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Title: Open-source Release of CGMF and Integration into the MCNP6.3 Code

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Open-source Release of CGMF and Integration into the MCNP6.3 Code

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2021 MCNP® User Symposium
July 12-16, 2021

LA-UR-21-26275

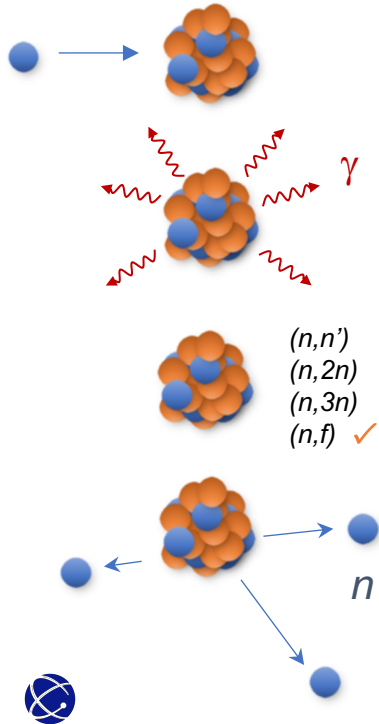
Overview

- Motivation for CGMF in the MCNP6.2 release
- CGMF on GitHub
 - Source code and Python toolkit
 - ReadTheDocs documentation
 - Computer Physics Communications publication
- Updates for the MCNP6.3 release
 - CGMF updates
 - New CGMF-MCNP integration
 - Verification



Motivation for CGMF in the MCNP6.2 release

Default MCNP Calculations



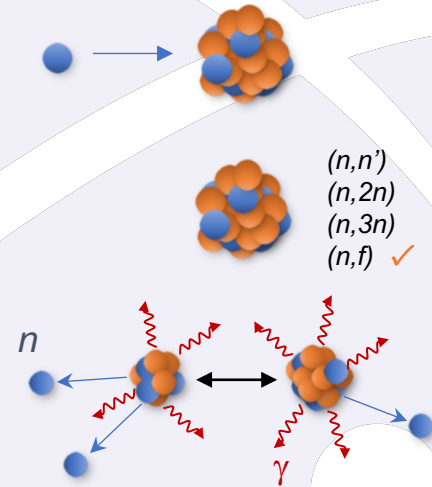
• Limitations

- OK on average \rightarrow criticality safety, shielding, reactor physics applications, etc.
- Wrong order for selection of reaction channels and reaction output
- Cannot perform correlated simulations or time-coincident detector response calculations

• Previous workarounds:

- Sampling $P(\nu)$ in MCNP
- LLNL fission library
- Detector response simulations in MCNPX-PoliMi

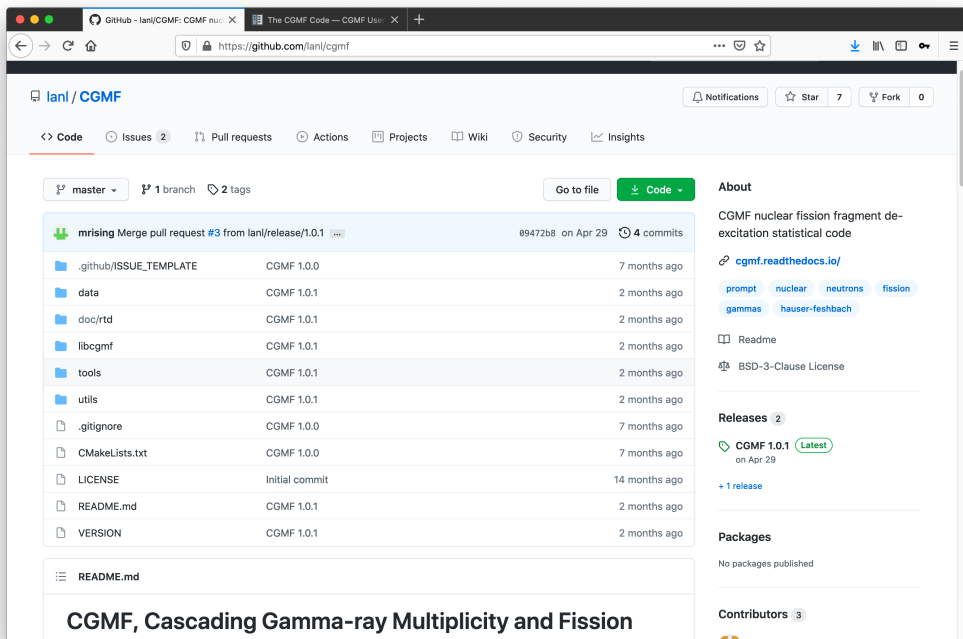
MCNP with CGMF Calculations



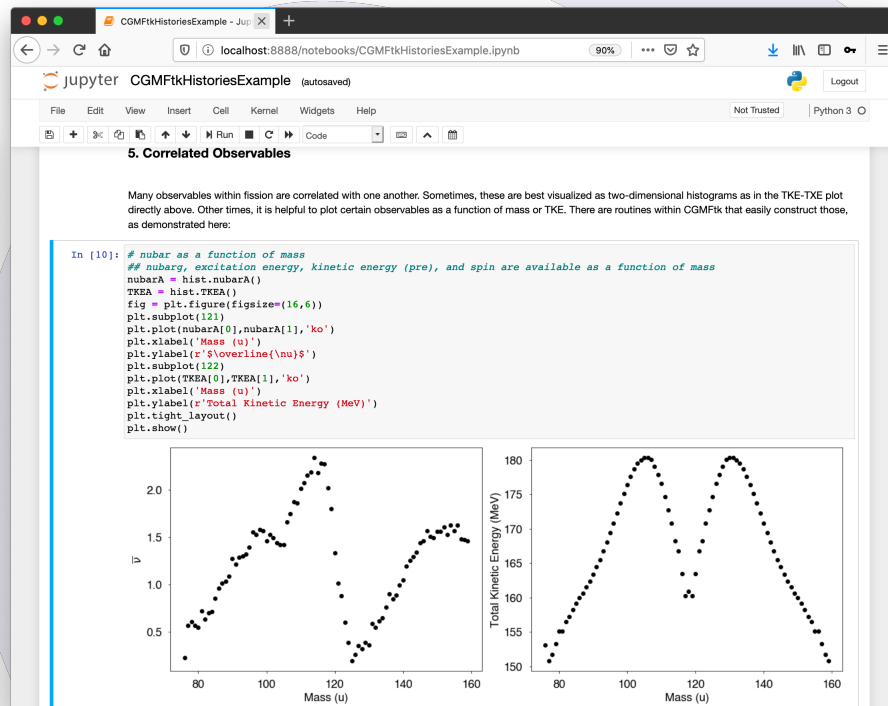
Developed a new paradigm to simulate nuclear reactions on an event-by-event basis for “low-energy” fission physics applications

CGMF on GitHub - <https://github.com/lanl/cgmf>

Source code, data, and Python tools



The screenshot shows the GitHub repository page for `lanl/CGMF`. The repository is in the `master` branch and has 1 branch and 2 tags. The file list includes `.github/ISSUE_TEMPLATE`, `data`, `doc/rtd`, `libcgmf`, `tools`, `utils`, `.gitignore`, `CMakeLists.txt`, `LICENSE`, `README.md`, and `VERSION`. The repository description is "CGMF nuclear fission fragment de-excitation statistical code". The latest release is `CGMF 1.0.1` from April 29, 2023. The repository is licensed under BSD-3-Clause License. The repository is also linked to `cgmf.readthedocs.io` and has a `Readme` and `BSD-3-Clause License` section. The repository is also linked to `cgmf.readthedocs.io` and has a `Readme` and `BSD-3-Clause License` section. The repository is also linked to `cgmf.readthedocs.io` and has a `Readme` and `BSD-3-Clause License` section.



The screenshot shows a Jupyter Notebook titled "CGMFtkHistoriesExample" running on a local host. The notebook displays the following Python code:

```
In [10]: # nubar as a function of mass
## nubar, excitation energy, kinetic energy (pre), and spin are available as a function of mass
nubarA = hist.nubarA()
TKEA = hist.TKEA()
fig = plt.figure(figsize=(16,6))
plt.subplot(121)
plt.plot(nubarA[0],nubarA[1],'ko')
plt.xlabel('Mass (u)')
plt.ylabel(r'$\overline{\nu}$')
plt.subplot(122)
plt.plot(TKEA[0],TKEA[1],'ko')
plt.xlabel('Mass (u)')
plt.ylabel(r'Total Kinetic Energy (MeV)')
plt.tight_layout()
plt.show()
```

The notebook also contains the following text:

5. Correlated Observables

Many observables within fission are correlated with one another. Sometimes, these are best visualized as two-dimensional histograms as the TKE-TXE plot directly above. Other times, it is helpful to plot certain observables as a function of mass or TKE. There are routines within CGMFtk that easily construct those, as demonstrated here:

The notebook displays two plots side-by-side. The left plot shows the average number of prompt neutrons ($\overline{\nu}$) as a function of mass (u), with data points in black circles and a line connecting them. The right plot shows the Total Kinetic Energy (MeV) as a function of mass (u), also with data points in black circles and a line connecting them. Both plots show a clear correlation between mass and the respective observable.

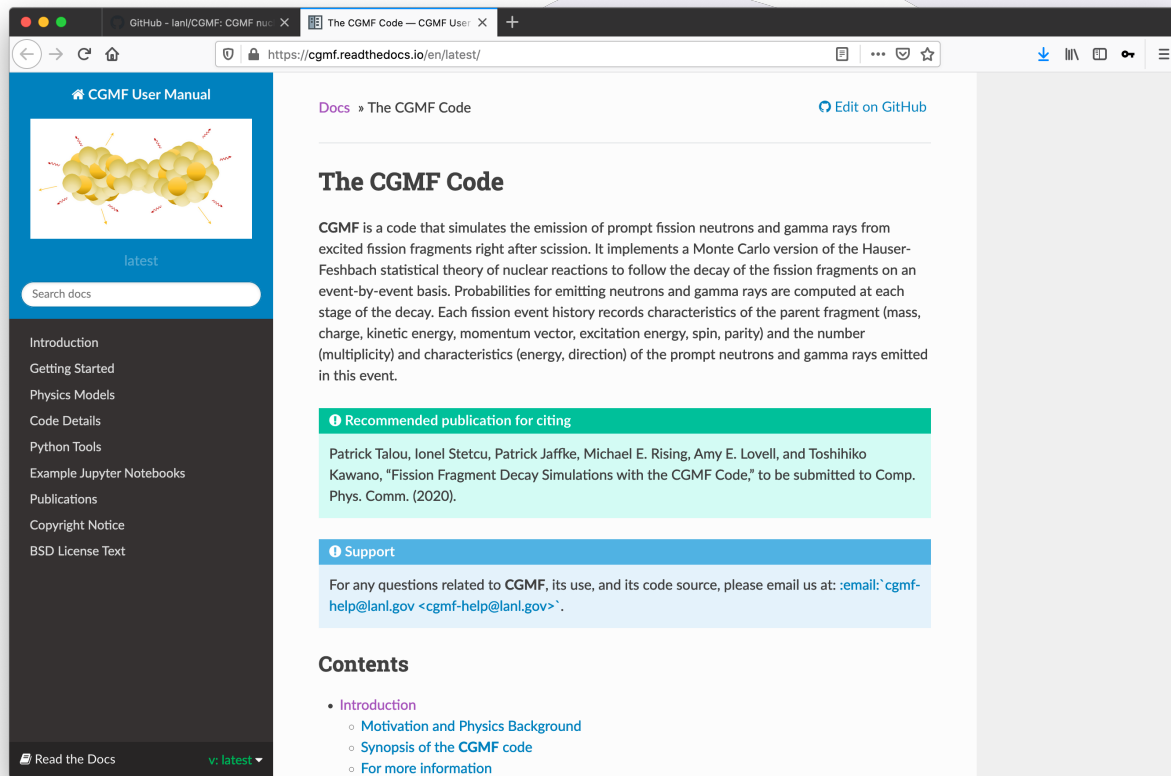
Python Jupyter notebooks distributed



CGMF on GitHub - <https://cgmf.readthedocs.io/en/latest/index.html>

- ReadTheDocs documentation
- Computer Physics Communications publication coming out soon

Patrick Talou, Ionel Stetcu, Patrick Jaffke, Michael E. Rising, Amy E. Lovell, and Toshihiko Kawano, "Fission Fragment Decay Simulations with the CGMF Code," accepted in *Comp. Phys. Comm.* (2021).



The screenshot shows a web browser displaying the CGMF User Manual page. The page has a dark blue header with the title "CGMF User Manual" and a search bar. Below the header is a navigation menu with links to "Introduction", "Getting Started", "Physics Models", "Code Details", "Python Tools", "Example Jupyter Notebooks", "Publications", "Copyright Notice", and "BSD License Text". The main content area is white and features a section titled "The CGMF Code" with a detailed description of the code's purpose and capabilities. Below this is a "Recommended publication for citing" section with a green background, followed by a "Support" section with a blue background. At the bottom, there is a "Contents" section with a list of links.

CGMF User Manual

latest

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Introduction
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The CGMF Code

CGMF is a code that simulates the emission of prompt fission neutrons and gamma rays from excited fission fragments right after scission. It implements a Monte Carlo version of the Hauser-Feshbach statistical theory of nuclear reactions to follow the decay of the fission fragments on an event-by-event basis. Probabilities for emitting neutrons and gamma rays are computed at each stage of the decay. Each fission event history records characteristics of the parent fragment (mass, charge, kinetic energy, momentum vector, excitation energy, spin, parity) and the number (multiplicity) and characteristics (energy, direction) of the prompt neutrons and gamma rays emitted in this event.

Recommended publication for citing

Patrick Talou, Ionel Stetcu, Patrick Jaffke, Michael E. Rising, Amy E. Lovell, and Toshihiko Kawano, "Fission Fragment Decay Simulations with the CGMF Code," to be submitted to *Comp. Phys. Comm.* (2020).

Support

For any questions related to CGMF, its use, and its code source, please email us at: `email:cgmf-help@lanl.gov <cgmf-help@lanl.gov>`.

Contents

- [Introduction](#)
 - [Motivation and Physics Background](#)
 - [Synopsis of the CGMF code](#)
 - [For more information](#)



Updates for the MCNP6.3 release

- CGMF updates

- Spontaneous fission

- $^{238}, ^{240}, ^{242}, ^{244}\text{Pu}$
- $^{252}, ^{254}\text{Cf}$

New Fissionable
Systems Compared to
MCNP6.2 Release

- Neutron-induced fission

- $^{233}, ^{234}, ^{235}, ^{238}\text{U}, ^{237}\text{Np}$, and $^{239}, ^{241}\text{Pu}$

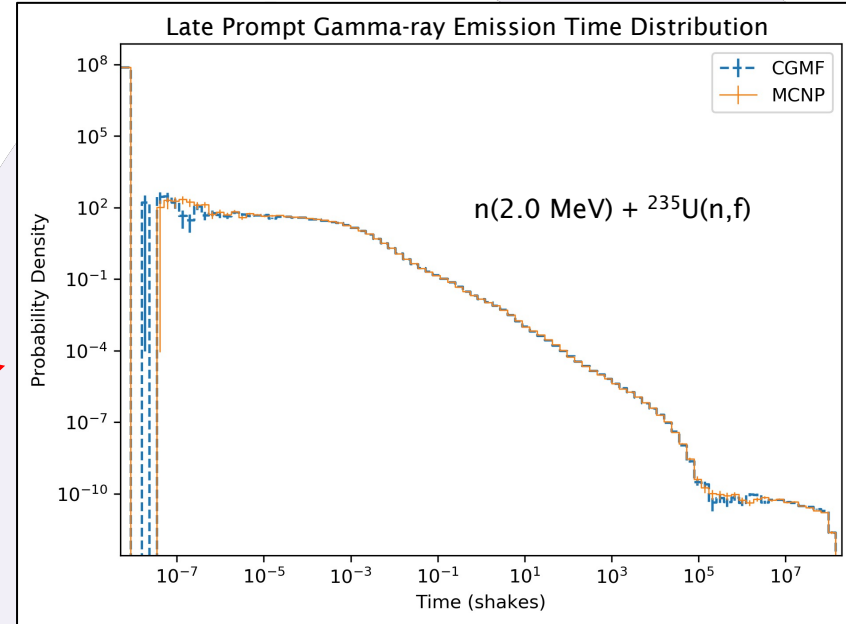
- Late-time prompt fission gamma rays

- Fission fragment angular distributions

- Pre-equilibrium neutron emission

- New CGMF-MCNP integration

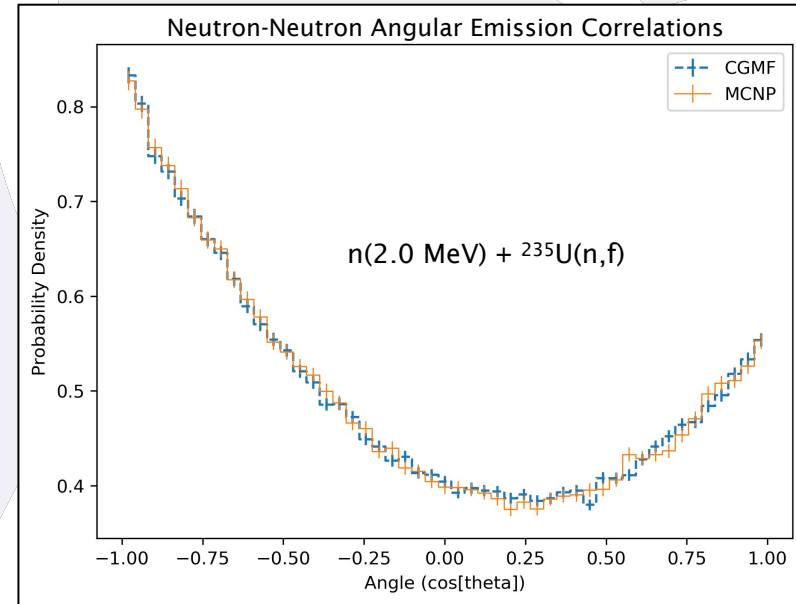
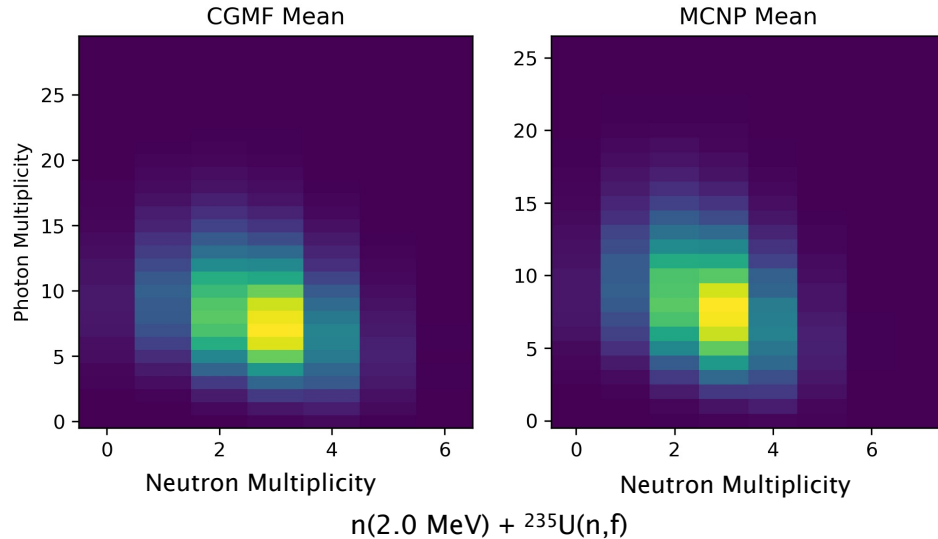
- Through the new MCNP CMake build system (`find_package`)
- Built as library, linked to MCNP executable
- Same library can also be linked to CGMF executable



Updates for the MCNP6.3 release

- Verification of the integrated CGMF code and MCNP interface
 - Done with new HDF5 PTRAC and MPI

Neutron-Photon Fission Multiplicity Correlations



Note: No change to MCNP input options. To use CGMF → **FMULT METHOD=7**

Acknowledgements

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Questions?

Contact: mrising@lanl.gov

