_0^{lab}) \sigma_s(E \rightarrow E', \vec{\Omega} \rightarrow \vec{\Omega}') d\mu_0^{lab}$$

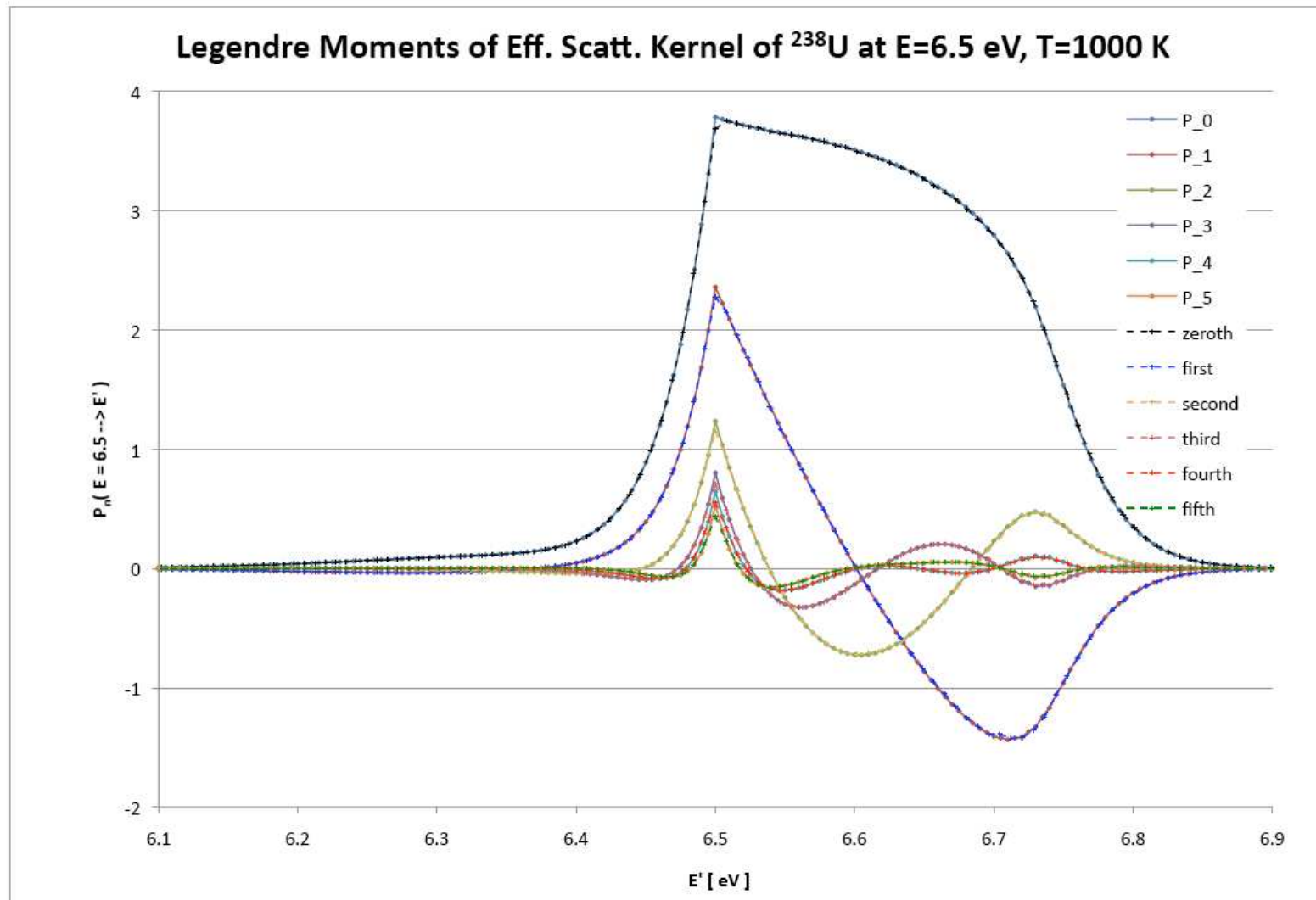
First Moment of the Scattering Kernel
of ²³⁸U at E=6.5 eV and T=1000 K



Second Moment of the Scattering Kernel
of ²³⁸U at E=6.5 eV and T=1000 K



Resonance dependent Legendre moments



G. Arbanas et al. M&C 2011

With faster, more capable computers, there are many new R&D efforts in progress to develop new MC analysis capabilities

- Some of the R&D efforts were not possible until now, due to computer limitations on speed &/or memory
- Other R&D efforts are addressing new methods to eliminate approximations made in MC codes 20-30 years ago, that are now significant due to much smaller uncertainties

Of course, everyone's R&D project is of the highest importance to the future of mankind.....

**I've listed my 10 personal favorites on the next few slides.
These are not ranked in any particular order.**

Two of the top future oriented Monte Carlo R&D efforts dedicated to Doppler Broadening effects

4. On-the-fly Doppler broadening of neutron cross-sections (Yesilyurt, U Mich / ORNL)

- Permit a continuous distribution of material temperatures
- Essential for multiphysics calculations, with neutronics/CFD coupling

G. Yesilyurt, W.R. Martin, F.B. Brown, “On-The-Fly Doppler Broadening for Monte Carlo Codes”, ANS M&C-2009, Saratoga Springs, NY, May 3-7 (2009).

8. Improved treatment of the neutron free-gas scattering model at epithermal energies (Becker, Dagan)

- Include important resonance scattering effects
- Fixes long-standing approximation

B. Becker, R. Dagan, G. Lohnert, “Proof and Implementation of the Stochastic Formula for Ideal Gas, Energy Dependent Scattering Kernel”, *Annals of Nuclear Energy* 36, 470-474 (2009).

Forest Brown SNA+MC Tokyo 2010

Top 6 future oriented Monte Carlo R&D efforts connected to Doppler Broadening; temperature effects

6. Depletion analysis of fuel assemblies and reactors (Leppanen, VTT; KAPL/Bettis; many others)

- including equilibrium Xenon and control searches

Leppanen, J., 2009. PSG2/Serpent – A Continuous-energy Monte Carlo Reactor Physics Burnup Calculation Code, User's Manual (February 2, 2009). VTT Technical Research Centre of Finland.

T.M. Sutton, et al., "The MC21 Monte Carlo Transport Code", M&C+SNA-2007, Monterey, CA, April 15-19 (2007).

Forest Brown SNA+MC Tokyo 2010

Challenges for SERPENT: Stochastic Doppler Broadening (will be addressed later in the work shop)

Weighting method:

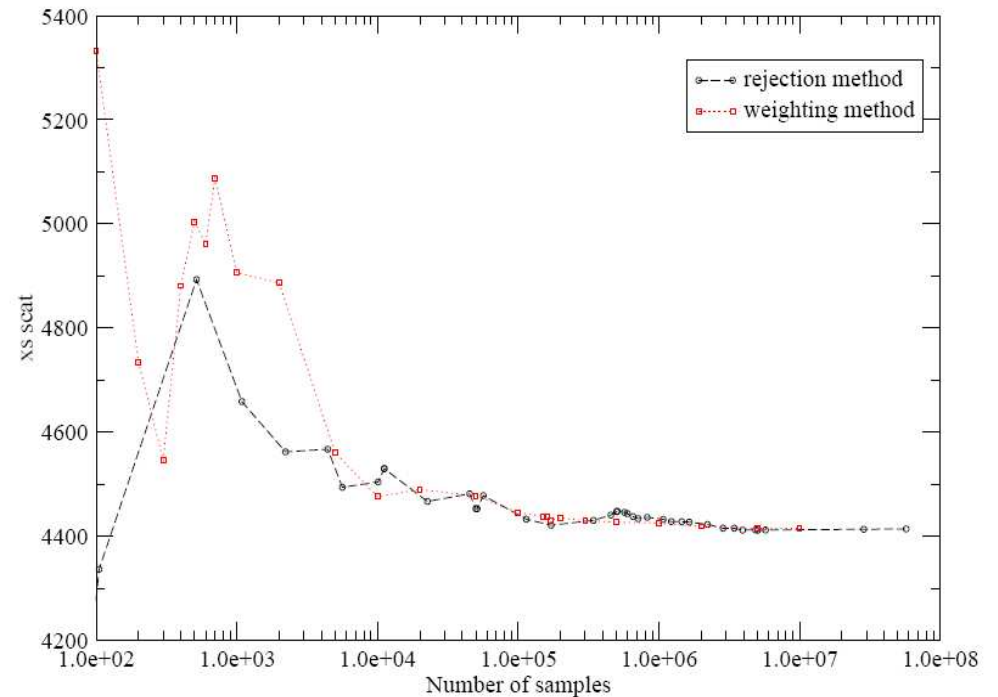
$$\sigma_s^T = \frac{\sum_{i=1}^N w_{1,i} \sigma_s(v_{r,i}, 0)}{N} \quad w_{1,i} = \frac{v_r}{v}$$

Rejection method:

$$1: \left\{ \frac{v_r}{v + V} \right\} \quad 2: \left\{ \frac{\sigma_s(v_r, 0)}{\sigma_s^{\max}(v_\xi, 0)} \right\}$$

$$\sigma_s^T = \sigma_{\max} \frac{\sum_{N} \text{accepted tallies}}{\sum_{N} \text{accepted + rejected tallies}}$$

Scattering cross section evaluation (1200K) at the peak resonance of 36.67 for U238



What is an Antithetic Variate?

Introduced by Hammersley and Morton, 1956.

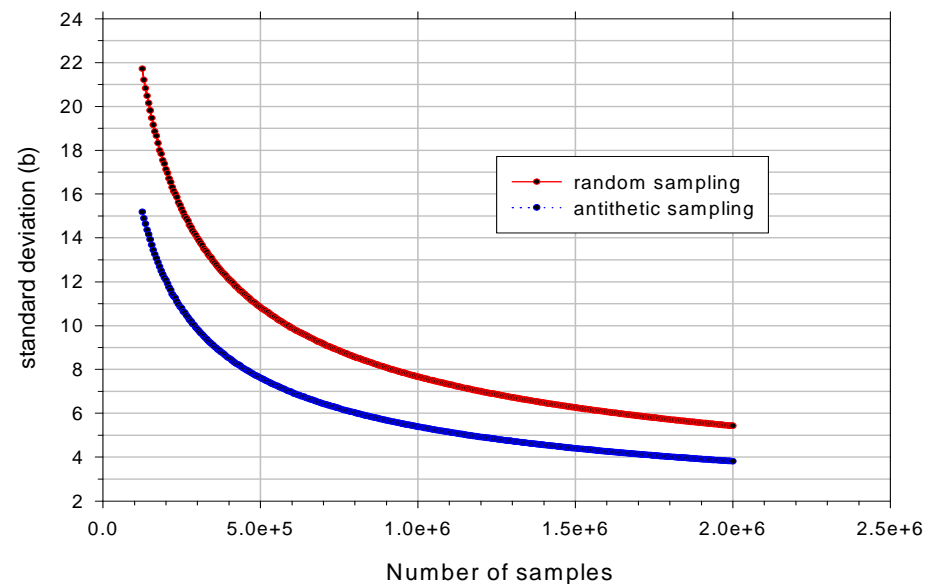
Based on the following observation:

Suppose there exists two estimators t_1 and t_2 . Then the variance of their average is

$$\text{var}([t_1 + t_2]/2) = \{\text{var}(t_1) + \text{var}(t_2) + 2*\text{covar}(t_1,t_2)\}/4$$

So, if the covariance is negative, total variance is reduced relative to what it would otherwise be. If this occurs the variates t_1 and t_2 are antithetic

CONVERGENCE RATE



Summary

- Serpent is a good tool for the testing of the impact of the resonance dependent scattering kernel:
 - It can give corrections for core parameters of different levels
 - The probability table method could be implemented for an accurate study of the Mc method itself (validity of rejection methods etc.) and for learning better the solid state effects for heavy nuclides like U238.
 - The validity of the Legendre moments
 - Extension of the Studies to stochastic Doppler Broadening
 - Variance reduction methods in view of the scattering kernel solver