MCNP6.2 Status & Developments: FY16 and early FY17

NA-22 Collaboration Meeting
Santa Fe, NM  USA

Michael E. Rising
XCP-3 Group, LANL

March 6-7, 2017
Outline

- **What was done in FY16**
  - New models integrated
    - LLNL Fission Library 2.0.1
    - FREYA 2.0
    - CGMF 1.0.9
  - Verification Testing

- **What is being done now**
  - Release of MCNP6.2
  - Validation Testing

- **What will be done in FY17**
  - New MCNP6.2 tools released
  - Code upgrades and modernization

- **What else...**
What was done in FY16
Looking back at previous collaboration meetings

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
What was done in FY16
New models integrated (1)

- LLNL Fission Library 2.0.1
  - Produces same results from previous version
  - Now includes FREYA 2.0

- FREYA 2.0
  - Code and data included
  - Spontaneous fission: $^{238}$U, $^{238}$Pu, $^{240}$Pu, $^{242}$Pu, $^{244}$Cm, and $^{252}$Cf
  - Neutron-induced fission: $^{233}$U, $^{235}$U, $^{238}$U, $^{239}$Pu, and $^{241}$Pu

- CGMF 1.0.9
  - Code and data included (also upgraded CGM)
  - Spontaneous fission: $^{240}$Pu, $^{242}$Pu, and $^{252}$Cf
  - Neutron-induced fission: $^{235}$U, $^{238}$U, and $^{239}$Pu
What was done in FY16
New models integrated (2)

- Standalone versus MCNP-integrated for verification
- Completed and cleaned up interface to models
- Regressions tests (~30) run and give exact results on Linux, Mac OS/X and Windows systems
- Added comments to output file indicating
  - Which model is being used (and the backup option)
  - What isotopes are available for the selected model
- Continue-run and MPI-capable
- Performance:
  - CGMF

MCNP6
  - Inputs
  - Sources
  - Physics

Fission Event Multiplicity & Correlations Interface

LLNL Fission Library / FREYA

CGM / CGMF

Others (Jandel, Lestone, etc.)
What was done in FY16
MCNP6.2 user options (1)

- FMULT option within MCNP turns on neutron multiplicity sampling and allows the user to,
  - Modify spontaneous fission average multiplicity and yield rate
  - Change Watt energy spectrum parameters for spontaneous fission
  - Provide Gaussian FWHM width for spontaneous and induced fission multiplicity distributions
  - Select a sampling algorithm and data source
- Does not handle fission gamma-ray emission
- Each neutron emitted,
  - Direction is isotropic and independently sampled
  - Energy is sampled independently from the same energy distribution (uncorrelated)

What was done in FY16
MCNP6.2 user options (2)

• How do users access these models in MCNP?
  • FMULT data card with method keyword
    • method = 5 → LLNL Fission Library
    • method = 6 → FREYA
    • method = 7 → CGMF
  • If FREYA/CGMF cannot handle a specific spontaneous or neutron-induced fission isotope, the LLNL Fission Library is used
  • If the LLNL Fission Library cannot handle a specific spontaneous or neutron-induced fission isotope, the default FMULT parameters are used
  • Some additional information printed to output file:

    warning. Using FMULT, not CGMF, for spontaneous fission of 98250.

* = this isotope was used in the simulation, but the nuclear data came from **CGMF + LLNL fission library.
** CGMF handles neutron-induced (n,f) fission of Pu-239.
The remaining (n,f) nuclear data will come from the LLNL fission library.
### What was done in FY16

**MCNP6.2 user options (3)**

- **MCNP6.2** $^{252}$Cf spontaneous fission input files

<table>
<thead>
<tr>
<th>Default MCNP</th>
<th>LLNL Fission Library</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test of spontaneous fission multiplicity</td>
<td></td>
</tr>
<tr>
<td>1 1 -1e-10 -1 imp:n=1</td>
<td></td>
</tr>
<tr>
<td>99 0 1 imp:n=0</td>
<td></td>
</tr>
<tr>
<td>1 so .001</td>
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</tr>
<tr>
<td>m1 98252 1</td>
<td></td>
</tr>
<tr>
<td>sdef par=-sf</td>
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<tr>
<td>c</td>
<td></td>
</tr>
<tr>
<td>fmult 98252 method=3 data=3 shift=1</td>
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<td>c</td>
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<tr>
<td>nps 1000000</td>
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<tr>
<td>mode n p</td>
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<tr>
<td>cut:n 2j 0 0</td>
<td></td>
</tr>
<tr>
<td>c</td>
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<tr>
<td>*f11:n 1</td>
<td></td>
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<td>f11:n 1</td>
<td></td>
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<tr>
<td>c</td>
<td></td>
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<tr>
<td>*f21:p 1</td>
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<tr>
<td>f211:p 1</td>
<td></td>
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<td></td>
</tr>
</tbody>
</table>

[Method=6 → FREYA, Method=7 → CGMF]
What was done in FY16
Verification testing (1)

- Documented in report LA-UR-16-27710 and presented at 2016 ANS
  ANNTCP Conference in Santa Fe, NM
- Average multiplicity and energy

**CGMF**

<table>
<thead>
<tr>
<th>Quantity</th>
<th>²⁵²Cf(sf)</th>
<th>n(1.0273 MeV)+²³⁹Pu</th>
<th>n(thermal)+²³⁵U</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Standalone</td>
<td>MCNP</td>
<td>Standalone</td>
</tr>
<tr>
<td>$\tilde{\nu}_N$</td>
<td>3.7415(13)</td>
<td>3.7439(16)</td>
<td>3.0512(11)</td>
</tr>
<tr>
<td>$\tilde{\chi}_N$</td>
<td>2.0927(8)</td>
<td>2.0920(10)</td>
<td>2.0322(9)</td>
</tr>
<tr>
<td>$\tilde{\nu}_\gamma$</td>
<td>8.2721(32)</td>
<td>8.2680(37)</td>
<td>7.9039(31)</td>
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<tr>
<td>$\tilde{\chi}_\gamma$</td>
<td>0.8561(3)</td>
<td>0.8558(3)</td>
<td>0.9287(3)</td>
</tr>
</tbody>
</table>

**FREYA**

<table>
<thead>
<tr>
<th>Quantity</th>
<th>²⁵²Cf(sf)</th>
<th>n(1.0273 MeV)+²³⁹Pu</th>
<th>n(thermal)+²³⁵U</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Standalone</td>
<td>MCNP</td>
<td>Standalone</td>
</tr>
<tr>
<td>$\tilde{\nu}_N$</td>
<td>3.7464(13)</td>
<td>3.7463(13)</td>
<td>3.0101(12)</td>
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<tr>
<td>$\tilde{\chi}_N$</td>
<td>2.2840(10)</td>
<td>2.2815(10)</td>
<td>2.1534(10)</td>
</tr>
<tr>
<td>$\tilde{\nu}_\gamma$</td>
<td>7.7291(28)</td>
<td>7.7364(28)</td>
<td>6.8770(24)</td>
</tr>
<tr>
<td>$\tilde{\chi}_\gamma$</td>
<td>0.9052(3)</td>
<td>0.9051(3)</td>
<td>1.0097(4)</td>
</tr>
</tbody>
</table>
What was done in FY16 Verification testing (2)

- Neutron and Gamma-ray Multiplicity
- $^{252}$Cf spontaneous fission
What was done in FY16
Verification testing (3)

• Neutron and Gamma-ray Energy Spectra
• $^{252}$Cf spontaneous fission
What was done in FY16 Verification testing (4)

- Neutron and Gamma-ray Multiplicity Correlations
- $n$(thermal)$+^{235}\text{U}$ neutron-induced fission

![Graphs showing neutron and photon multiplicity correlations for CGMF and FREYA models]
What was done in FY16
Verification testing (5)

- Neutron and Gamma-ray Multiplicity Correlations
- $n(\text{thermal}) + ^{235}\text{U}$ neutron-induced fission
What was done in FY16 Verification testing (6)

- Neutron-Neutron Angular Correlations
  - $n(1.0273 \text{ MeV}) + ^{239}\text{Pu}$ fission
  - $n(\text{thermal}) + ^{235}\text{U}$ fission
  - $^{252}\text{Cf}$ spontaneous fission
What was done in FY16
Verification testing (7)

• Why is this so important?
  • With the size of MCNP at ~500K source code lines, integration of these
kinds of features is complicated and prone to mistakes
  • Previously, when zero neutrons were emitted in neutron-induced fission,
    zero gamma rays were also emitted
  • This bug has been fixed for MCNP6.2

• New MCNPTools available with MCNP6.2 release
  • Used the PTRAC (sources, collisions, terminations, etc.) feature
    • Tabulated all averages, distributions and correlations from the MCNP simulations
    • How the MCNP zero neutron/gamma-ray bug was discovered

• Integrated fission event generator models appear to be implemented
correctly!
What is being done now
Release of MCNP6.2

- Soon! (April/May 2017)
- Finalizing documentation and references
- Testing on all supported platforms

What’s new in MCNP6.2?
- New/upgraded fission multiplicity models
  - LLNL Fission Library / FREYA
  - CGMF
- ISC : Intrinsic Source Constructor
  - Used to generate radiation sources for transport code input (SDEF)
- MCNPTools
  - Library that provides object-oriented access to MCNP outputs
    - MCTAL files
    - MESHTAL B (MCNP5/FMESH) files
    - PTRAC files
What is being done now
Validation testing (1)

- Presented at 2016 ANS ANNTP Conference in Santa Fe, NM (J. Verbeke)
- Used MCNPTools to convert PTRAC to format for post-processing
- Re-run these simulations with CGMF and FREYA in MCNP6.2

Cf source Birthday-cake liquid scintillator array
c c CELLS
17 13 -0.874 -17 imp:n,p,h=1 $ scintillator 17
18 13 -0.874 -18 imp:n,p,h=1 $ scintillator 18
...
c c SURFACES
...

mode n p h $ transport neutrons, photons, protons
nps 18981035 $ # of neut / sec = 39,761 neuts/s,
c # of neut in 1801 secs = 71,609,561 neuts.
c # of fiss in 1801 secs = 71,609,561/3.772690
  = 18,981,035 fiss.
phys:n 1.e8 5j 1 $ keep recoil particle (7th entry)
fmult 98252 method=7
ptrac file=bin max=1e9 write=all type=p,h
event=col,bnk,ter,sur filter=17,93,icl

c

MCNPX Model Depiction of Liquid Scintillator Detector Array at LLNL
What is being done now
Validation testing (2)

- University of Michigan differential measurements of angular correlations
- Priority is to compare against experimental measurements
- Follow-up of 2014 NSE paper by S.A. Pozzi et al.
- Submitted an abstract to IRRMA X meeting in Chicago, IL, July 9-13
- Transport and post-processing code comparisons
  - MCNP6 / DRiFT
  - MCNP6 / MPPPost
  - MCNPX-PoliMi / MPPPost
  - MCNPX-PoliMi / DRiFT
What is being done now
Validation testing (3)

- To perform MCNP6 / MPPost and MCNPX-PoliMi / DRiFT calculations, the outputs may need to be converted
- Tested PTRAC to MCNPX-PoliMi collision output file conversion script
  - Again, used MCNPTools for PTRAC reading
  - Agreement is very reasonable with small discrepancies
    - Deposited energy differences – inelastic scatter on Carbon (<0.009% source with > 1keV diff)
    - Incident energy differences – elastic scatter on Hydrogen (<0.004% source with > 1keV diff)
What is being done now
Validation testing (4)

• **Starting last summer, alpha testing new models began**
  - Students from CNEC and CVT are participating
  - Testing list-mode output through PTRAC
  - Collaboration with Univ. of Michigan (UMich), LLNL & LBNL

• **In progress validation models include**
  - NISC experiments (K. Meierbachtol, M. Andrews)
  - UMich scintillator array (M. Marcath, M. Rising)
  - LLNL scintillator array (J. Verbeke, M. Rising)
  - LANL detector arrays at LANSCE, DANCE & NEUANCE (C. Walker – LANL, M. Pinilla – KSU)
  - Subcritical BeRP ball experiments (J. Arthur – UMich)
  - Criticality validation (D. Timmons - UNM)
  - Others…
What will be done in FY17
New MCNP6.2 tools released

• In MCNP6.2 release:
  • (M)ISC : MCNP / general intrinsic source constructor
  • MCNPTools : MCNP outputs

• To be released at a future date:
  • DRiFT : Detector Response Function Toolkit

• Presented at workshop at 2016 ANS ANNTP Conference in Santa Fe, NM
  (look on website under technical references and workshops)
  • LA-UR-16-27559 : MCNP6 basics
  • LA-UR-16-27301 : fission multiplicity models
  • LA-UR-16-27265 : ISC and MCNPTools info
  • LA-UR-16-27166 : DRiFT
What will be done in FY17
Code upgrades and modernization

- In general, MCNP will see major infrastructure and coding changes in the upcoming years
  - Modernization
    - Common software engineering practices
    - Utilize software engineering tools (git, cmake, etc.)
  - Minimize impact on users

- Improve parallel capabilities
  - OMP threading for models
  - PTRAC / event logger improvements
    - MPI capable
    - Thread safe
  - Physics algorithm improvements
    - Closer to analog
    - ENDF/B-VIII – separate photon production channels
What else…
Where has this been presented

• **Meetings and workshops in FY14-FY16**
  • 2014 ANS Winter Meeting – M. Rising *et al.* in NNP Division
  • 2015 ANS M&C + SNA + MC – MCNP workshop
  • 2015 UNM Seminar – M. Rising
  • 2016 ANS PHYSOR & NCSP TPR – UNM student work
  • 2016 ANS ANNTP Conference – MCNP workshop
  • 2016 NECDC – same as PHYSOR/NCSP work above

• **Upcoming meetings and workshops in FY17**
  • 2017 Nuclear Engineering Capability Review – LANL
  • 2017 ANS Summer Meeting – M. Rising & A. Sood in RPS Division
  • 2017 IRRMA X Conference – M. Andrews, M. Rising & M. Marcath
  • 2017 ANS NCSD Topical Meeting – MCNP workshop
  • Others…
What else...
Conclusions

- Needs to have **validation tests** documented and included
  - Would have been nice to have more results prior to MCNP6.2 release
  - All of the ongoing work is extremely promising
- **Should be continue-run, MPI-capable and thread-safe**
  - Need performance improvements (for CGMF especially)
  - Other MCNP features like PTRAC need work too

- MCNP tasks for this LCP should be attainable
  - Physics algorithm improvements ➔ priority after MCNP6.2 release
  - Parallel code capabilities ➔ priority after MCNP6.2 release
  - List-mode analyzer utilities ➔ some already made available
  - Perform MCNP6 simulations of NISC experiments ➔ ongoing
THANK YOU!

Questions?