LA-UR-15-29286
Approved for public release; distribution is unlimited.

Title: MCNP6: Simulating Correlated Data in Fission Events

Author(s): Rising, Michael Evan
Sood, Avneet

Intended for: NA-22 Collaboration Meeting in Santa Fe, NM, Dec. 3-4

Issued: 2015-12-03

MCNP6: Simulating Correlated Data in Fission Events

Michael E. Rising and Avneet Sood

XCP-3 Division
Los Alamos National Laboratory

NA-22 Collaboration Meeting
Santa Fe, NM USA

December 3-4, 2015

Outline

- **Introduction**
  - Background
  - Review of MCNP6 development and integration strategy
- **FY15 Progress**
  - Implemented interface and tested performance
  - Updated LLNL Fission Library (v. 1.8 → v. 1.9.1)
  - Verification and validation testing
  - Partially integrated CGMF v. 1.0.6
- **FY16 Q1 Progress**
  - Updated new CGM
  - Nearly completed CGMF integration
- **Final Thoughts**

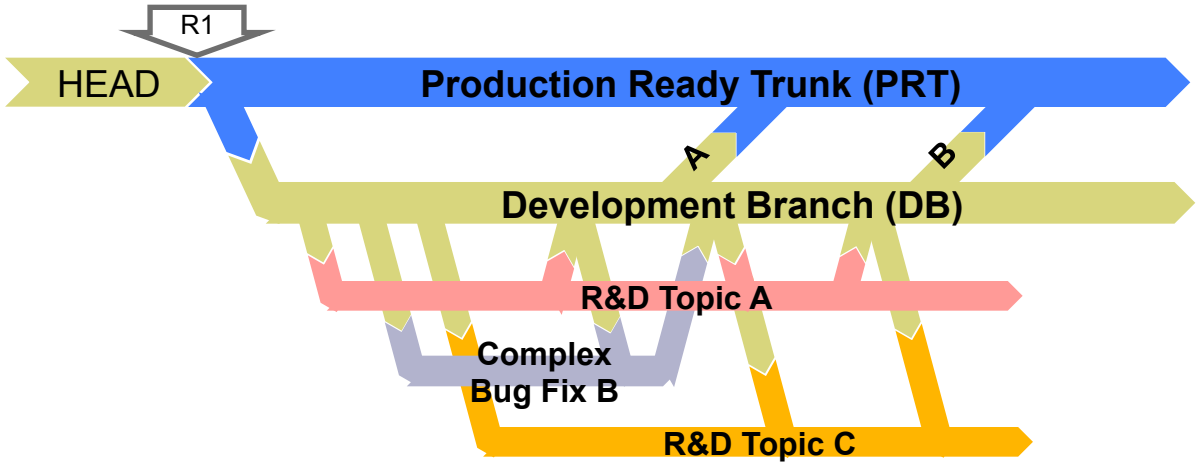
Background

- **Application of interest**
  - Global security and nuclear nonproliferation
  - Detection of special nuclear material (SNM)
  - Passive and active interrogation techniques
  - Coincident neutron and photon leakage
- **Key issues**
  - Average nuclear data quantities are insufficient
  - Cannot predict correlated signatures of shielded SNM
- **Approach to obtain predictive capability**
  - Use transport code MCNP for modeling neutrons and photons
  - Fission event generators are under development
  - Implement in MCNP and compare to experiment

Background

- **Default MCNP6 secondary emission physics:**
  - Neutrons – integer sampling of
  - Photons
    - Based on total photon production data
    - Emission determined before type of reaction is known
    - Integer number of photons changes with isotope, energy, etc.
  - No correlations between emitted particles
- **Parallel processing:**
  - OMP threading disabled for certain features
    - Most MCNPX physics models
      - High-energy physics like CEM, LAQGSM, INCL, ABLA, etc.
      - Multiplicity packages CGM & LLNL Fission Library
      - Delayed particle physics from CINDER
    - PTRAC (list-mode style output) and event logging

Development Strategy



- **Maintain a production-ready trunk of source**
- **Parallel development branch**
  - Minor bug fixes
  - Restructuring / modernization
  - New feature integration and testing
- **Research & development branches**
  - Complex bug fixes
  - New feature development
  - Initial implementation, testing and verification

Integration Strategy

First…

- ✓ Standalone executable for verification
- ✓ Have a user- and developer-friendly interface

Second…

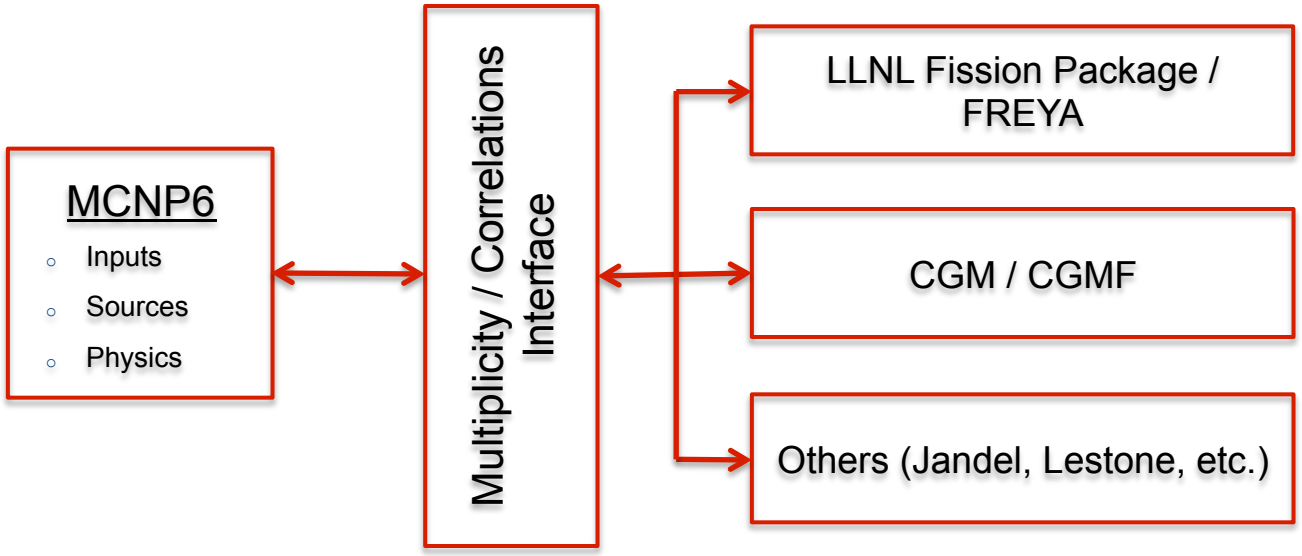
- ✓ Need thermal to 20 MeV for neutron-induced fission
- ~ Develop and pass all tests with standard configuration and compilers
- ❑ Indicators to users how the model is being used

Third…

- ❑ Needs to have validation tests documented and included
- ~ Further testing on more platforms, configurations, compilers, etc.
- ~ Should be continue-run, MPI-capable and thread-safe
- ~ Should be tested for performance and memory-usage

Integration Strategy

- **New interface:**
  - Features are less intrusive into MCNP6 source
  - Less chance for error in similar sections of code
  - Model options controlled in interface
  - New/updated event generators easier to integrate



FY15 Progress: Implemented Interface

- **Fortran module in MCNP6 source**

```
! Copyright LANS/LANL/DOE - see file COPYRIGHT_INFO
module corr_mult_interface_mod
  ! Interface for correlated/multiplicity secondary emission even
  !   CGM/CGMF (LANLs multplicity package) --- Includes many reac
  !   LLNL Fission Library --- Including FREYA, fission only
  !   Lestone correlated neutron multiplicity (future)
  !   Jandel correlated gamma multiplicity (future)
```

```
subroutine corr_mult_gennfevent(ZA,ERG,TME,NUBAR)
  ! Description:
  ! CORR_MULT_GENNFEVENT takes fission event info
  ! and calls cgmf or LLNL fission library

  ! .. external
  external genfissevt
  external cgmf_genfissevent

  integer,    intent(in) :: ZA
  real(dknd), intent(in) :: ERG
  real(dknd), intent(in) :: TME
  real(dknd), intent(in) :: NUBAR

  if( USING_CGMF ) then
    call cgmf_genfissevent(ZA,ERG,TME/1.0e8_dknd)
  if( USING_LLNL ) then
    call genfissevt(ZA,TME/1.0e8_dknd,NUBAR,ERG)
  endif

end subroutine corr_mult_gennfevent
```

```
subroutine corr_mult_init()
  ! Description:
  ! CORR_MULT_INIT uses rang to set RNG of models.

  ! .. used variables
  use mcnp_iofiles, only : hdpath

  ! .. used routines
  use mcnp_random, only : rang

  ! .. external
  external setrndg, setrngcgm
  external setcorrel
  external setdatapath


  if( .not. USING_CORR_MULT ) then
    return
  endif

  if( USING_CGM .or. USING_CGMF ) then
    call setrngcgm(rang)
    call setdatapath(hdpath//CHAR(0))
  endif
  if( USING_LLNL ) then
    call setrngd(rang)
    call setcorrel(3)
  endif

end subroutine corr_mult_init
```

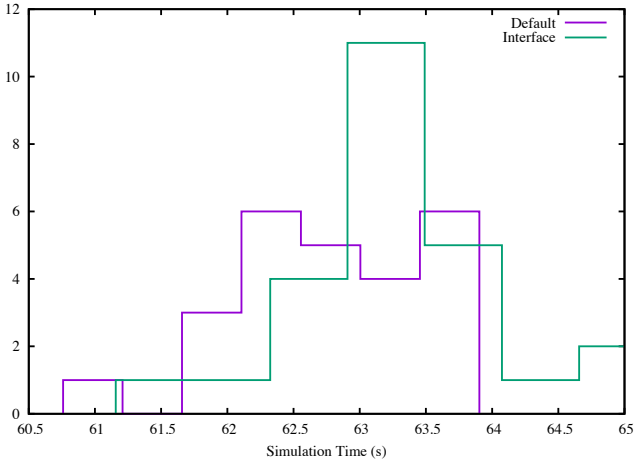
FY15 Progress: Tested Performance

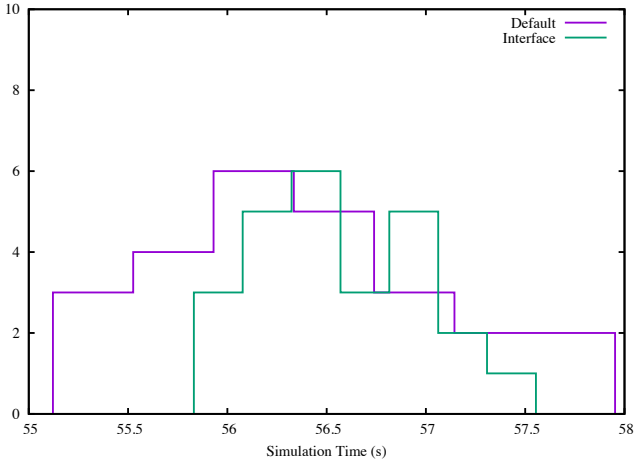
- **Added if test and function call**
  - When initialization occurs → no impact
  - When **each** fission event is generated
  - When **each** piece of secondary particle information is retrieved
    - Number of emissions
    - Energy
    - Direction vector
    - Time/Age
- **Think millions or billions of histories**
  - 1 extra if test and function call for **each** fission event
  - 6 extra if tests and function calls for **each** type of particle
- **Does this matter?**

FY15 Progress: Tested Performance

- **Worst case:**
  - Source monoenergetic particles
  - Force immediate collision
  - Stream secondary particles (no tallies)

	Test Times (s)			
	U Test		Pu Test	
	Default	Interface	Default	Interface
Linux 'time'	62.107	62.590 (+0.78%)	55.706	55.795 (+0.16%)
MCNP time avg	62.795	63.339 (+0.87%)	56.318	56.571 (+0.45%)
MCNP time unc	1.21%	1.29%	1.24%	0.74%

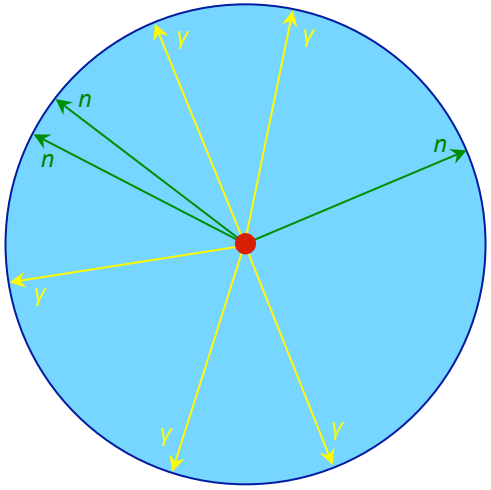




- **Slow down is less than 1%**
- **For realistic transport problems it will be negligible**

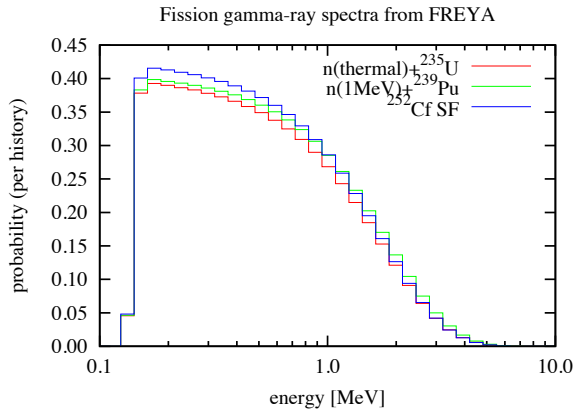
FY15 Progress:
Updated LLNL Fission Library

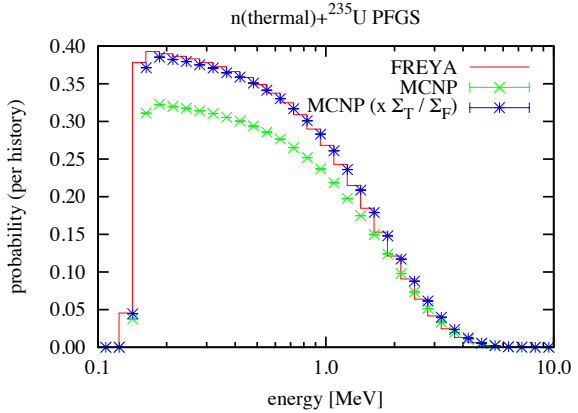
- **Moved from version 1.8 to 1.9.1**
  - Now FREYA is default over library tabulated data
  - Few bug fixes and Fortran compliance issues resolved
- **MCNP6 test problems**
  - Common test problems for these features:
    - Point source at origin of sphere
    - Force immediate collision from source
    - Secondary particles stream to sphere
    - Tallies on sphere surface
  - Changed regression answers:
    - 5/7 LLNL Fission Library specific tests (n+^{238}U and n+^{232}Th unchanged)
    - 2/14 CGM specific tests (n+^{239}Pu and n+^{235}U changed)
  - All 7 test problem changes were expected!
    - Currently, FREYA does not have n+^{238}U and n+^{232}Th
    - Currently, CGM uses LLNL Fission Library for fission gamma-rays

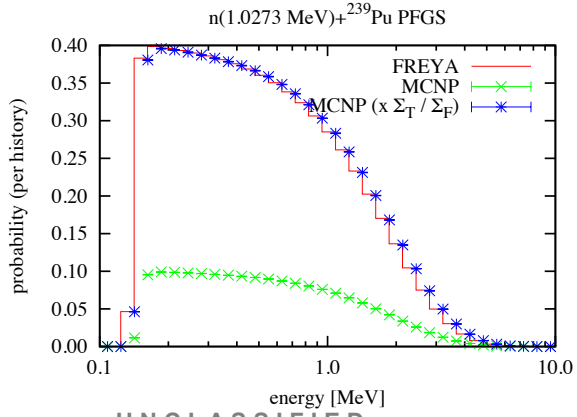


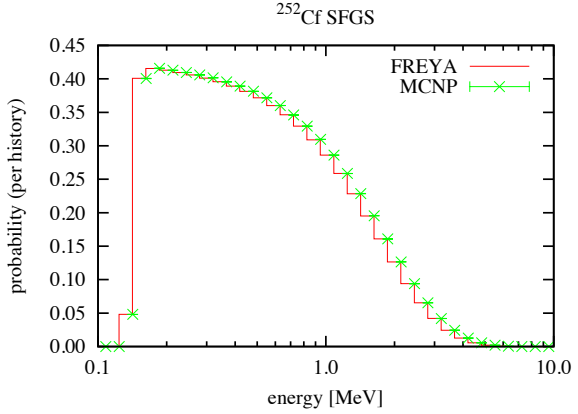
FY15 Progress: Verification Testing

- **Primary tests include ^{235}U(n,f), ^{239}Pu(n,f) and ^{252}Cf(sf)**
- **Standalone compared to integrated event generators**
- **LLNL Fission Library**
  - version 1.9.1
  - using FREYA
- **CGMF next…**
- **Easy tests**
  - total $\bar{\nu}_n$ & $\bar{\nu}_\gamma$
  - $\bar{\chi}_n$ & $\bar{\chi}_\gamma$ (shown)
- **Normal tests**
  - $P(\nu_n)$ & $P(\nu_\gamma)$
- **Hard tests**
  - Correlations, $n-n$ $\gamma-\gamma$ $n-\gamma$



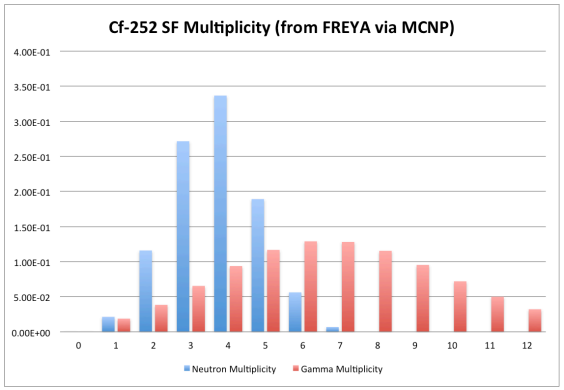




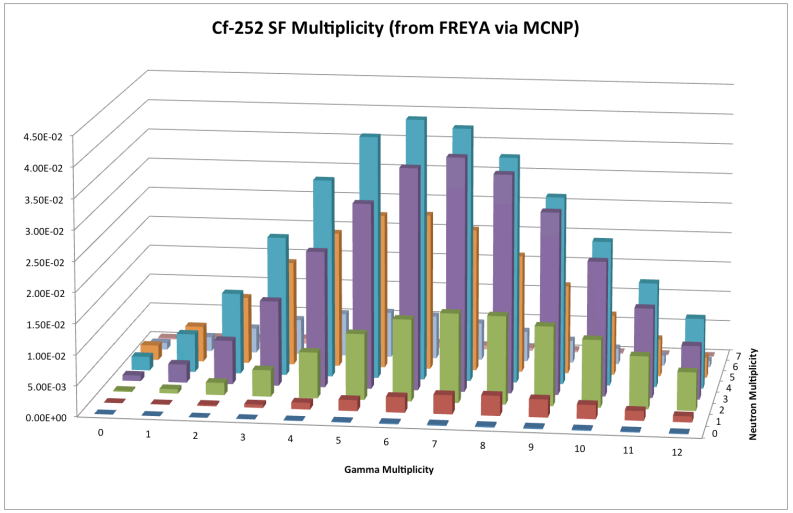


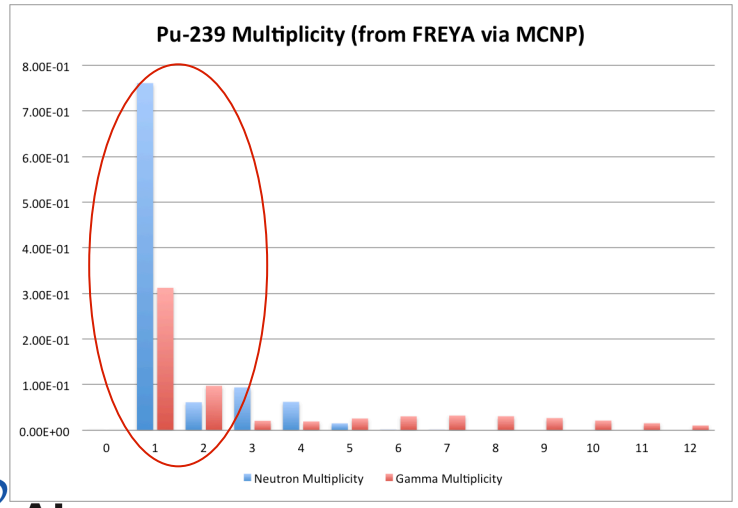
FY15 Progress: Verification Testing

- **Checking multiplicity distributions**



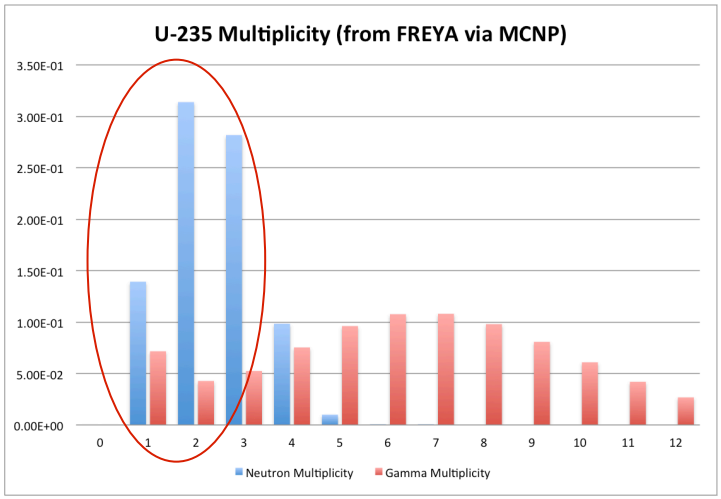
Cf-252 SF



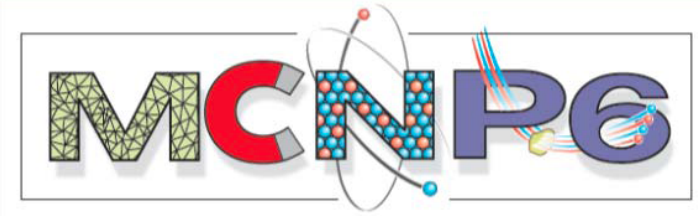


n(~1MeV)+^{239}Pu

n(thermal)+^{235}U



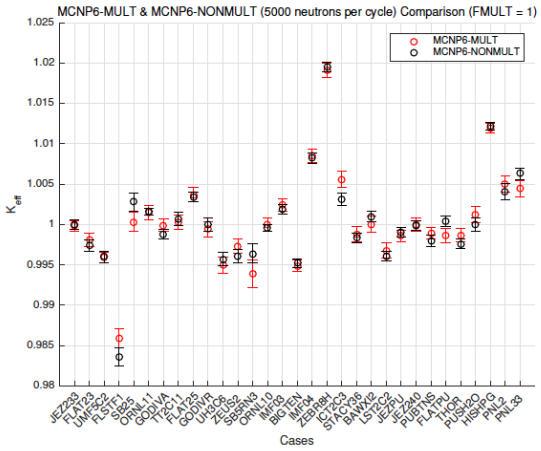
FY15 Progress: Validation Testing



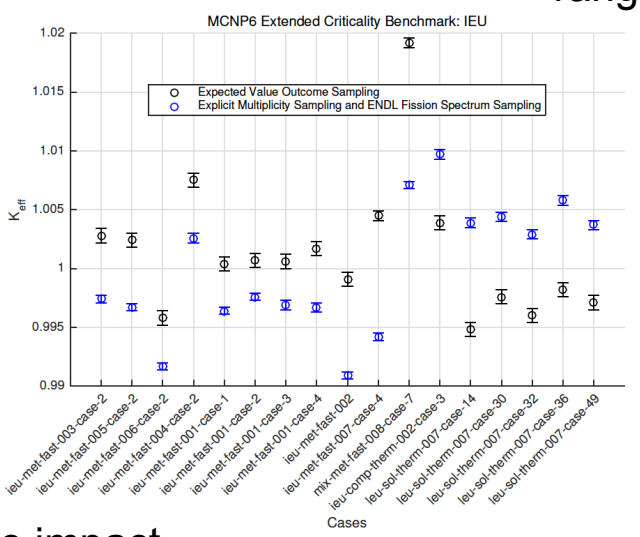
- **Investigated impact on criticality calculations (NCSP supported)**
  - Extensive V&V benchmark test suites in MCNP already
  - For example, ICSBEP Handbook used for all (serious) MC codes
- **By default in MCNP**
  - Neutron multiplicity for fission is based on expected value of wgt · $\nu\Sigma_F^{mat} / \Sigma_T^{mat}$ neutrons per collision in the material
    - Energy & direction for each are sampled independently (no correlation)
  - The spectrum used for the fission neutrons is randomly chosen using probabilities $\nu\Sigma_F^{iso} / \nu\Sigma_T^{mat}$ for the nuclides in the material
    - Energy is sampled using ENDF spectrum data for the selected nuclide
    - Prompt vs delayed neutron selected first, then energy
    - Energy is sampled independently for each one (no correlation)
  - The direction for fission neutrons is sampled isotropically
    - Directions are sampled independently for each neutron (no correlation)
  - For criticality problems with photons, photons are sampled independent of neutrons (no correlation between neutrons & photons)

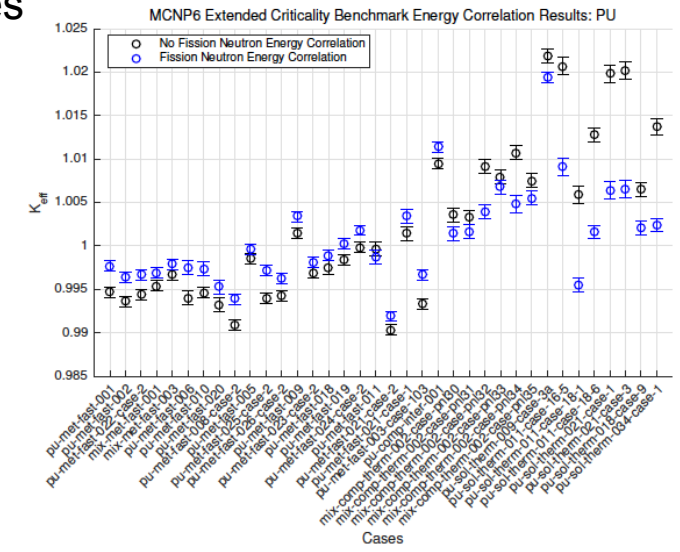
FY15 Progress: Validation Testing

- **Criticality Validation Test Suite**
  - 31 experimental benchmarks
  - Covers several materials, compositions & energy ranges



- **Extended Criticality Validation Test Suite**
  - 119 experimental benchmarks
  - LEU, IEU, HEU, U233 and Pu materials, compositions & energy ranges



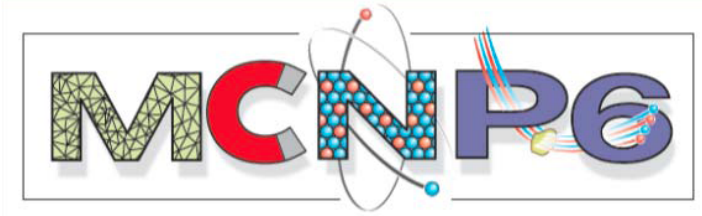


- **Punchline:**
  - multiplicity → *no impact
  - spectrum → definite impact
  - energy correlation → ???

*if nubar is preserved

Figures taken from: M. Ortega, M.S. Thesis, University of New Mexico, NM.

FY15 Progress:
Partially Integrated New CGMF



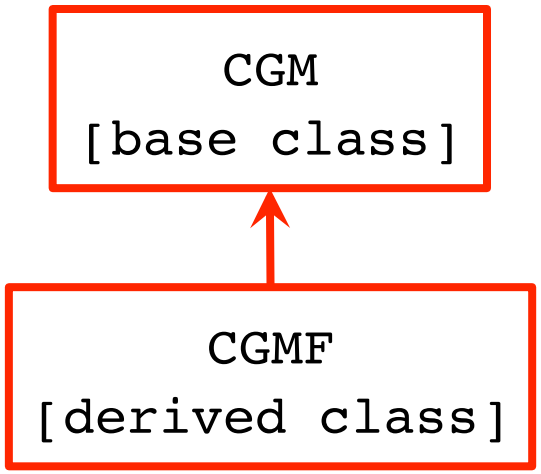
- **Received CGMF v. 1.0.6 on 9/3/15**
  - Updated manual
  - Includes initial interface to MCNP
  - n+^{239}Pu now incident energy dependent
  - Modest updates to CGMF-only routines from v. 1.0.3
  - Several changes made to underlying CGM routines
- **Performed a quick initial test**
  - Could build standalone and run standard tests
  - CGMF interface approach would work for integration
- **Planned integration strategy**
  - With CGM in MCNP6 already, want to preserve capability
  - But with the improvements that come along with the new routines
  - Bottom line: integration requires careful step-by-step process
    - Migrate new source files individually
    - Run MCNP CGM test cases to identify differences

FY16 Q1 Progress: Updated New CGM

- **MCNP6 includes 14 CGM test problems (regression)**
  - Templates based on local LANL linux platform
  - Intel fortran compiler 12.1.5 (moving to 15.0.5) and gcc
  - OMP (threading) is in default build with tests based on single thread execution
- **In comparison to CGM tests/templates already distributed with MCNP**
  - Identified ~6 parameters that cause changes
  - Identified ~7 methods that cause changes
  - Found 1 error (in MCNP) in the random number usage
- **For now, original CGM parameters & methods are default**
- **Recently, the primary CGM function/driver was converted to C++ class**
  - Has no impact on tests/templates
  - Can be used as base class for CGMF C++ class
    - Removes some duplicate methods
    - Unifies the global variable usage

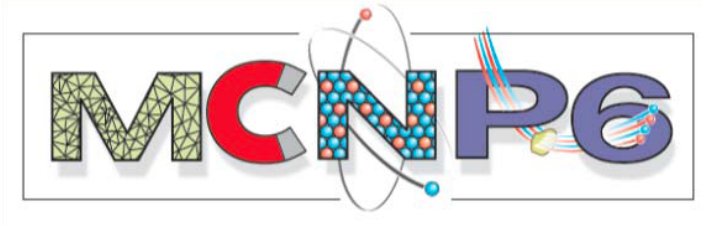
FY16 Q1 Progress:
Nearly Completed CGMF Integration

- **Migrated remaining CGMF-only source files to MCNP6**
- **Created a CGMF C++ class which derives from the CGM base class**
  - Both build as standalone with simple drivers
  - Both build in MCNP6 system (with CGM functioning correctly)



- **Minor CGMF issues need to be resolved before V&V testing**

Final Thoughts



1 **Need to finish up**

- CGMF
  - CGM update
  - Integration of CGMF
  - Verification testing
  - Performance testing

2 **Next efforts on**

- Adding more user support on details of the model being used
- Work on continue run and parallel
  - MPI compatible
  - OMP thread safe
- Test more platforms (Windows, etc.)

3 **Validation is very important**

- Using criticality for now
- Need experimental list-mode comparisons to predictions
- Code-to-code comparisons would be valuable as well

4 **Finally, before the FY16 MCNP release**

- Need local LANL code review
- User guide for how to use multiplicity options and general guidance
- V&V documentation

Thank You