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Author(s): Timmons, Daniel Herbert
Rising, Michael Evan
Prinja, Anil Kant

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Evaluating the MCNP6.2 Correlated Fission Multiplicity Models for Criticality Calculations

[1,2]Daniel Timmons, [1]**Michael E. Rising** and [2]Anil K. Prinja

[1]Los Alamos National Laboratory
[2]University of New Mexico

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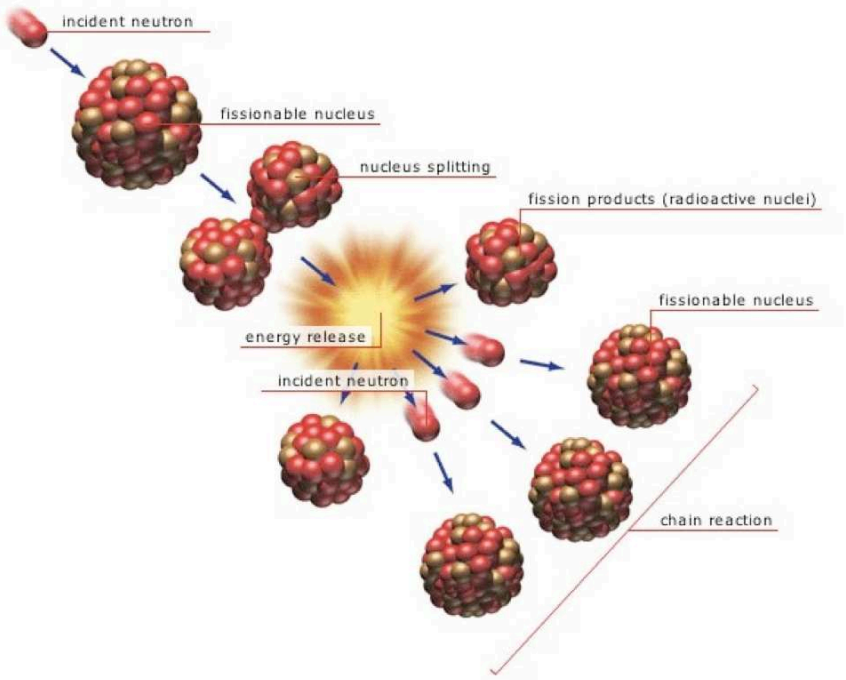
- Conclusions & Future Work



Background & Motivation

Background

- MCNP6.2 release included the ability to use FREYA and CGMF for fixed-source calculations
- FREYA was initially developed at LBNL/LLNL while CGMF was developed at LANL
- These high-fidelity models are used to simulate spontaneous, neutron-induced, and photo-fission (future work) events
- These fission physics models, primarily targeted toward nuclear nonproliferation applications, have not been validated for use in k-eigenvalue calculations

Motivation & Plan

- Using the well-known criticality benchmark experiments will aid in validating the correlated fission multiplicity models for more general use in a variety of applications
- This would allow us to study new methods for use in subcritical experiment design and subsequent validation calculations
- The use of the models in criticality calculations allows us to study the differences between the weighted and analog simulations
- Allow MCNP to use FREYA and CGMF in KCODE calculations (ACE file / MCNP modifications discussed in later slides)

Correlated Fission Multiplicity Models

FREYA – Fission Reaction Event Yield Algorithm

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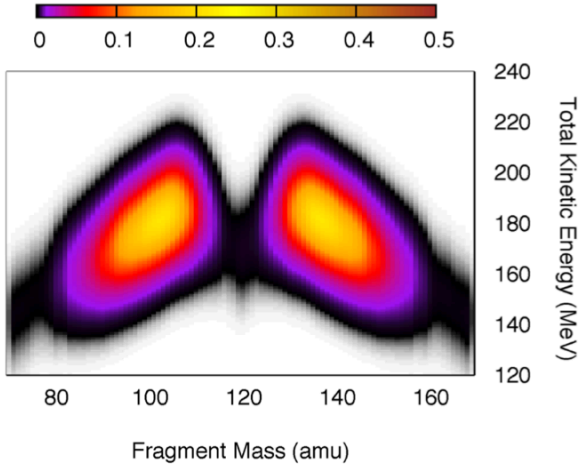
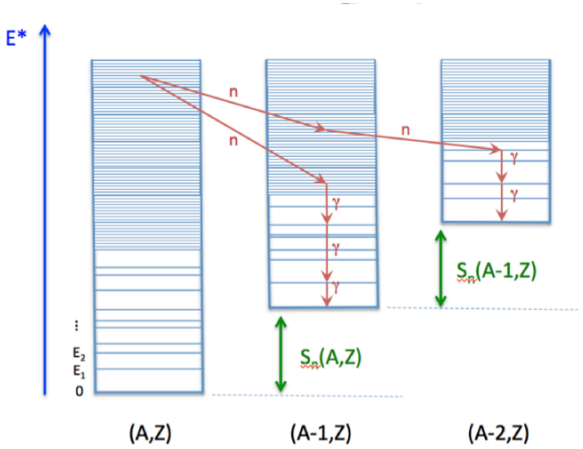
- Developed at LBNL and LLNL
- Determines mass split of the compound nucleus on experimental mass yields
- Determine the energy distribution between fragments
- Determine the energy given to post emission radiation
- Neutrons are emitted until below a threshold energy then gammas are emitted
- Neutron induced fission: ^{233}U, ^{239}Pu, ^{235}U, ^{241}Pu, ^{238}U
- Spontaneous Fission: ^{238}U, ^{238}Pu, ^{240}Pu, ^{242}Pu, ^{244}Cm, ^{252}Cf



CGMF – Cascading Gamma-ray Multiplicity + Fission

- Developed at LANL
- Determines mass split of the compound nucleus based on systematics of fission yields
- Determine the energy distribution between fragments
- Determine the energy given to post emission
- Hauser-Feshbach model is used to describe of the fission fragments to ground state
- Neutron induced fission: ^{239}Pu, ^{235}U, ^{238}U
- Spontaneous Fission: ^{240}Pu, ^{242}Pu, ^{252}Cf



ACE File Modifications

ACE File Modifications

- Data was generated with standalone FREYA and CGMF
- Computed data from models for ^{235}U and ^{239}Pu
  - Used “same” incident and outgoing energy bin structure as in ENDF/ACE
  - Average prompt fission multiplicity
  - Average prompt fission neutron spectrum
- Data points were placed into an ENDF/B-VII.1 ACE file
  - All other reactions/quantities left untouched
- Sensitivity coefficients (KSEN) computed for GODIVA and JEZEBEL
- Several other criticality benchmark cases were run to observe differences

ACE File Modifications

Numerical Results

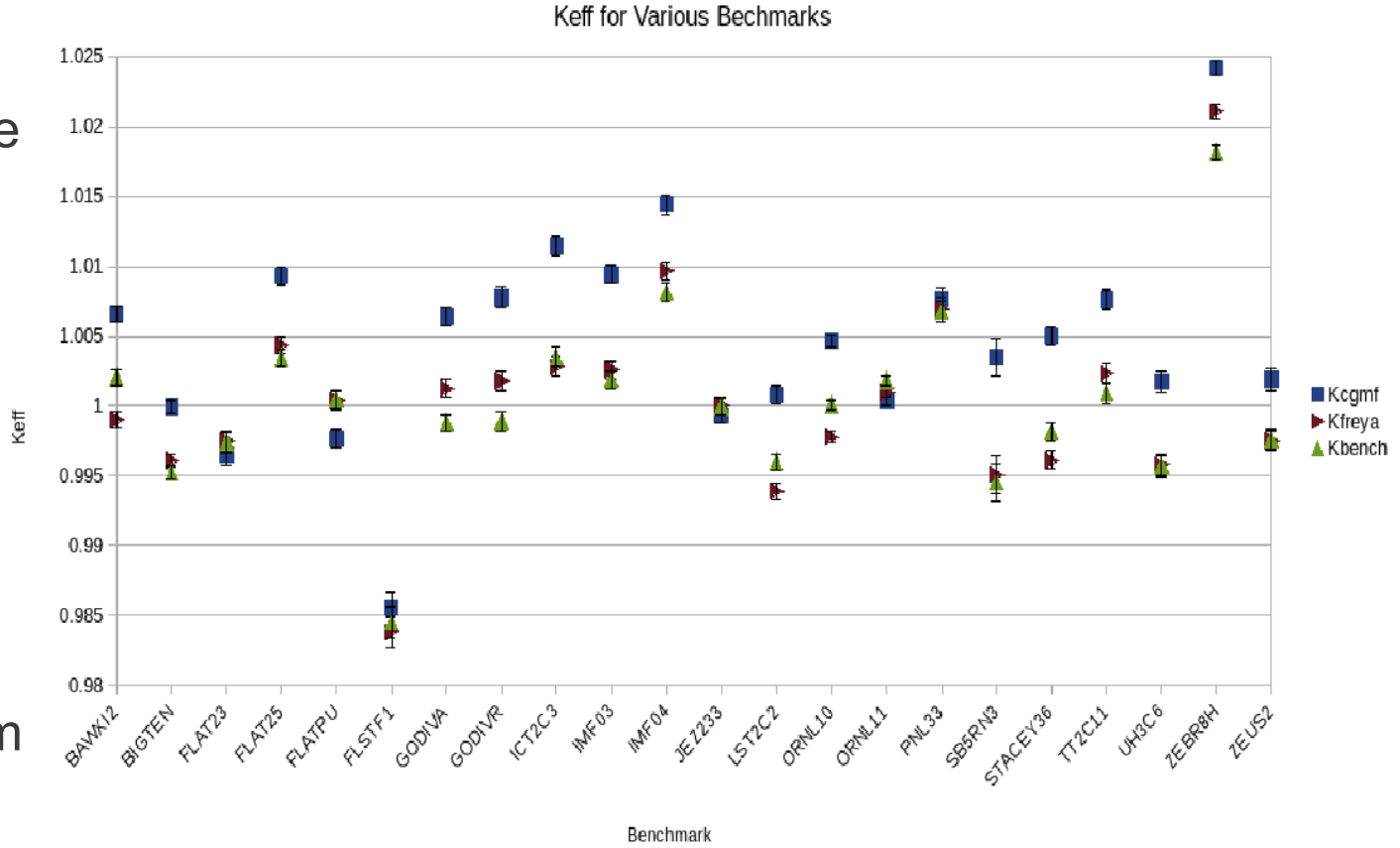
- This was done by running the event generator models and using the multiplicity and chi-energy spectrum data in place of the ACE data

	Method	Δkeff Sensitivity Calculation	Uncertainty	MCNP Calculation Δkeff	Uncertainty
GODIVA					
	CGMF	3.60E-02	3.07E-04	3.65E-002	4.75E-04
	FREYA	4.26E-02	7.94E-03	3.544E-002	2.16E-04
JEZEBEL					
	CGMF	-1.65E-02	1.72E-02	-1.684E-002	1.70E-04
	FREYA	-1.66E-02	3.31E-03	-1.675E-002	2.16E-04

ACE File Modifications

Numerical Results

- Many CGMF cases calculate higher k_{eff}
- Most cases show that FREYA is closer to the MCNP6.2 default based using data from ENDF/B-VII.1



MCNP6.2 Modifications

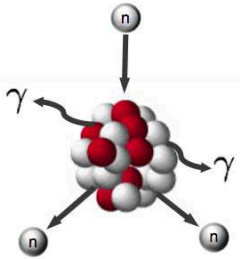
MCNP6.2 Modifications

- Need to allow for a more analog k-eigenvalue calculation using the full neutron multiplicity distribution
  - Fission site sampling based on the random selection of the fission reaction
    Think $\frac{\Sigma_f}{\Sigma_t}$, rather that the expected value of $wgt \cdot \frac{\nu\Sigma_f}{\Sigma_t}$
  - At fission sites, number $P(\nu)$, energy and direction of next-generation fission neutrons returned from models and placed in the bank
  - Renormalization of the fission bank population/weight is still required – because all particles have unit weight, splitting/rouletting of particles in the fission bank is done instead of scaling the weight of each particle

- Previously, these MCNP modifications had been done to study the effects of the LLNL Fission Library within criticality calculations

MCNP6.2 Modifications

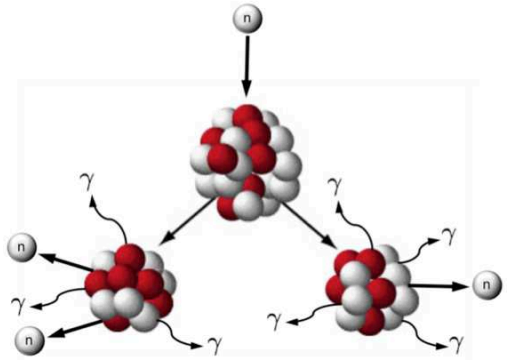
$$wgt \cdot \frac{\nu\Sigma_f}{\Sigma_t}$$



- Weighted Simulation
  - Average fission sites produced per collision
- Renormalization done by fission bank weight adjustment

1st Generation	2nd Generation	3rd Generation
$wgt_i = 1$	$wgt_i = 2$	$wgt_1 = 2$
		$wgt_{2,3} = 1$
$\sum wgt_i = 4$	$\sum wgt_i = 4$	$\sum wgt_i = 4$
$\nu = 1$, $\nu = 1$	$\nu = 1$, $\nu = 2$	$\nu = ?$, $\nu = ?$

$$\frac{\Sigma_f}{\Sigma_t}$$



- Analog Simulation
  - $P(\nu)$ fission sites produced per sampled fission reaction
- Renormalization done by fission bank splitting/rouletting

1st Generation	2nd Generation	3rd Generation
$wgt_i = 1$	$wgt_i = 1$	$wgt_i = 1$
$\sum wgt_i = 4$	$\sum wgt_i = 4$	$\sum wgt_i = 4$
$\nu = 1$, $\nu = 1$	$\nu = 2$, $\nu = 3$	$\nu = ?$, $\nu = ?$

MCNP6.2 Modifications

Numerical Results

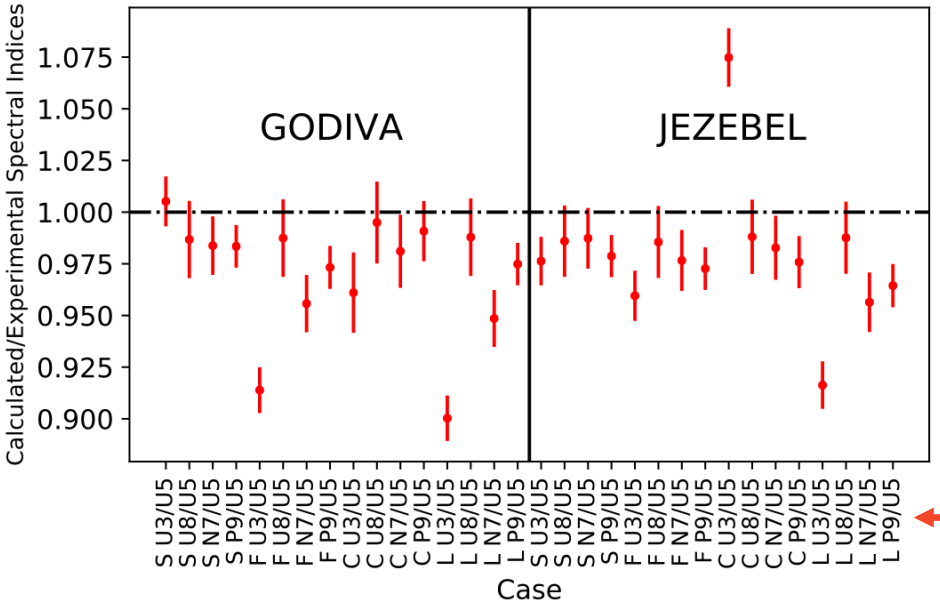
- CGMF and FREYA are supplemented with the LLNL Fission Library where the available nuclide does not exist for the model
- It is of note that CGMF is significantly slower than any other applied method
- Initially the changes to MCNP6.2 were tested on Godiva, Jezebel, and more
  - The k_{eff} and the spectral information (next slide) for each system have been studied

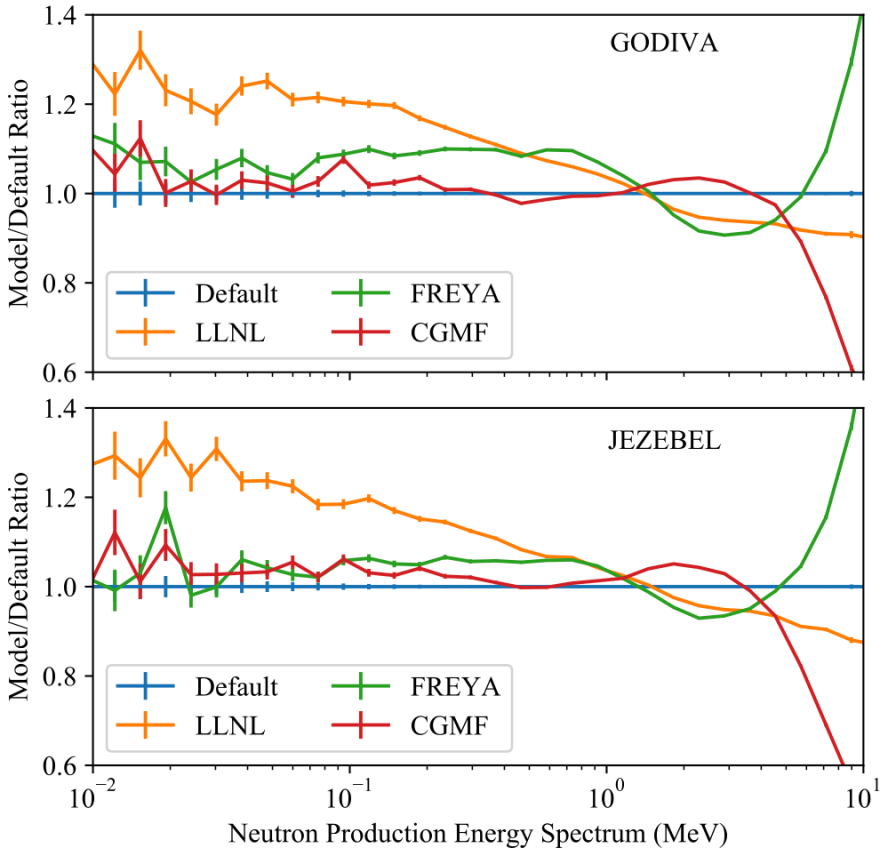
Model	GODIVA k_{eff}	JEZEBEL k_{eff}	FLAT23 k_{eff}	FLAT25 k_{eff}
Default	0.99987(19)	0.99987(19)	0.99915(30)	1.00331(30)
LLNL	0.99897(34)	0.99515(31)	0.99673(37)	1.00005(37)
FREYA	1.00053(34)	1.00097(31)	1.00121(39)	1.00568(37)
CGMF	0.99589(32)	0.99500(30)	0.99730(55)	0.99928(55)

MCNP6.2 Modifications

Numerical Results

- Spectral indices (*SI* defined below) can provide more information about system differences



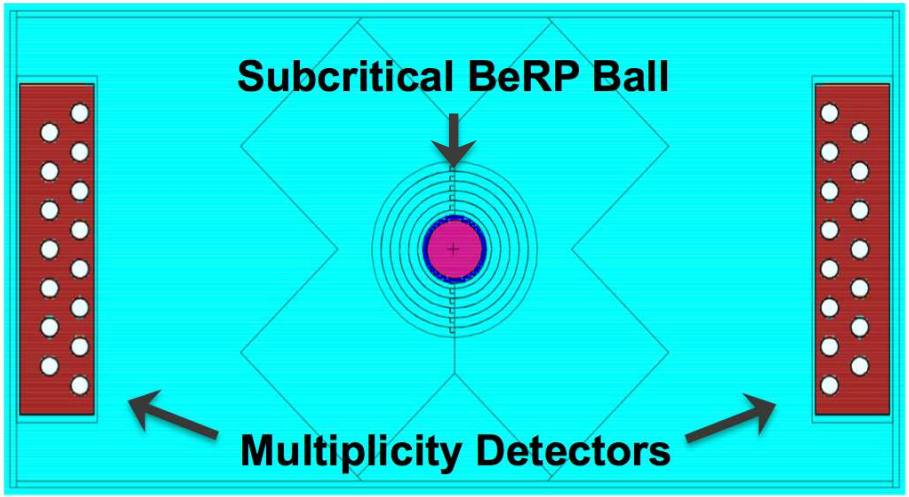


$$SI = \frac{\int_E \phi \Sigma_f^X \, dE}{\int_E \phi \Sigma_f^{235U} \, dE}$$

S=Standard U3=U-233
F=FREYA U8=U-238
C=CGMF N7=Np-237
L=LLNL P9=Pu-239

Initial Subcritical Simulations

Initial Subcritical Simulations



- Another use of the modified MCNP6.2 is to study subcritical benchmark calculations, which generally include:
  - Fixed-source calculation mode
  - Analog neutron multiplicity (FMULT)
  - Reading of the particle track (PTRAC) output
- As $k_{eff} \rightarrow 1.0$, the fixed-source approach can become intractable
- The population control (renormalization) in KCODE can help make these calculations more efficient
- Above, the BERP Ball can be surrounded by many Ni or W shells
  - The multiplicity (NPOD) detectors include several He-3 tubes

Initial Subcritical Simulations

- With the help of our colleagues in NEN-2 at LANL, some tools were used to analyze the results from the k-eigenvalue particle track (PTRAC) output
  - A wrapper was made to automate reading the time from the PTRAC file, analyzing the data, and collecting the results

- Three results were observed:
  - The singles count rate for a single NPOD detector
  - The doubles count rate for a single NPOD detector
  - The leakage multiplication rate (M_L)
    - Number of neutrons that leak out per source neutron

Initial Subcritical Simulations

- To modify the times a normal distribution is used to with a mean equal to that of what the output file for a fixed source case did, which is roughly half of the count time
- In order to ensure the same number of events, which the single count rate is dependent on, a direct ratio method was used between the fixed source case and the KCODE case to find the number of active cycles necessary
- With both of these it is possible to nearly match the results of the benchmark
  - Only the 1.0” Ni shell results will be shown here

Initial Subcritical Simulations

Numerical Results

BeRP Ball Reflected by 1" Ni Shell

	Benchmark	MCNP6.2	Modified MCNP6.2 (Fixed-Source)	Modified MCNP6.2 (KCODE+LLNL)
Singles	15107 ± 4.6	15150 ± 7.18	15150 ± 7.18	15054 ± 7.06
Doubles	7461 ± 23.6	7470 ± 16.0	7470 ± 16.0	7465 ± 16.3
M_L	5.42 ± 2.5E-2	5.46 ± 5.8E-3	5.46 ± 5.8E-3	5.46 ± 5.8E-3

For a single case: Fixed-Source: **44.8 min**

KCODE: **39.4 min**

Conclusions & Future Work

Conclusions

- Beginning to understand how the FREYA and CGMF models perform for criticality benchmarks when using their average data (nubar, PFNS) in ACE files and when used inline within MCNP6.2 as an event generator
- As expected, because these models have never been tuned (like the ENDF/B nuclear data) to criticality benchmarks, there is disagreement between the pure ENDF/B results and the FREYA/CGMF results
- Using KCODE with the multiplicity models to simulate the PTRAC output of the subcritical benchmarks is just beginning to be studied

Future Work

- Determine the source of the differences
  - It was noted that the output k_{eff} was different for LLNL, FREYA, and CGMF
- Modify the timing on the post processing of the PTRAC file
- Modify parameters/variables in CGMF and FREYA to bring the results closer to benchmark measurements
- Test further on more criticality cases
- Automate a new subcritical V&V suite

Acknowledgements

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Questions?