Simulations of Neutron Multiplicity Experiments with Nuclear Data Perturbations

S.R. Bolding[1], C.J. Solomon[2]

[1] *Texas A&M University, College station, TX*
[2] *Los Alamos National Laboratory, Los Alamos, NM*

ANS National Meeting, 14 November 2013

Outline

Nuclear Energy University Programs
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Neutron Multiplicity Distributions

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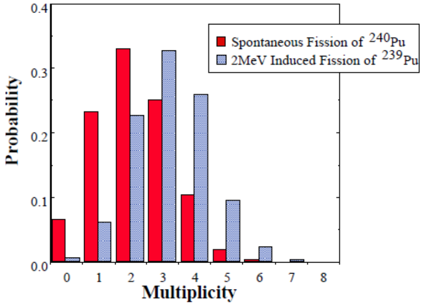

Figure: Multiplicity distributions [PANDA Manual, 1991]

- Provide passive multiplication information about a subcritical, fissionable system

Constructing a Multiplicity Distribution (Ideal Case)

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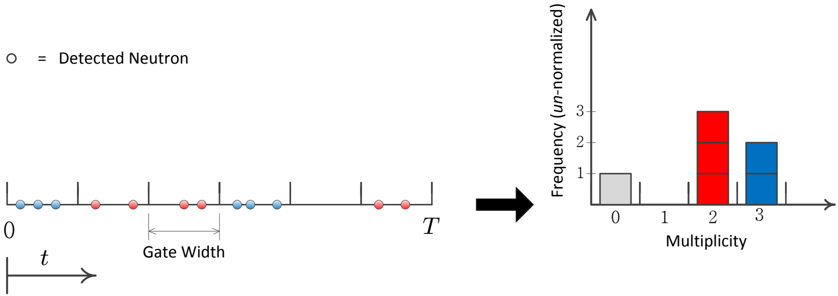
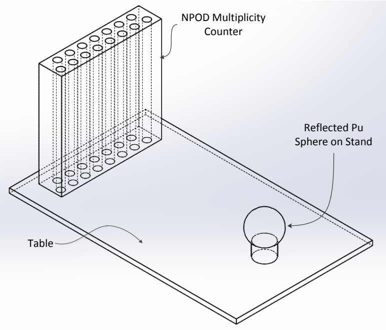


- Normalize to form a PDF

Multiplicity Experiments



*Not to scale

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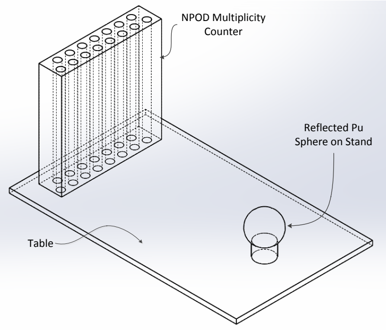

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- Performed at LANL for validating subcritical simulations
- Experimental Parameters
  - 94% ^{239}Pu sphere
  - 5 Different HDPE shells:
    - None, 0.5 cm, 1.0 cm, 1.5 cm, 3.0 cm

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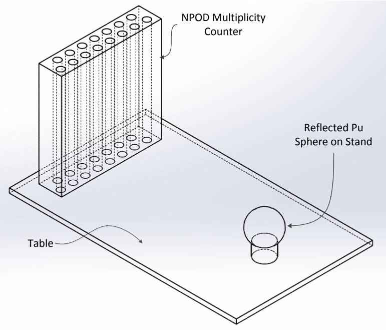

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- Experimental Parameters
  - 94% ^{239}Pu sphere
  - 5 Different HDPE shells:
    - None, 0.5 cm, 1.0 cm, 1.5 cm, 3.0 cm
- Measured multiplicity distributions are well verified
- Repeated with ^{252}Cf

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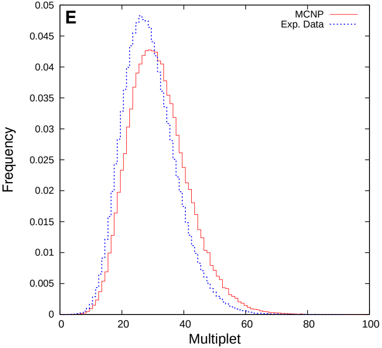

Pu with 3.0-cm HDPE reflector

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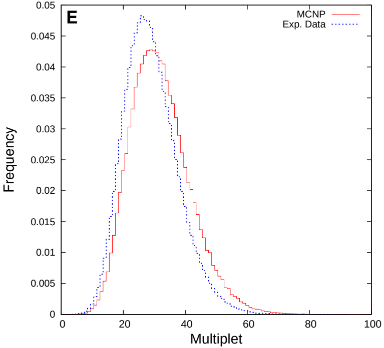
    - Caused by nuclear data of ^{239}**Pu**
    - Adjusted energy-integrated $\overline{\nu}$



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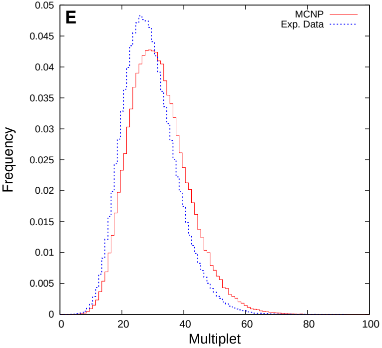
  - Adjusted energy-integrated $\overline{\nu}$
- **ENDF** ^{239}Pu $\overline{\nu}$ adjusted to match k_{eff}
  - $\overline{\nu}$ is $\sim 2\,\sigma$ above measured data for $E < 1.5$ MeV



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- Compare $\overline{\nu}(E)$ results to energy-independent shifts of microscopic cross sections σ_i
  - Are these experiments a validation tool for $\overline{\nu}$?

Outline

Covariance and Correlation Matrices

Consider N *dependent* random variables $X_i : i = 1, 2, \ldots, N$

- Covariance Matrix $\mathbf{\Sigma}$:

$$\Sigma_{ij} = \mathrm{Cov}(X_i, X_j)$$

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- Correlation Matrix $\mathbf{C}$:

$$C_{ij} = \frac{\Sigma_{ij}}{\sqrt{\Sigma_{ii}\Sigma_{jj}}}, \qquad C_{ij} \in [\mathbf{-1}, \mathbf{1}]$$

Sampling Correlated Random Values

1. Decompose correlation matrix:

$$\mathbf{V}\mathbf{V}^T = \mathbf{C}$$

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- Cholesky decomposition for $\mathbf{V}\mathbf{V}^T$

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3. Generate new set of $\overline{\nu}$:
   - IF E in E_g:

$$\boxed{\overline{\nu}\,'(E) = \sigma_{rel}(E_g)\nu(E)\widetilde{\mathbf{R}}(E_g) + \overline{\nu}(E)}$$

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- Adjust energy-integrated cross sections (or $\overline{\nu}$)

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- Compute average number of standard deviations shifted $\# s(\sigma_i)$

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Comparing Results of Simulations

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- Reduced χ^2 values for the 5 multiplicity experiments and criticality benchmark

$$\chi^2_{red,mult,m} = \frac{1}{N_{bins} - 1} \sum_{i=1}^{N_{bins}} \frac{(P_i^{\mathrm{exp}} - P_i^{\mathrm{mcnp}})^2}{\sigma^2(P_i^{\mathrm{exp}}) + \sigma^2(P_i^{\mathrm{mcnp}})}$$

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- Compute a Cost Function:

$$\boxed{\text{Cost} = \sum_{m=1}^{5} \chi^2_{red,mult,m} + \chi^2_{red,k_{\text{eff}}}}$$

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Summary of Procedure

- FOR each trial :
  1. Generate a unique set of perturbed nuclear data
  2. Run **MCNP5_mult** simulations (5 multiplicity, JEZEBEL)
  3. Produce multiplicity distributions
  4. Compute χ^2_{red} values and cost
- The lowest cost is the most accurate trial

Outline

Energy-dependent $\overline{\nu}$ perturbations

- Cost results from 500 trials:

Trial	Cost	$\chi^2_{k_{\mathrm{eff}}}$
$\overline{\nu}$ -1.14%	164.24	33.66
303	**197.07**	**4.18**
55	267.9	0.01
Original	426.86	0.27

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- MCNP criticality test suite for trial 303:
  - 39 different ^{239}Pu criticality benchmarks
  - $RMSD = \sqrt{\frac{\sum_{i=1}^{N_{cases}} (k_{\text{eff},i} - k_{\text{eff},i}^{ref})^2}{N_{cases}}} \times 100\%.$

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Trial	$RMSD$
$\overline{\nu}$ -1.14%	1.23%
303	0.51%
Original	0.49%

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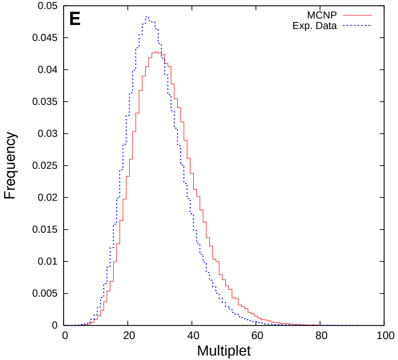
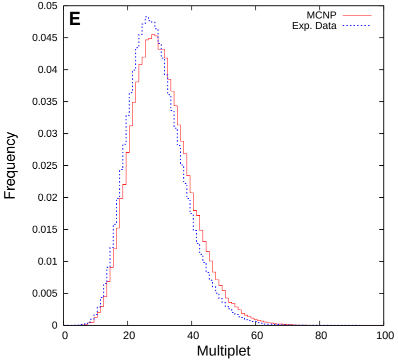
Energy-dependent $\overline{\nu}$ perturbations – 3.0 cm HDPE reflector

Original $\overline{\nu}$ Data



Trial 303: Lowest Cost



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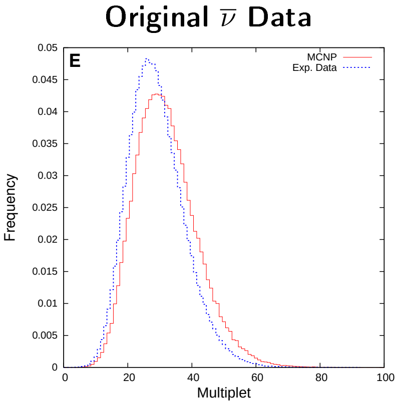
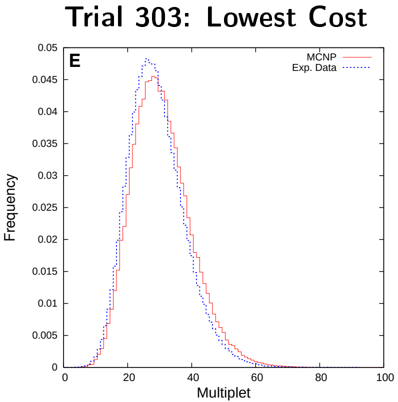
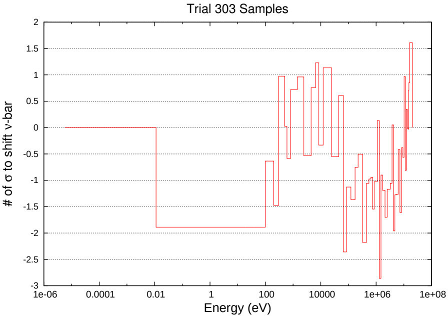
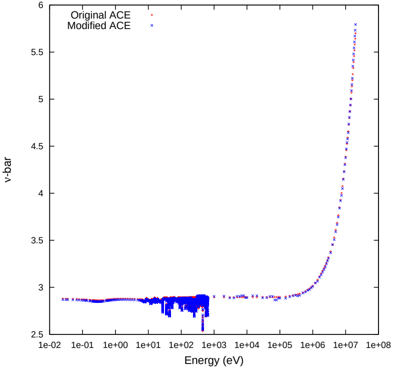




- Trial 303 data reduced bias in 1st and 2nd moments, averaged over all 5 simulations, by $\sim 35\%$

Trial 303 $\overline{\nu}$ Data





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Capture Cross Section – 3.0 cm HDPE reflector

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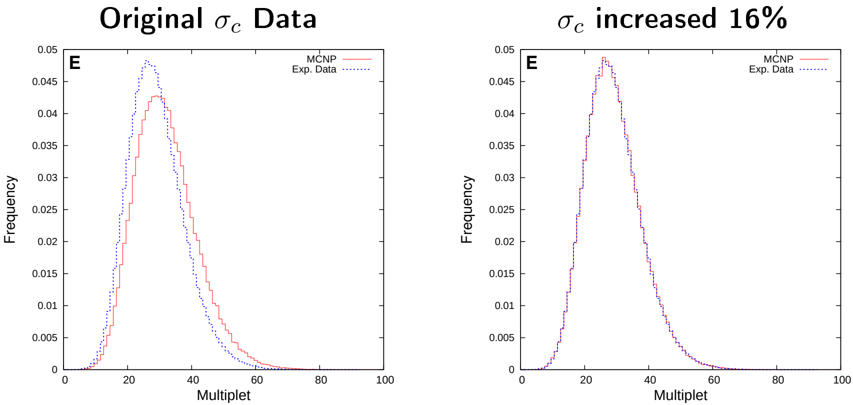


- Correction is less for other experiments, and $\#s(\sigma_c) = 7\ \sigma$

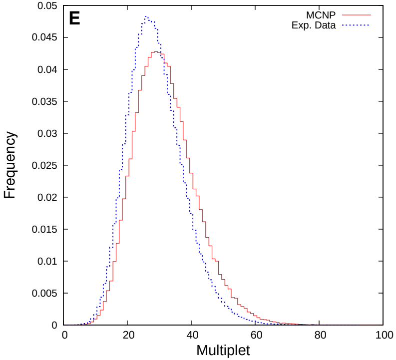
Fission Cross Section – 3.0 cm HDPE reflector

- Adjust elastic scattering (σ_s) to compensate change in σ_f, for $E > 1$ keV

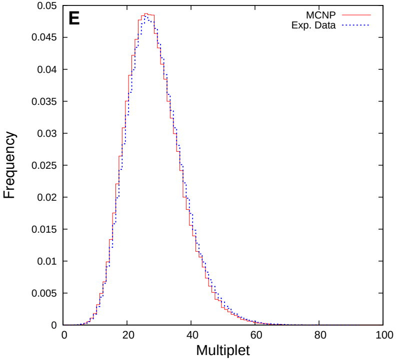
Fission Cross Section – 3.0 cm HDPE reflector

- Adjust elastic scattering (σ_s) to compensate change in σ_f, for $E > 1$ keV

Original σ_f Data



σ_f decreased 1.5%



- High accuracy for all simulations: $\sum_{i=1}^{5} \chi^2_{red,mult,m} = 14.6$

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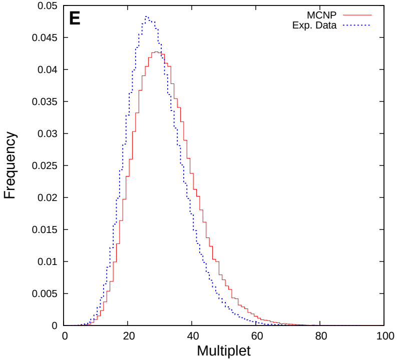
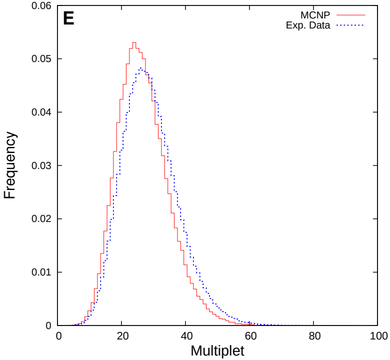
Energy-Integrated $\overline{\nu}$ Shift – 3.0 cm HDPE reflector

Original $\overline{\nu}$ Data



-1.14% $\overline{\nu}$ *Data*



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- Covariance sampling methodology has been developed and demonstrated, with promising results
  - Ideally sample all cross sections and $\overline{\nu}$ simultaneously

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Questions?

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Backup Slides

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Sample Statistics

- Consider independent random samples $\{x_i : i = 1, 2, \dots, N\}$ of a variable X with some PDF $f(x)$
- Statistics are some $f(x_1, x_2, \dots, x_N)$
  - Sample Mean: $\overline{x} = \dfrac{1}{N} \sum_{i=1}^{N} x_i$
  - Sample Variance: $s^2 = \dfrac{1}{N-1} \sum_{i=1}^{N} (x_i - \overline{x})^2$
- As $N \to \infty$, approach population (true) mean and variance

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Energy-dependent $\overline{\nu}$ perturbations

Comparison of Moments

Reflector	Moment	ENDF/B-VII.1 $\overline{\nu}$			Trial 303 $\overline{\nu}$			Experimental	
		Value	σ_{rel}	# σ away	Value	σ_{rel}	# σ away	Value	σ_{rel}
None	1	1.76E+001	2.68E-003	14.11	1.74E+001	2.68E-003	10.13	1.69E+001	1.38E-003
	2	3.31E+002	2.94E-003	24.43	3.24E+002	2.95E-003	17.59	3.08E+002	1.52E-003
0.5	1	2.40E+001	2.67E-003	16.72	2.37E+001	2.67E-003	11.75	2.29E+001	1.51E-003
	2	6.13E+002	2.90E-003	29.51	5.97E+002	2.90E-003	20.84	5.61E+002	1.65E-003
1.0	1	3.17E+001	2.66E-003	23.52	3.11E+001	2.66E-003	16.67	2.97E+001	1.77E-003
	2	1.07E+003	2.89E-003	41.52	1.03E+003	2.89E-003	29.59	9.38E+002	1.93E-003
1.5	1	3.80E+001	2.67E-003	28.61	3.70E+001	2.67E-003	19.27	3.51E+001	1.84E-003
	2	1.54E+003	2.92E-003	50.25	1.46E+003	2.91E-003	34.14	1.32E+003	2.01E-003
3.0	1	3.19E+001	2.70E-003	34.04	3.06E+001	2.70E-003	19.44	2.90E+001	1.75E-003
	2	1.11E+003	3.04E-003	58.05	1.02E+003	3.03E-003	33.72	9.17E+002	1.96E-003

Nuclear Data Formats

- **ACE** format

```
94239.70c  236.998600 2.53010E-08   08/25/07
94-Pu-239 at 293.6K from endf/b-vii.0 njoy99.248                     mat9437
   808738    94239    72098       48       45       14        0        6
        0        0        0        0        0        0        0        0
        1   360491   371402   371450   371498   371546   371594   598924
   598970   658265   658310   733847   805945   805959   805973   806478
   806492   806492   806506   808735   371781   808738   715724   724200
   724211   724253   724259        0        0        0        0        0
   1.00000000000E-11   1.03125000000E-11   1.06250000000E-11   1.09375000000E-11
```

- **ENDF** format

```
7.000000+6 4.519930-9 7.520000+6 0.000000+0                    943715102   56
0.000000+0 0.000000+0          0          0          0          0943715  099999
0.000000+0 0.000000+0          0          0          0          09437 0   0    0
9.423900+4 2.369986+2          0          0          0          1943731452    1
0.000000+0 0.000000+0          0        452          0          1943731452    2
0.000000+0 0.000000+0          1          5       1326          51943731452    3
1.000000-5 8.000000-3 1.000000+2 2.000000+2 3.000000+2 5.000000+2943731452    4
```

Capture Cross Section - Case 4

- Adjust elastic scattering (σ_s) to compensate for change in σ_c

$$\boxed{\sigma_s' = \sigma_s - \epsilon_c} \qquad \epsilon_c = \alpha\,\sigma_c \qquad \sigma_c' = \sigma_c + \epsilon_c$$

- Only for $E > 1keV$

Trial	χ^2_{mult}	$\chi^2_{k_{eff}}$	$\#s(\sigma_c)$
$\overline{\nu}$ -1.14%	130.58	33.7	n/a
$\alpha = 10.0\%$	345.1	0.22	4.04
$\alpha = 4.0\%$	390.9	0.01	1.62
$\alpha = 1.0\%$	417.9	0.01	0.40
Original	426.6	0.27	0

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Fission Cross Section – Case 1

Trial	χ^2_{mult}	$\chi^2_{k_{eff}}$	$\#s(\sigma_t)$	$s(\#s(\sigma_t))$
-4.0%	1318.2	167.72	-1.16	0.82
-2.0%	101.0	48.31	-0.58	0.41
-1.6%	27.1	22.97	-0.47	0.33
-1.4%	17.4	22.79	-0.41	0.29
-1.2%	23.1	14.25	-0.35	0.25
-1.0%	47.7	9.37	-0.29	0.21
-0.5%	178.7	1.33	-0.14	0.10
$\overline{\nu}$ -1.14%	130.58	33.7	n/a	n/a
Original	426.6	0.27	0	0

Changing Fission and Capture Cross Sections

- Adjust fission to compensate for change in capture

$$\boxed{\sigma_f' = \sigma_f - \epsilon_c} \qquad \epsilon_c = -\alpha\,\sigma_f \qquad \boxed{\sigma_c' = \sigma_c + \epsilon_c}$$

Trial	χ^2_{mult}	$\#s(\sigma_c)$
$\alpha = 10\%$	90.66	4.31
$\alpha = 4\%$	222.47	1.72
$\alpha = 2\%$	314.82	0.86
$\overline{\nu}$ -1.14%	130.58	n/a
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Changing Fission and Capture Cross Sections

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- $\sigma_{\mathbf{f}} >> \sigma_{\mathbf{c}}$

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Effect of altering σ_t

Monoenergetic neutrons, unit atom density, two reaction types: $\sigma_t = \sigma_a + \sigma_b$

- Perturb σ_a: $\sigma_a' = \sigma_a + \epsilon_a, \quad \sigma_t' = \sigma_t + \epsilon_t \quad \sigma_b' = \sigma_b$
- Interaction Probability:

$$\begin{aligned} P(\text{Interaction } i, x) &= P(\text{Interaction}, x) * P(\text{Interaction } i \mid \text{Interaction}, x) \\ &= \left[1 - e^{-\sigma_t x}\right] \frac{\sigma_i}{\sigma_t}, \end{aligned}$$

- Probability for σ_b':

$$P'(\text{Interaction } b) = p_b'(x) = \left[1 - e^{-\sigma_t{}' x}\right] \frac{\sigma_b}{\sigma_t'}$$

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Effect of altering σ_t

- Expand probability for σ_b' with Taylor series:

$$p_b'(x) = \left[1 - (1 - \sigma_t' x + \frac{(\sigma_t' x)^2}{2} + \mathcal{O}(\sigma_t'^3 x^3))\right] \frac{\sigma_b}{\sigma_t'}$$

$$p_b'(x) = \sigma_b\, x - \frac{\sigma_t' x^2}{2} - \mathcal{O}(\sigma_t'^2 x^3)).$$

- Change in probability:

$$\Delta p_b(x) = p_b'(x) - p_b(x) = -\frac{(\sigma_t' - \sigma_t) x^2}{2} + \mathcal{O}((\sigma_t'^2 - \sigma_t^2) x^3)$$

$$\boxed{\Delta p_b(x) = -\frac{\epsilon_a x^2}{2} + \mathcal{O}((\sigma_t'^2 - \sigma_t^2) x^3)}$$

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Simulations

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Simulations

- Perform **MCNP5_mult** simulations
  - Use modified nuclear data from created **ACE** files
  - The 5 different Pu sphere multiplicity experiments
  - JEZEBEL fast critical benchmark

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Simulations

- Perform **MCNP5_mult** simulations
  - Use modified nuclear data from created **ACE** files
  - The 5 different Pu sphere multiplicity experiments
  - JEZEBEL fast critical benchmark
- Generate multiplicity distributions with **mtool.pl** script
  - Non-paralyzable dead time correction

Comparing Results of Simulations

Comparing Results of Simulations

- Reduced χ^2 values for the 5 multiplicity experiments and criticality benchmark

$$\chi^2_{red,mult,m} = \frac{1}{N_{bins}-1}\sum_{i=1}^{N_{bins}} \frac{(R_i - S_i)^2}{\sigma^2(R_i)+\sigma^2(S_i)}$$

$$\chi^2_{red,k_{\text{eff}}} = \frac{(k_{\text{eff}}^{\text{MCNP}} - k_{\text{eff}}^{ref})^2}{\sigma^2(k_{\text{eff}}^{\text{MCNP}}) + \sigma^2(k_{\text{eff}}^{ref})}$$

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- Compute a FOM:

$$\boxed{FOM = \sum_{m=1}^{5} \chi^2_{red,mult,m} + \chi^2_{red,k_{\text{eff}}}}$$

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Modifying Nuclear Data

Modifying Nuclear Data

- Covariance data: **ENDF/B-VII.1** library

- MCNP input nuclear data: **ACE** format

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- Random samples of $\overline{\nu}(E)$, rather than linear optimization (LO)
  - LO would not preserve statistical accuracy
  - Under-constrained problem, infinite solutions

Capture Cross Section

- Adjust total cross section (σ_t) to compensate for change in σ_c

$$\boxed{\sigma_t' = \sigma_t + \epsilon_c} \qquad \epsilon_c = \alpha\,\sigma_c \qquad \sigma_c' = \sigma_c + \epsilon_c$$

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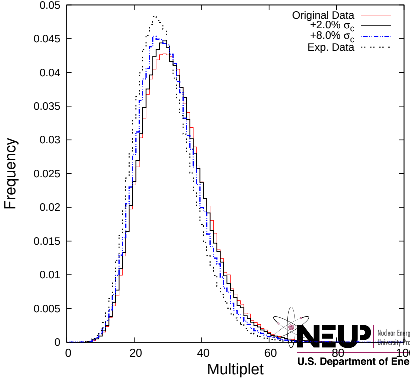
$\alpha = \mathbf{16.0\%}$	142.6	1.86	3.47	6.90
$\alpha = 8.0\%$	237.5	0.51	1.74	3.45
$\alpha = 2.0\%$	371.2	0.02	0.43	0.86
$\alpha = 1.0\%$	396.4	0.16	0.22	0.43
Original	426.6	0.27	0	0



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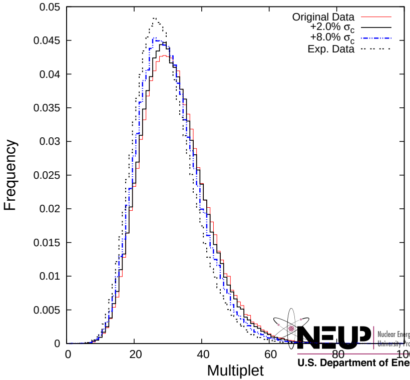

Fission Cross Section

- Adjust elastic scattering (σ_s) to compensate for change in σ_f

$$\boxed{\sigma'_s = \sigma_s + \epsilon_f} \qquad \epsilon_f = -\alpha\, \sigma_f \qquad \sigma'_f = \sigma_f - \epsilon_f$$

- Only for $E > 1keV$

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$$\boxed{\sigma'_s = \sigma_s + \epsilon_f} \qquad \epsilon_f = -\alpha\,\sigma_f \qquad \sigma'_f = \sigma_f - \epsilon_f$$

- Only for $E > 1keV$

Trial	χ^2_{mult}	$\chi^2_{k_{eff}}$
$\alpha = 2.0\%$	65.8	29.6
$\alpha = 1.5\%$	14.6	24.4
$\alpha = 1.0\%$	56.5	9.4
$\alpha = 0.5\%$	195.7	3.0
$\overline{\nu}$ -1.14%	130.58	33.7
Original%	426.6	0.0

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Future Work

- More energy-dependent $\overline{\nu}$ trials

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- Energy-dependent σ_f trials

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- More energy-dependent $\overline{\nu}$ trials
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  - Need constrained global optimization method

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