CGMF Documentation

Release 1.0.6

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CHAPTER ONE

SUMMARY

- **Program Title**: CGMF
- **Expanded Title**: Monte Carlo Hauser-Feshbach Decay of Fission Fragments
- **Current Version**: 1.0.6
- **License**: Copyrighted Los Alamos National Laboratory (**for now**)
- **Programming Language**: C++
- **Computing Platform**: any computer with a C++ compiler; tested with GNU g++, gcc version 4.2.1
- **Operating System**: tested on Mac OS X 10.7, 10.8, 10.9.5, and GNU/Linux 2.6.18
- **Parallel Version?**: Yes. MPI version included.

CHAPTER

TWO

INTRODUCTION

Note: Current Version: 1.0.6

Date: August 28, 2015

2.1 Motivation and Physics Background

The fission of a heavy nucleus into two or more lighter fragments is usually accompanied with the emission of *prompt* neutrons and photons. In our current understanding of the fission process, the fission fragments are produced in a certain state of deformation and intrinsic excitation, eventually resulting in the production of excited fission fragments. Very quickly, those primary fragments will evaporate neutrons and photons to reach a more stable configuration, either a ground-state or a long-lived isomer. The post-neutron emission fission fragments, also called fission products, will possibly further β-decay, leading to another burst of β-delayed neutron and photon emissions.

The study of the prompt fission neutrons and photons is significant to better model the nuclear fission process, constrain the collective and intrinsic configurations of the nascent fragments near the scission point, and understand the sharing of the available excitation energy between the two fragments. This study is also highly relevant for applications, ranging from nuclear energy safety and efficiency to non-proliferation and stockpile stewardship missions.

Until recently, most of the nuclear data evaluation work related to prompt fission neutrons and photons was limited to their average number, or multiplicity, and their average energy spectrum. Even for those somewhat simple quantities, scarce experimental data exist only, limited to some important isotopes and incident neutron energies. Phenomenological models have been developed over the years, e.g., the so-called Los Alamos model (LAM), mostly for calculating the average prompt fission neutron spectrum (PFNS). Evaluated data on prompt fission always originated from very scarce experimental data, leaving important gaps even in the most modern nuclear data libraries such as ENDF/B-VII.1.

The **CGMF** code was developed to model the de-excitation of the fission fragments on an event-by-event basis, following the successive emissions of neutrons and photons. This is radically different from what had been done in the past, allowing an unprecedented level of predictions on distributions and correlations of neutrons, photons and fission fragments. The development of this code is accompanied by a host of new fission experiments that look at increasing details and correlations among the vast quantity of fission data. Correlations and distributions of post-scission data will be very useful to constrain the free parameters entering in the **CGMF** code and models.

2.2 Synopsis of the CGMF code

The **CGMF** code is based on two older codes developed at LANL: **FFD** [LA-CC-10-003] and **CGM** [LA-CC-11-018]. It performs Monte Carlo simulations of the decay of excited fission fragments by emission of prompt neutrons and gamma rays. The Hauser-Feshbach statistical theory of compound nuclear reactions is used to compute the emission probabilities at each step of the cascade. Monte Carlo histories are then recorded and analyzed.

The average prompt fission neutron multiplicity $\overline{\nu}$, the prompt fission neutron multiplicity distribution $P(\nu)$, the average prompt fission neutron multiplicity as a function of mass, charge and kinetic energy of the fragment, $\overline{\nu}(A, Z, TKE)$, etc, can all be extracted from **CGMF** calculations. Similar quantities can also be obtained for prompt gamma rays. In addition, $n - n$, $n - \gamma$, and $\gamma - \gamma$ correlations can be studied both in energy and angle.

The **FFD** code was the first fission fragment evaporation code to be developed, and used the Weisskopf-Ewing approximation to evaporate neutrons. Characteristics of the emitted prompt neutrons could be retrieved, but only little information could be inferred for the prompt γ-ray data, and no specific discrete transitions in particular fragments could be tagged. Meanwhile, the **CGM** code was being developed as a general Monte Carlo implementation of the traditional statistical nuclear reaction codes, e.g., GNASH, EMPIRE, TALYS, COH, using the very well-established Hauser-Feshbach statistical theory of nuclear reactions. With **CGM**, one can follow the decay of an excited compound nucleus by evaporation of photons, neutrons, and light charged particles until it reaches its ground-state or a long-lived isomer. Monte Carlo histories could be followed one-by-one to study correlations and *exclusive* data.

Initially written in FORTRAN 95, significant parts of **FFD** were re-written into C++ classes to work seamlessly with the C++ code **CGM**, leading to the release of the **CGMF** code that applies the physics of **CGM** to the de-excitation of fission fragments.

2.3 For more information

This user manual is intended to become the main reference for the **CGMF** code. However, several publications and presentations might be of interest to the reader wanting more information on how the code is actually used for practical studies. Here, we just mention a few of them. A larger publication list can be found at the end of this manual.

- "Monte Carlo approach to sequential neutron emission from fission fragments," S. Lemaire, P. Talou, T. Kawano, M. B. Chadwick, and D. G. Madland, Phys. Rev. C 72, 024601 (2005). *This publication was our first attempt to compute prompt fission neutron data in a Monte Carlo statistical evaporation approach. It used our previous* **FFD** *code.*
- "Monte Carlo Simulation for Particle and Gamma-Ray Emissions in Statistical Hauser-Feshbach Model," T. Kawano, P. Talou, M. B. Chadwick, and T. Watanabe, J. Nucl. Sci. Tech. 47, No.5, 462 (2010). *This publication discusses for the first time the Monte Carlo implementation of the Hauser-Feshbach statistical theory present in the* **CGM** *code.*
- "Advanced Monte Carlo Modeling of Prompt Fission Neutrons for Thermal and Fast Neutron-Induced Fission Reaction on Pu-239," P. Talou, B. Becker, T. Kawano, M. B. Chadwick, and Y. Danon, Phys. Rev. C 83, 064612 (2011). *A good example of an application of the* **FFD** *code to study the prompt fission neutron data for Pu-239. It also contains a long description of how the initial fission fragment yields are reconstructed from partial experimental data.*
- "Monte Carlo Hauser-Feshbach Predictions of Prompt Fission Gamma Rays- Application to $n_{\mathrm{th}}+$ U-235, $n_{th}+$ Pu-239 and Cf-252 (sf)," B. Becker, P. Talou, T. Kawano, Y. Danon, and I. Stetcu, Phys. Rev. C 87, 014617 (2013). *This publication discusses results obtained with a very early version of the* **CGMF** *code.*
- "Properties of Prompt Fission Gamma Rays," I. Stetcu, P. Talou, T. Kawano and M. Jandel, Phys. Rev. C 90, 024617 (2014).

CHAPTER

THREE

THE PHYSICS OF CGMF

CGMF follows the de-excitation of primary fission fragments through the evaporation of neutrons and photons until they reach a ground-state or a long-lived excited state. The statistical Hauser-Feshbach theory is used to infer the probabilities of evaporating a neutron or a photon at each step of the decay. Some details on the physics used is described in this Chapter.

3.1 Initial Fission Fragment Yields

CGMF does not calculate the initial pre-neutron fission fragment yields. Instead, it reads or reconstructs those yields in mass, charge and kinetic energy, $Y(A, Z, TKE)$, from experimental data or systematics. Several theoretical efforts are underway to predict fission fragment yields from dynamical fission calculations. We will incorporate the results of those works as they become available.

In the present version of **CGMF**, only binary fission events are considered. Ternary fission where an alpha-particle is emitted along with the two fragments is not treated, nor more complicated "fission" splitting, e.g., accompanied with cluster emission. In addition, the neutron emission is assumed to happen only once both fragments are *fully accelerated*. In other words, no *scission* neutrons are considered at this point. However, multi-chance fission processes such as (n,n'f), (n,2nf), etc., as well as pre-equilibrium contributions are taken into account at higher incident energies.

3.1.1 Mass Yields

Thermal Neutrons and Spontaneous Fission

For important fission reactions such as the thermal neutron-induced fission cross-section of Pu-239 and U-235, enough reliable experimental data exist to reconstruct those initial yields reasonably well. This was done for instance in the case of thermal neutron-induced fission on Pu-239 in *[Talou:2011]*. In that case, the fission fragment mass distribution $Y(A)$ was obtained from a least-square fit of several experimental data sets, as shown in Fig. *MassYields*.

Incident Neutron Energies up to 20 MeV

At higher incident neutron energies, experimental data become scarce or non-existent, and one has to rely on theoretical models to construct the fragment yields. In the version 1.0.6 of the code, we have implemented a simplified energy dependence for the mass yields. It consists in using a three Gaussian model, whose parameters have been adjusted to reproduce experimental data, when available. For a particular incident neutron energy E_n, the yield for the fragment mass A is given by:

$$Y(A; E_n) = G_0(A) + G_1(A) + G_2(A),$$

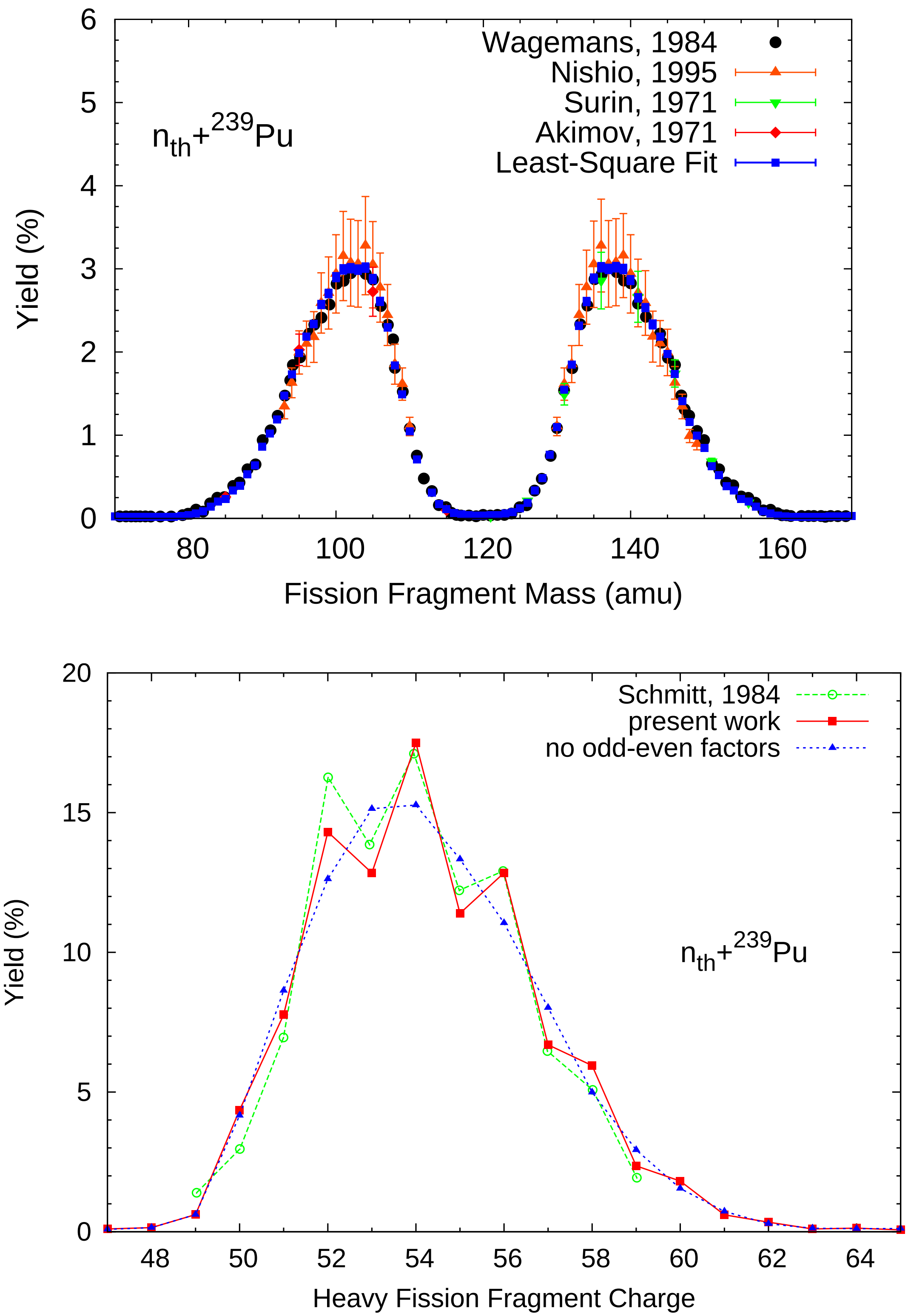


Fig. 3.1: Primary fission fragment mass (top) and charge (bottom) yields for thermal neutron-induced fission of Pu-239. Experimental data on the mass yields were used in a least-square fit to produce the black line. The charge distribution was reconstructed following the Wahl systematics for each fragment mass, as explained below.

where G_0 corresponds to a symmetric mode,

$$G_0(A) = \frac{W_0}{\sigma_0\sqrt{2\pi}}\exp\left(-\frac{(A-\overline{A})^2}{2\sigma_0^2}\right),$$

and G_1 and G_2 to two asymmetric modes

$$G_{1,2}(A) = \frac{W_{1,2}}{\sigma_{1,2}\sqrt{2\pi}}\left[\exp\left(-\frac{(A-\overline{A}-D_{1,2})^2}{2\sigma_{1,2}^2}\right)+\exp\left(-\frac{(A-\overline{A}+D_{1,2})^2}{2\sigma_{1,2}^2}\right)\right].$$

Here, $\overline{A} = A_f/2$ with A_f the mass of the fissioning system, which can differ from the original compound nucleus if pre-fission neutrons are emitted. The parameters D_i are governed by spherical and deformed shell closures. Their values decrease by 1/2 for each pre-fission neutron emitted. The energy-dependence for the width parameters is given by:

$$\sigma_i = \sigma_i^{(0)} + \sigma_i^{(1)}E_n + \sigma_i^{(2)}E_n^2$$

for $i = 1, 2$. The width of the symmetric mode σ_0 is assumed to be energy independent.

The weights W_i of the Gaussians depend slowly on the incident energy, with an increasing symmetric component. For $W_{1,2}$, we adopt the following energy dependence:

$$W_i = \frac{W_i^0}{1+\exp[(E_n-E_1)/E_2]},$$

with two adjustable parameters $E_{1,2}$. The weight W_0 for the symmetric mode is obtained through the normalization condition

$$W_0 + W_1 + W_2 = 2.$$

If neutrons are emitted prior to fission, the fissioning nucleus is formed with a residual excitation energy smaller than the initial excitation energy. In this case, an "equivalent" incident neutron energy is defined as the neutron energy that would produce the $(A_0 - \nu_{pre})$ fissioning nucleus, with ν_{pre} pre-fission neutrons, at the same residual excitation energy. Hence, E_n becomes

$$E_n = E^* - S_{n|A_0-\nu_{pre}}.$$

The same equivalent incident energy is used in the Wahl parameterization for the charge distribution.

In the current version of the code, we impose that E^* be greater or equal than the fission barrier height in the $(A_0-\nu_{pre})$ nucleus, and therefore neglect any subbarrier fission events.

Note: Initial parameterizations for the three-Gaussian model were taken from the **FREYA** code. Newer parameterizations based on better fits to known experimental data are being investigated.

3.1.2 Charge Yields

Wahl systematics *[Wahl:2002]* are then used to obtain the charge distribution for a given mass following:

$$P(Z|A) = \frac{1}{2}F(A)N(A)\left[erf(V) - erf(W)\right], \tag{3.1}$$

where

$$V = \frac{Z-Z_p+0.5}{\sigma_z\sqrt(2)} \text{ and } W = \frac{Z-Z_p-0.5}{\sigma_z\sqrt(2)}$$

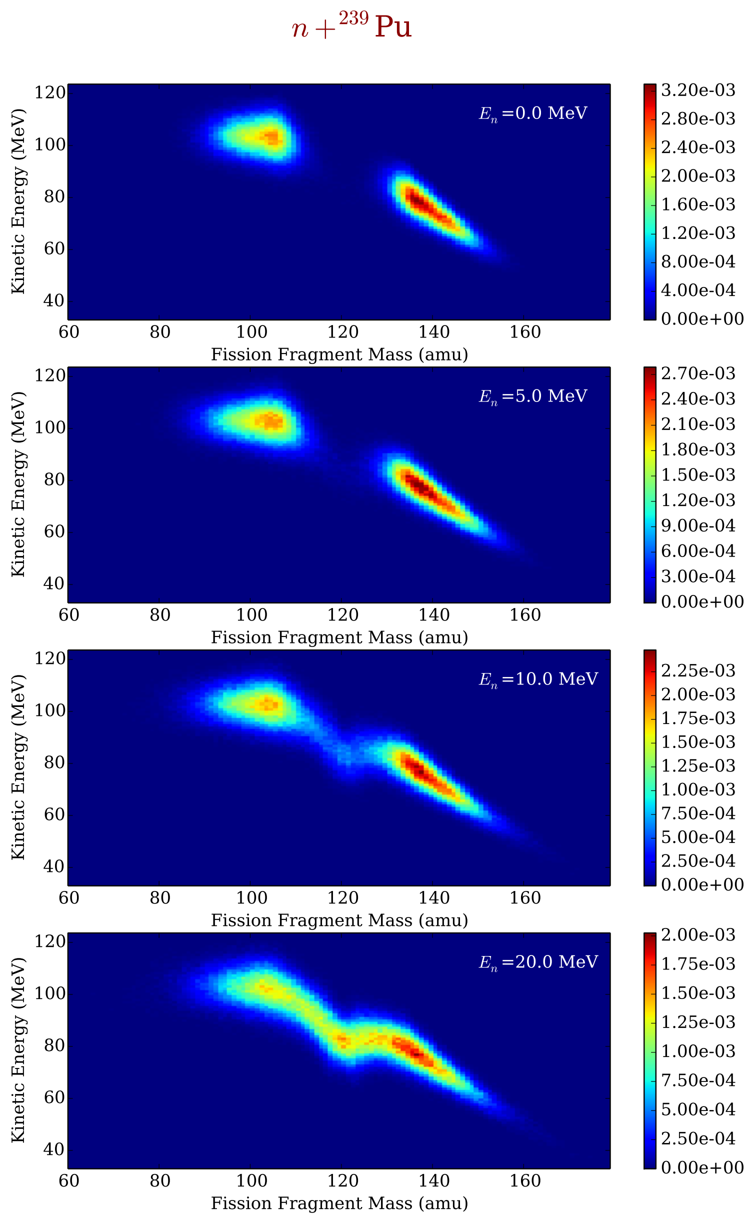


Fig. 3.2: Fission fragment yields as a function of mass and kinetic energy, for several incident neutron energies in the neutron-induced fission reaction on Pu-239. Multi-chance fission and pre-equilibrium contributions are taken into account as the incident neutron energy increases.

and $erf(x)$ represents the error function. The factor $N(A)$ is simply a normalization factor. The most probable charge is given by

$$Z_p = A_h \frac{Z_c}{A_c} + \Delta Z, \tag{3.2}$$

where Z_c, A_c are the charge and mass of the fissioning compound nucleus, σ_z is the charge width parameter and ΔZ is the charge deviation. The odd-even factor $F(A)$ is computed as

$$\begin{aligned}
F(A) &= F_Z \times F_N && \text{for } Z \text{ even and } N \text{ even} \\
F(A) &= F_Z / F_N && \text{for } Z \text{ even and } N \text{ odd} \\
F(A) &= F_N / F_Z && \text{for } Z \text{ odd and } N \text{ even} \\
F(A) &= 1/(F_Z \times F_N) && \text{for } Z \text{ odd and } N \text{ odd}
\end{aligned}$$

The average charge distribution is obtained by convoluting $Y(Z|A)$ over the fragment mass distribution $Y(A)$, and the result is shown in figure *fig-YZ-Einc* for the heavy fission fragments only.

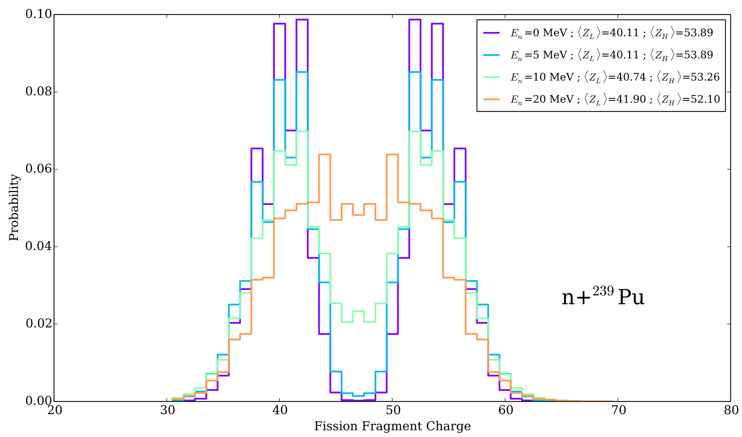


Fig. 3.3: Fission fragment charge distribution as a function of incident neutron energy for the Pu-239 (n,f) reaction.

3.1.3 Total Kinetic Energy (TKE) Distributions

The average total kinetic energy $\overline{TKE}$ is an important quantity that determines in great part the total excitation energy available in the system for the evaporation of neutrons and photons. Since most neutrons are emitted prior to photon emission, the average total prompt neutron multiplicity, $\overline{\nu}$, strongly depends on an accurate value for $\overline{TKE}$. For the simulation of single fission events, TKE distributions have to be known for all fragments.

For thermal neutron-induced fission reactions on important isotopes as well as spontaneous fission, some reliable and rather consistent experimental data exist, albeit less so in the symmetric region where fission events are rare.

To reconstruct the total kinetic energy dependence of the fission fragment yields, one can use experimental information on the average TKE as a function of the fragment mass A as well as its width $\sigma_{TKE}(A)$. Continuing on the example above for thermal neutron-induced fission of Pu-239, we have performed a least-square fit of $\overline{TKE}(A)$ as seen in Fig. *fig-TKEA*.

The TKE distribution for each fragment mass is then reconstructed using

$$P(TKE|A) = \left(2\pi\sigma^2_{TKE}(A)\right)^{-1/2} \times \exp\left[-\frac{\left[TKE - \overline{TKE}(A)\right]^2}{2\sigma^2_{TKE}(A)}\right].$$

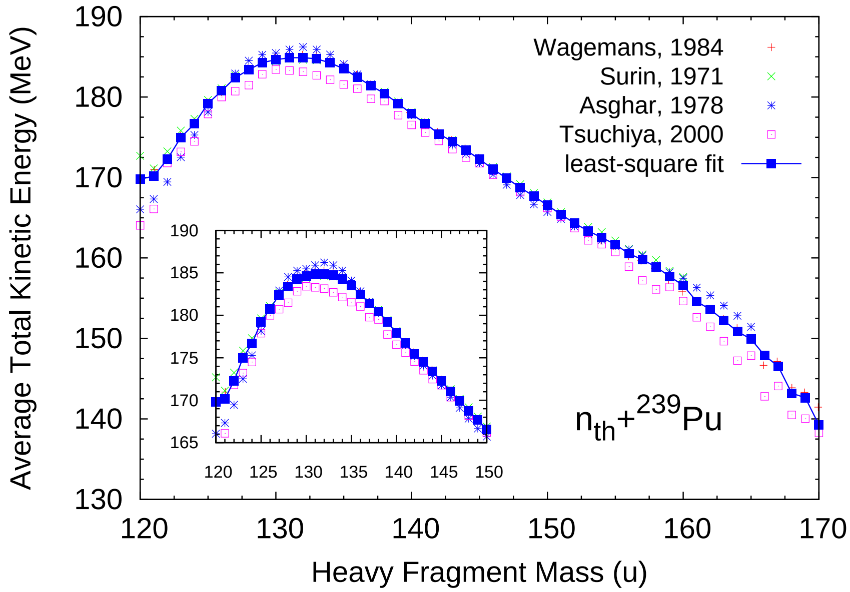
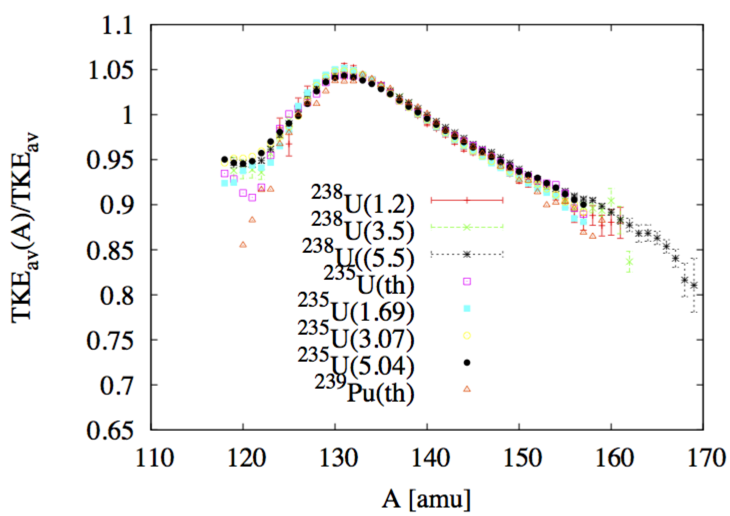


Fig. 3.4: Average total kinetic energy as a function of the heavy fragment mass in the case of the thermal neutron-induced fission of Pu-239.

In a first approximation, one can assume that the shape of $\overline{TKE}(A)$ as well as $\sigma_{TKE}(A)$ are independent of the particular fissioning system and the energy of the incident neutron (see Fig. *fig-TKEA-Isotopes*). We therefore assume that only the absolute scaling of $\overline{TKE}$ changes with energy.



Note: The mass-dependent average total kinetic energy does change with incident energy, reflecting changes in the shell corrections as the excitation energy is increased. A more refined treatment of this quantity will be tackled in the future.

The energy-dependence of $\overline{TKE}$ is poorly known for most systems. However, recent experimental data have shed some light on this issue. In the current version of the code, we assume that for each pair of fission fragments, TKE can be represented by a normal distribution $\mathcal{N}_{(\langle TKE \rangle, \sigma_{TKE})}(A, E_n)$, and assume that the energy dependence is entirely encoded in the average value $\overline{TKE}$.

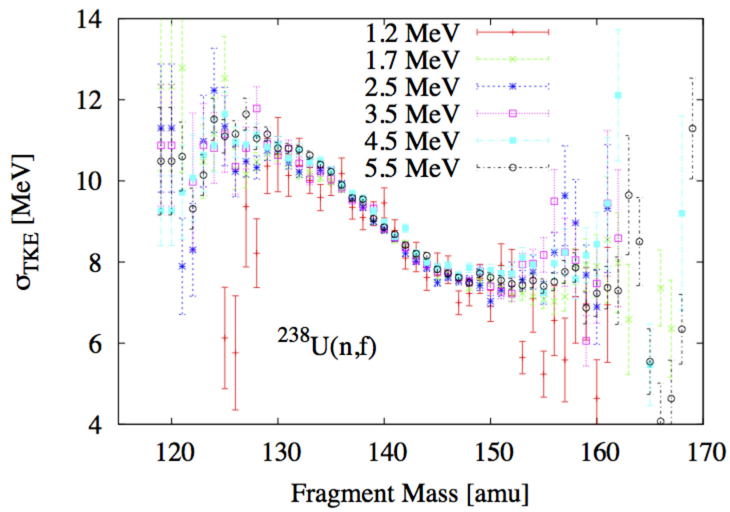


Fig. 3.5: Experimental data available for the mass and incident energy dependence of $\overline{TKE}$ and σ_{TKE} are shown for several fissioning systems and incident neutron energies.

In the current code implementation, the mass and energy-dependent distributions $TKE(A, E_n)$ are obtained as

$$\overline{TKE}(A, E_n) = \overline{TKE}(A, E_{th}) \times \frac{\overline{TKE}(E_n)}{\sum_A Y(A, E_n)\overline{TKE}(A, E_{th})}$$

The energy dependence of $\overline{TKE}(A)$ is given by the Madland systematics *[Madland:2006]*, which are simple linear or quadratic fits to experimental data for selected isotopes. Making the distinction between the total fission fragment (pre-neutron) kinetic energy, TKE_{pre}, and the total fission product (post-neutron) kinetic energy, TKE_{post}, those systematics read:

For **n+U-235**,

$$\begin{aligned} TKE_{pre} &= (170.93 \pm 0.07) - (0.1544 \pm 0.02)E_n \text{ (MeV)}, \\ TKE_{post} &= (169.13 \pm 0.07) - (0.2660 \pm 0.02)E_n \text{ (MeV)}. \end{aligned} \tag{3.3}$$

For **n+U-238**,

$$\begin{aligned} TKE_{pre} &= (171.70 \pm 0.05) - (0.2396 \pm 0.01)E_n + (0.003434 \pm 0.0004)E_n^2 \text{ (MeV)}, \\ TKE_{post} &= (169.8 \pm 0.05) - (0.3230 \pm 0.01)E_n + (0.004206 \pm 0.0004)E_n^2 \text{ (MeV)}. \end{aligned} \tag{3.4}$$

And for **n+Pu-239**,

$$\begin{aligned} TKE_{pre} &= (177.80 \pm 0.03) - (0.3489 \pm 0.02)E_n \text{ (MeV)}, \\ TKE_{post} &= (175.55 \pm 0.03) - (0.4566 \pm 0.02)E_n \text{ (MeV)}. \end{aligned} \tag{3.5}$$

Madland's fits were only constructed up to the threshold for second-chance fission. We assume however that they are valid at higher energies as well for the initial fissioning nucleus. Above the second-chance fission threshold, the average TKE does not necessarily follow a linear or quadratic behaviour though, as successive neutron emissions modify the fissioning nucleus and its excitation energy. We further assume that Madland's energy-dependence parameterizations remain valid for the nuclei A-1, A-2, etc. Only the reference thermal value of $\overline{TKE}(E_{th})$ is changed according to Viola's systematics *[Viola:1985]*

$$\overline{TKE}_{th} = (0.1189 \pm 0.011)\frac{Z^2}{A^{1/3}} + (7.3 \pm 1.5) \text{ MeV}. \tag{3.6}$$

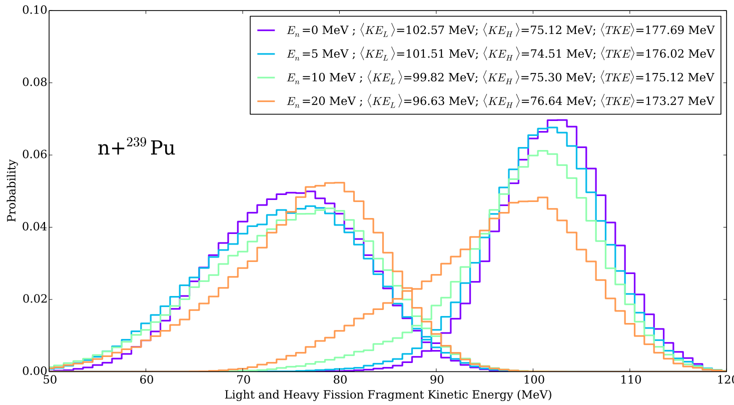


Fig. 3.6: Fission fragment kinetic energy distribution as a function of incident neutron energy for the Pu-239 (n,f) reaction.

3.1.4 Complete $Y(A, Z, TKE)$ Yields Reconstruction

Finally, the full pre-neutron emission fission fragment distributions can be reconstructed as:

$$Y(A, Z, TKE) = Y(A) \times P(Z|A) \times P(TKE|A) \tag{3.7}$$

The resulting $Y(A, TKE)$ distribution is shown here:

The approach described above to evaluate the pre-neutron emission fission fragment yields is not unique, and depends on the type of experimental data that have been measured. In some cases, the two-dimensional $Y(A, TKE)$ distribution has been measured *[Hambsch:2007] [Romano:2010]*, and therefore only the charge distribution for every fragmentation has to be computed to obtain the full distribution. In the majority of cases, however, no such information is available and one has to rely on systematics and/or phenomenological models. The present version of **CGMF** is limited to the few isotopes and reactions that have been well measured. The extension to other isotopes and reactions is planned for the near future.

3.2 Pre-Fission Neutrons

If the initial excitation energy in the compound nucleus is high enough, there is a chance that neutrons are evaporated prior to fission. We then talk about first-chance (n, f), second-chance $(n, n'f)$, third-chance $(n, 2nf)$, etc., fissions. The probabilities for each multi-chance fission event to occur can be computed from the Γ_n/Γ_f ratio as a function of the incident neutron energy. This ratio depends in turn on the fission barrier heights in the various compound nuclei $A, A-1, A-2$, etc. The **CoH-3.0.4** code was used to calculate those ratios for different actinides. As an example, we show here the case of n+Pu-239, in comparison with ENDF/B-VII.1 and JENDL-4.0 evaluations. The **CoH** calculations tend to predict a much higher second-chance fission probability at the expense of the first-chance, compared to the evaluations. These quantities are not observables though, and it is therefore difficult to judge about the validity of those curves at this point.

In **CGMF**, those multi-chance fission probabilities are sampled to determine the number of pre-fission neutrons. Then, the energies of those neutrons are obtained by sampling the corresponding neutron spectra. In the case of the first emitted neutron, the spectrum corresponds to a weighted sum of a pre-equilibrium and an evaporation components. The fraction of pre-equilibrium neutrons is also calculated in the **CoH** code using the exciton model. Then, the first neutron-out spectrum is given by:

$$\chi_1 = f_{pe}\chi_{pe} + (1 - f_{pe})\chi_{evap}.$$

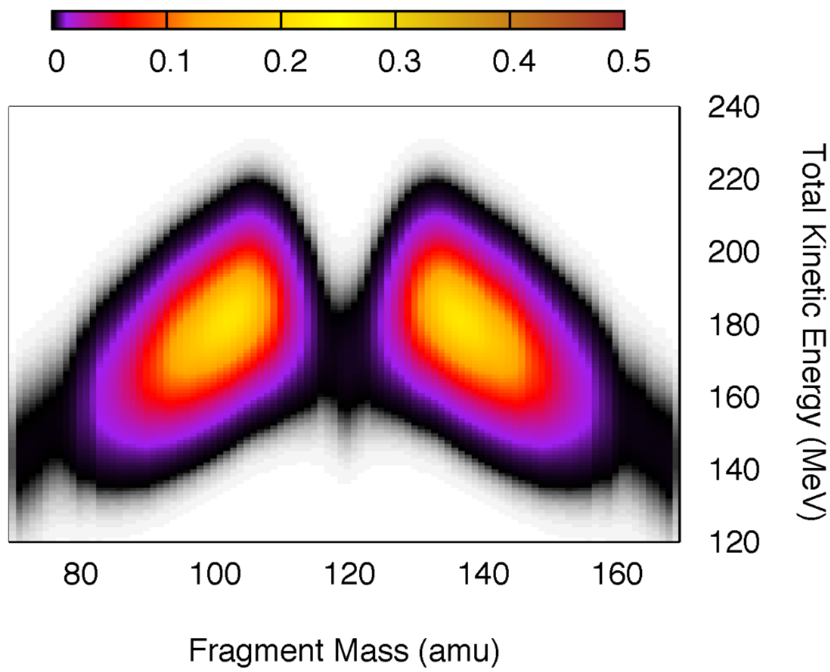


Fig. 3.7: Mass and Total Kinetic Energy yields reconstructed using Eq. (3.7) in the thermal neutron-induced fission of Pu-239.

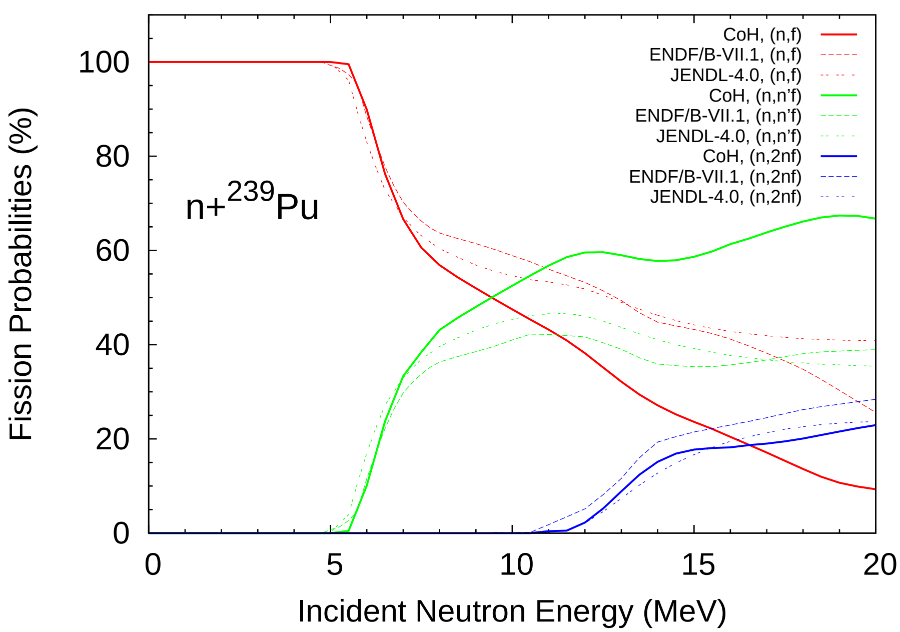


Fig. 3.8: Multi-chance fission probabilities in the neutron-induced fission reaction on Pu-239 as calculated with the **CoH** code (and used in **CGMF**), and in comparison with the ENDF/B-VII.1 and JENDL-4.0 evaluations.

The energy-dependent fraction f_{pe} can be fitted by a simple function:

$$f_{pe}(E_{inc}) = \frac{1}{1+\exp\left[(12.49-E_{inc})/10.21\right]} - 0.042E_{inc} - 0.25.$$

As can be seen in Fig. *fig-PE*, it is a very reasonable approximation for neutron-induced reactions on U-235, U-238 and Pu-239.

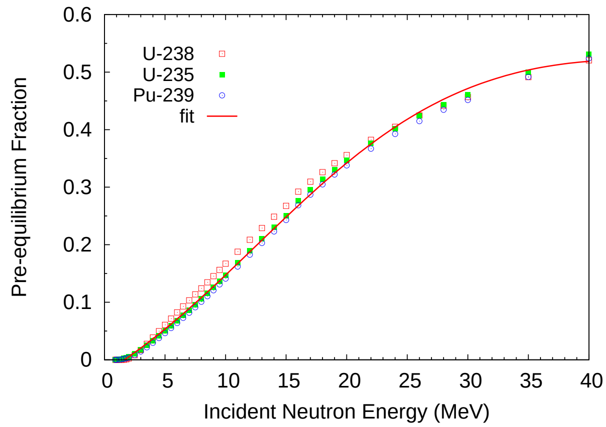


Fig. 3.9: Pre-equilibrium fractions calculated with the **CoH** code. There is only a slight dependence on the target nucleus, and the fit formula (solid line) is used by default in **CGMF** instead.

3.3 Excitation Energy, Spin and Parity Distributions

The total excitation energy (TXE) available to the two fragments is constrained by the energy conservation rule

$$\begin{aligned} TXE &= Q_f - TKE, \\ &= E_{inc} + B_n + M_n(A_f,Z_f)c^2 - M_n(A_1,Z_1)c^2 - M_n(A_2,Z_2)c^2 - TKE \end{aligned} \tag{3.8}$$

where TKE is the total kinetic energy, i.e. the sum of the kinetic energies of fragment 1 and fragment 2, and M_n are the nuclear masses for the fissioning nucleus, and the fragments 1 and 2 respectively. Once TKE is known, the total excitation energy TXE is also known. However, the partitioning of this energy between the two fragments is a more complicated matter, which is discussed at more length in the section below.

3.3.1 Excitation Energy Partitioning

As mentioned above, the total excitation energy (TXE) is known as long as the total kinetic energy (TKE) and nuclear masses are known. What is not completely known however is the way TXE is distributed among the light and the heavy fragments.

Several interesting and competing ideas have been proposed to explain how TXE is shared among the two fragments *[Schmidt:2010] [Talou:2011]*, but no fully compelling proof has been given so far supporting those theories. They all rely on some assumptions regarding the configurations of the fission fragments near the scission point. In the present version of **CGMF**, this excitation energy partitioning is treated as a free parameter, which can be tuned to be best reproduce the average prompt fission neutron multiplicity as a function of the fragment mass, $\overline{\nu}_p(A)$. Indeed, to the first order, the neutron multiplicity reflects the excitation energy of the fragment, while the average neutron energy reflects the temperature of the fragment.

We introduce the ratio of the temperatures between the light and heavy fragments:

$$R_T = \frac{T_l}{T_h}, \tag{3.9}$$

and use the Fermi gas formula to infer the sharing of the excitation energy. This ratio parameter depends on the fragment pair masses A_l and A_h. At this stage, it is only a convenient way to parameterize the partitioning of TXE, and nothing more. Note that this parameter can also be confusing as it uses a ratio of temperatures, while its correct purpose is to share excitation energies. It was introduced at first in the context of the Los Alamos model (LAM) *[Madland:1982]* to compute the average prompt fission neutron spectrum. In its original formulation, the LAM uses a distribution of temperatures to represent the intrinsic excitations in the fragments, and uses the same distribution for both the light and the heavy fragments. In other words, $R_T = 1.0$.

In **CGMF**, R_T can be chosen to be mass-dependent to best reproduce $\overline{\nu}_p(A)$. In most cases, it means that $R_T > 1.0$ as more excitation energy is pumped into the light fragment at the expense of the heavy fragment. This result is in large part due to the deformation energies of the nascent fragments, the heavy fragment being closer to a sphere thanks to shell closures, while the light fragment is largely deformed. This is not true everywhere however, and for very asymmetric fragmentations the inverse becomes true.

We are working on a more physically and mathematically sound proof of this empirical result, in particular in order to expand **CGMF** calculations to other isotopes and energies more reliably.

Figure *fig-Ui* shows an example of a distribution of initial excitation energies in the light and heavy fragments, as well as the total energy, in the case of Cf-252 spontaneous fission.

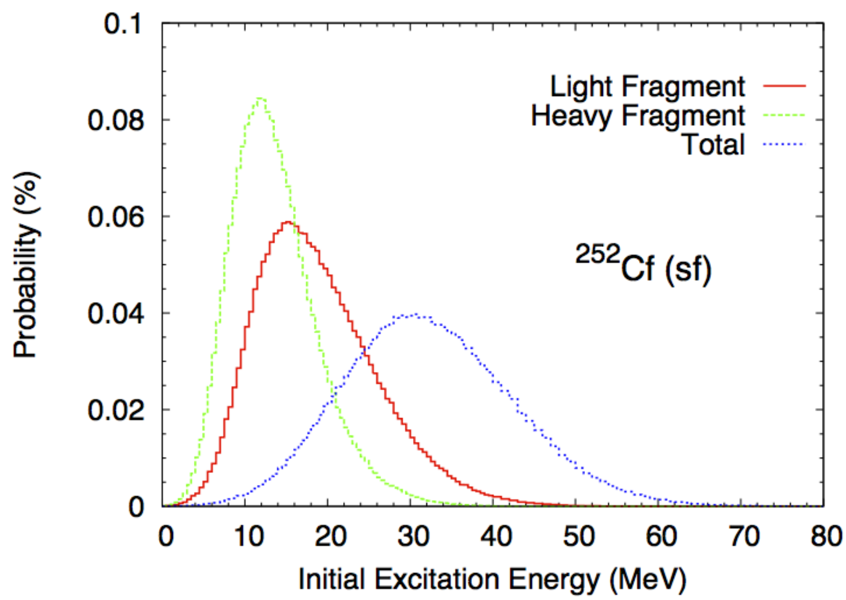


Fig. 3.10: Typical initial excitation energy distributions in the light and heavy fragments, as well as the total, computed in the case of Cf-252 spontaneous fission.

3.3.2 Spin and Parity Distributions

The spin of the fragments also follows a conservation rule

$$\vec{J_1} + \vec{J_2} + \vec{l} = \vec{J_f} \tag{3.10}$$

where $\vec{J}_1$ and $\vec{J}_2$ are the fission fragment total spins, $\vec{J}$ is the total angular momentum of the fissioning nucleus, and $\vec{l}$ is the relative orbital angular momentum between the two fragments. In the present version of **CGMF**, $\vec{J}_1$ and $\vec{J}_2$ follow a Gaussian distribution around a mean value that is chosen to best reproduce some of the observed prompt photon characteristics. The relative orbital angular momentum l is left free, so there is no correlation between $\vec{J}_1$ and $\vec{J}_2$ at this point. This question will be revisited in future versions of the code. Also, negative and positive parities are chosen to be equally probable, so the spin and parity distribution in the fragments reads

$$\rho(J,\pi) = \frac{1}{2}(2J+1)\exp\left[-\frac{J(J+1)}{2B^2(Z,A,T)}\right] \tag{3.11}$$

where B is defined in terms of the fragment temperature as

$$B^2(Z,A,T) = \alpha\frac{\mathcal{I}_0(A,Z)T}{\hbar^2},$$

and $\mathcal{I}_0(A,Z)$ is the ground-state moment of inertia of the fragment (A,Z). α is an adjustable parameter that is used globally to reproduce prompt fission γ data.

Typical values calculated for the light and heavy fragments are 6-8 $\hbar$, in rather good agreement with values cited in the literature (see *[Wilhelmy:1972]* for instance).

3.4 Statistical Hauser-Feshbach Theory

The Hauser-Feshbach theory *[Hauser-Feshbach:1952]* describes the decay of a compound nucleus in statistical equilibrium through the evaporation of particles and photons until a ground-state or long-lived isomer is reached. This is schematically represented in Fig. 2.6.

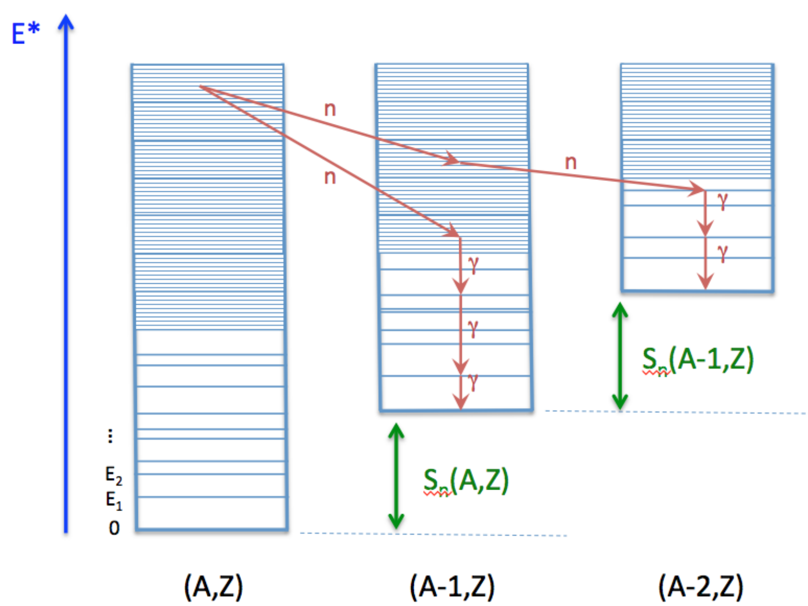


Fig. 3.11: Schematic drawing explaining the representation of a nucleus in the **CGMF** code, and individual decay paths followed through Monte Carlo simulations.

In this schema, a fragment (A,Z) is represented by its ground-state at energy zero, a set of low-lying discrete excited states, and by a set of energy-bins at higher excitation energy where the density of levels becomes too high for individual levels to be separated experimentally. In practice, this picture is not a clear-cut between resolved and unresolved levels. Some levels may have been identified above the continuum threshold region, but it may also be known, from a statistical analysis of the observed levels, that a significant portion of levels has not been observed or that a large fraction of observed levels could not be assigned a specific spin or/and parity. In this case, the matching energy between the discrete and continuum regions is often lowered to well-known levels.

Fission fragments are neutron-rich, and often relatively far from the valley of $beta$-stability where most experiments have been performed. The known spectroscopy of neutron-rich nuclei is very poor compared to stable nuclei, which means that often very few discrete levels are known. In this case, the matching of the discrete region to the continuum is complicated and very sensitive to the number of specific levels included in the analysis. One also has to rely on systematics of level density parameters to describe the continuum region. Those systematics have been established for stable nuclei and large uncertainties can be expected in the description of nuclei far from stability.

In Fig. 2.6, a couple of decay paths, starting from the same initial excitation energy-bin, are drawn (red arrows) to illustrate the emission of neutrons and photons. In a traditional deterministic Hauser-Feshbach reaction code, the daughter nuclei are all populated at the same time. In a Monte Carlo code such as **CGMF**, only one path is chosen at a given step.

The Hauser-Feshbach theory is statistical in nature and the decay paths are governed by the probabilities for the system to evolve in a particular reaction channel that is open, i.e. physically possible given constraints in energy, spin and parity. We will denote a channel c by:

$$c \equiv (A_i, Z_i, U_i, J_i, \pi_i; A_f, Z_f, U_f, J_f, \pi_f)$$

In the case of neutron or photon emissions only, we always have $Z_i = Z_f$, and $A_i = A_f$ (photon) or $A_f = A_i - 1$ (neutron).

The probability of decaying through a particular channel c is given by the product of the channel transmission coefficients and the density of levels in the final state. For photons, we have:

$$P(\epsilon_\gamma)dE \propto T_\gamma(\epsilon_\gamma)\rho(Z, A, E-\epsilon_\gamma)dE,$$

and for neutrons

$$P(\epsilon_n)dE \propto T_n(\epsilon_n)\rho(Z, A-1, E-\epsilon_n-S_n)dE,$$

where ϵ_γ and ϵ_n are the center-of-mass energies of the emitted photon and neutron, respectively.

3.5 Neutron Transmission Coefficients

Neutron transmission coefficients $T_n^{lj}(\epsilon)$ are obtained through optical model calculations. In this model, the Schroedinger equation describing the interaction of incoming waves with a complex mean-field potential is solved, providing the total, shape elastic and reaction cross-sections. It also provides the transmission coefficients that are used in the compound nucleus evaporation calculations.

The transmission coefficients for a channel c are obtained from the scattering matrix S as

$$T_c = 1 - |\langle S_{cc} \rangle|^2 . \tag{3.12}$$

To calculate the neutron transmission coefficients for fission fragments, it is important to rely on a global optical model potential (OMP) that can provide results for all nuclei. By default, **CGMF** uses the global spherical OMP of Koning and Delaroche *[KD03]*.

It is important to note that the calculated spectrum of prompt neutrons does depend on the choice of the optical potential used to compute the neutron transmission coefficients. The OMP of Koning-Delaroche has been established to describe a host of experimental data, e.g., total cross-sections, S_0 and S_1 strength functions, etc. However, those data are only available for nuclei near the valley of stability. Some experimental information do indicate that this optical potential may not be very suitable to the fission fragment region, and therefore a relatively large source of uncertainty in the calculation of the neutron spectrum results from this open question.

3.6 Gamma-Ray Transmission Coefficients

The gamma-ray transmission coefficients are obtained using the strength function formalism from the expression:

$$T^{Xl}(\epsilon_\gamma) = 2\pi f_{Xl}(\epsilon_\gamma)\epsilon_\gamma^{2l+1}, \tag{3.13}$$

where ϵ_γ is the energy of the emitted gamma ray, Xl is the multipolarity of the gamma ray, and $f_{Xl}(\epsilon_\gamma)$ is the energy-dependent gamma-ray strength function.

For $E1$ transitions, the Kopecky-Uhl *[Kopecky:1990]* generalized Lorentzian form for the strength function is used:

$$f_{E1}(\epsilon_\gamma, T) = K_{E1}\left[\frac{\epsilon_\gamma \Gamma_{E1}(\epsilon_\gamma)}{\left(\epsilon_\gamma^2 - E_{E1}^2\right)^2 + \epsilon_\gamma^2 \Gamma_{E1}(\epsilon_\gamma)^2} + \frac{0.7\Gamma_{E1} 4\pi^2 T^2}{E_{E1}^5}\right]\sigma_{E1}\Gamma_{E1} \tag{3.14}$$

where σ_{E1}, Γ_{E1}, and E_{E1} are the standard giant dipole resonance (GDR) parameters. $\Gamma_{E1}(\epsilon_\gamma)$ is an energy-dependent damping width given by

$$\Gamma_{E1}(\epsilon_\gamma) = \Gamma\frac{\epsilon_\gamma^2 + 4\pi^2 T^2}{E_{E1}^2},$$

and T is the nuclear temperature given by

$$T = \sqrt{\frac{E^* - \epsilon_\gamma}{a(S_n)}}.$$

The quantity S_n is the neutron separation energy, E^* is the excitation energy of the nucleus, and a is the level density parameter. The quantity K_{E1} is obtained from normalization to experimental data on $2\pi\langle\Gamma_{\gamma_0}\rangle/\langle D_0\rangle$.

For $E2$ and $M1$ transitions, the Brink-Axel *[Brink:1955] [Axel:1962]* standard Lorentzian is used instead:

$$f_{Xl}(\epsilon_\gamma) = K_{Xl}\frac{\sigma_{Xl}\epsilon_\gamma\Gamma_{Xl}^2}{(\epsilon_\gamma^2 - E_{Xl}^2)^2 + \epsilon_\gamma^2\Gamma_{Xl}^2}. \tag{3.15}$$

In the current version of **CGMF** (ver. 1.0.6), only $E1, E2$, and $M1$ transitions are allowed, and higher multipolarity transitions are neglected.

3.7 Level density in the continuum

In **CGMF**, the Gilbert-Cameron *[Gilbert-Cameron:1965]* model of level densities is used for all fragments. In this model, a constant temperature formula is used to represent the level density at lower excitation energies, while a Fermi gas formula is used at higher excitation energies. Experimental data on the average level spacing at the neutron separation energy can be used to constrain parameters entering the Fermi gas formula, while low-lying discrete levels are used to constrain the constant-temperature parameters. Again, little data is available for nuclei far from stability where systematics have been developed, contribution to uncertainties in the final predicted data.

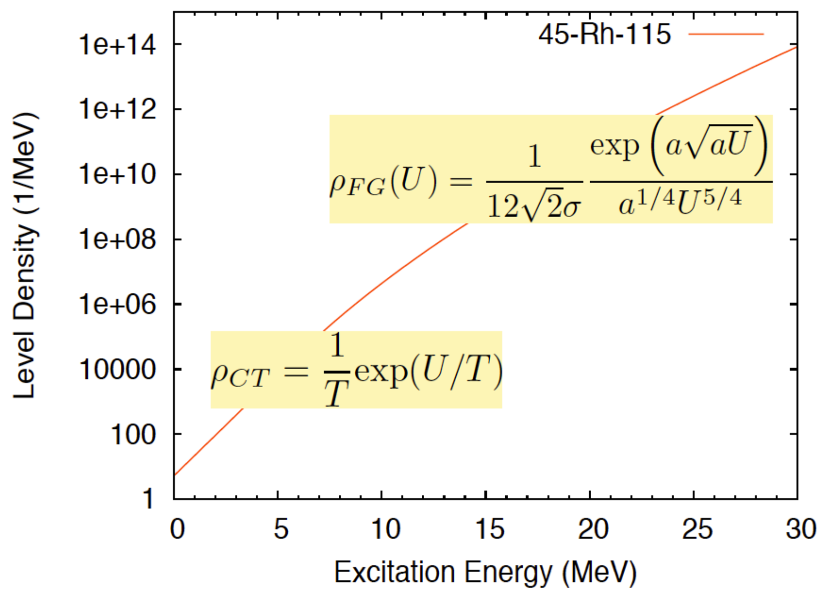
The constant temperature form is given by

$$\rho_{CT}(U) = \frac{1}{T}\exp\left(\frac{U + \Delta - E_0}{T}\right), \tag{3.16}$$

where T is the nuclear temperature and E_0 is a normalization factor. The quantity U is the excitation energy E minus the pairing energy Δ. At higher excitation energies, the Fermi gas form of the level density is used instead and is given by

$$\rho_{FG}(U) = \frac{\exp\left(2\sqrt{aU}\right)}{12\sqrt{2}\sigma(U)U(aU)^{1/4}}, \tag{3.17}$$

where a is the level density parameter. The constant temperature form of the level density is matched to cumulative low-lying discrete levels, when they are known. For fission fragments, which are neutron-rich and rather poorly known, this constant-temperature level density is sometimes used down to the ground-state, as shown in the following figure



In its original formulation, the Gilbert-Cameron formalism uses an energy-independent level density parameter a. To better describe the washing-out of shell effects at higher excitation energies, Ignatyuk *[Ignatyuk:1979]* developed a model that uses an energy functional for the level density parameter as

$$a(U) = \tilde{a}\left(1 + \delta W \frac{1 - \exp(-\gamma U)}{U}\right). \tag{3.18}$$

In this formula, $\tilde{a}$ is the asymptotic value of the level density parameter at high energy, δW is the shell correction energy, and γ is an empirical damping width to account for the washing-out of shell effects at high energy.

3.8 Isomeric States

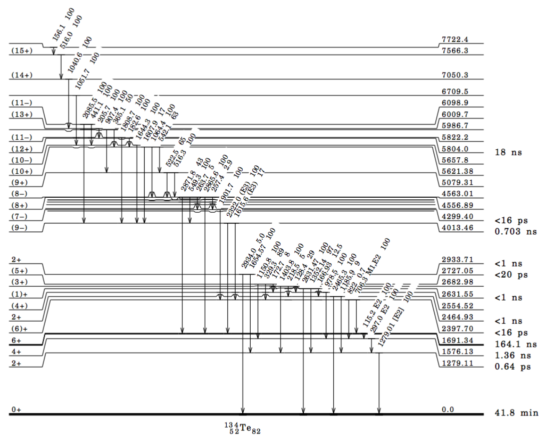
Many low-lying discrete levels that are reported in the ENSDF database have a measurable half-life, ranging from nanoseconds to seconds and even longer. **CGMF** takes this into account when calculating the gamma cascades in the fission products, and samples the exponential decay law according to the reported half-lives.

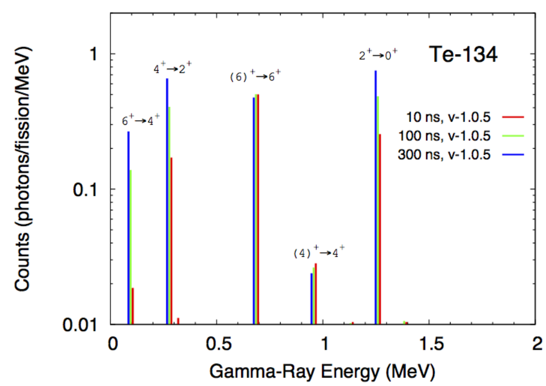
An experimental time coincidence window can be set in the `config.h` configuration file:

```
const double EXPERIMENTAL_TIME_WINDOW = 1e-8;
```

The time is given in seconds, so in the example above, 1e-8 corresponds to 10 ns. The default value is negative. In this case, all levels are set to decay to the ground-state, ignoring half-lives entirely. Since this value is stored in a configuration file, it is set at compilation time. If the user decides to change this value, he/she would need to recompile the code before using it.

As an example, the calculated intensities for specific gamma lines in Te-134, in the thermal neutron-induced fission of U-235, are shown in the figure below. Time-coincidence windows of 10, 100 and 300 ns were used in three separate calculations. Because of the presence of ~100 ns isomers in Te-134, some of these lines are more or less prominent depending on their half-lives. For example, the 6^+ state at 1.691 MeV has a half-life of 164 ns, decaying to the 4^+ state at 1.576 MeV. A too-short time gate (e.g., 10ns) cannot record this particular gamma line at 115 keV. Similarly, the decay of the 4^+ to 2^+ (297 keV) is also hindered since it depends on the decay of the higher excited 6^+ state.





CHAPTER

FOUR

CODE DETAILS

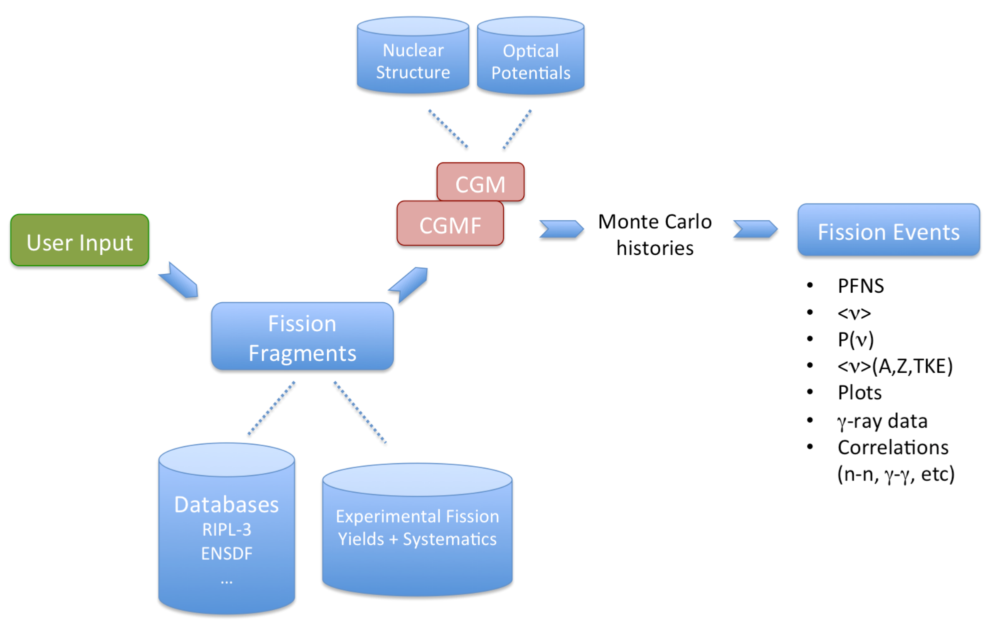
The **CGMF** code is written in C++. It is built around the **CGM** Monte Carlo statistical Hauser-Feshbach code, which provides the main computational methods for following the decay of the excited fission fragments. Two additional classes have been written out of the **FFD** code to prepare and sample the initial fission fragments, and to read out and analyze the Monte Carlo histories that are generated.

4.1 Code Organization & options

`cgmf.cpp` is the main driver of the code. It first reads in the user input parameters, and calls other routines from different classes to perform the requested calculations.

4.1.1 Algorithm

Here we describe the basic algorithm of `cgmf.cpp`.



First, the user input provided at the command line is parsed, and analyzed. The `ZAIDt` and `Einc` input parameters are mandatory. Note that some options available in **CGM** are now set fixed and hardwired for their use in **CGMF**.

Reading a history file

If the `-r` option is given, then the code reads a history file containing an ensemble of Monte Carlo histories previously generated by **CGMF**. In the case of large files, it is possible to add the `-n` option to provide a smaller number of events to be read and analyzed. In this case, the basic algorithm of the code is as follows:

```
fissionEvents = new FissionEvents (nevents);
fissionEvents->setZAIDcn (ZAIDt, Einc);
fissionEvents->readHistories (historyFile, nevents);
fissionEvents->analyzeResults ();
fissionEvents->computeFinalResults();
```

Note that all the methods used above only make use of the class `fissionEvents.cpp/.h`. A number of events (`nevents`) are read from the Monte Carlo history file using `readHistories()`, and they are analyzed in `analyzeResults()`. In this method, the characteristics of the fission fragments, the prompt neutrons and the prompt photons are stored in various histograms, e.g., `particles->Pnu[]`, `particles->nuTKE[]`, etc, where `particles` is a pointer to an `emittedParticleType`, which can be either neutrons or photons.

Finally, the method `computeFinalResults()` is used to transform histograms into average quantities, distributions and correlations among different physical quantities. For instance, the fission fragment yields are calculated and stored under `YA[]`, `YApost[]`, `YZ[]`, `YTKE[]`, `YUl[]`, etc. Prompt fission neutron and photon spectra are calculated from the original histograms and transformed onto the outgoing energy grid `SPECTRUM_ENERGY_GRID` defined in the `init()` method in `FissionEvents.cpp`.

Performing Monte Carlo Simulations

In the more general case where one wants to perform Monte Carlo simulations of the decay of the fission fragments, the algorithm is as follows:

First, a new instance of `FissionFragments` is created to initialize the fission reaction parameters and files:

```
ff = new FissionFragments ();
```

Next, instances of light and heavy fragments are created with the total number of Monte Carlo events `nevents` specified by the user:

```
lightFragments = new fissionFragmentType [nevents];
heavyFragments = new fissionFragmentType [nevents];
```

These objects are used to track all information pertinent to each of the fragments for each fission event.

Next, a set of `nevents` fission events are produced:

```
ff->generateInitialFissionFragmentHistories (lightFragments, heavyFragments, nevents);
```

This call produces all the initial characteristics (A, Z, KE, U, J, π) for each fission fragment in each fission event.

What follows is the main loop of the program, going over every fission event and performing the de-excitation of each fission fragment:

```
// -- BEGIN LOOP OVER FISSION EVENTS ----------------------------------------
for (int ievent=0; ievent<nevents; ievent++) {
  lf = lightFragments[ievent];
  hf = heavyFragments[ievent];
  fissionEvents->addFragments (lf, hf);
  specMCMain (lf.spin, lf.parity, 0.0, 0.0, 1, spc); // light fragment calc.
  specMCMain (hf.spin, hf.parity, 0.0, 0.0, 1, spc); // heavy fragment calc.
}
// -- END LOOP OVER FISSION EVENTS ------------------------------------------
```

`lf` and `hf` are pointers to the light and heavy fission fragment partners for the fission event `ievent`. The `addFragments(lf,hf)` method is used to record the characteristics of this particular fission event. Next is the main **CGM** computational method `specMCMain()`, which performs the Monte Carlo Hauser-Feshbach calculations of the decay of this particular excited nucleus. `specMCMain()` is called twice, once for each fragment. A description of this method is given below.

Past this main loop, the Monte Carlo histories are recorded in an output file:

```
fissionEvents->writeHistories ("histories.CGMF");
```

and the results analyzed with:

```
fissionEvents->analyzeResults ();
fissionEvents->computeFinalResults();
```

This last section of the code is identical to the one used after reading a Monte Carlo history file, as explained above.

4.1.2 User Options

The user options, given at the command line, are as follows:

- `-i ZAIDt` : ZAID (1000*Z+A) of the target nucleus, or fissioning nucleus in the case of spontaneous fission. [required]
- `-e Einc` : energy of the incident neutron (in MeV). For spontaneous fission, set to 0.0. [required]
- `-n nevents` : number of Monte Carlo events [default: 1,000,000]
- `-r historyFile` : to read and analyze a Monte Carlo history file already produced by **CGMF**
- `-h`: display the help page for **CGMF**

Note: other options are available, but won't be described in this release of the code and user manual.

If `nevents` is negative, then only the pre-neutron emission fission fragment yields $Y(A, Z, KE, U, J, \pi)$ are produced.

If the `-r` option is given, a **CGMF** output file is read and analyzed. This is especially useful when a large output file has been generated and needs to be re-analyzed differently. In this case, the number of events can also be read, and smaller samples of the entire file can be used instead.

4.1.3 Configuration File(s)

CGMF comes with two configuration files, one inherited from the **CGM** code and one required specifically for fission calculations. In this manual, we describe the settings that are relevant to the fission fragment decay calculations only.

config.h

The `config.h` file is inherited from **CGM**, but with some added options. Important variables are as follows:

```
#define  DATADIR   "/usr/local/share/cgmf"
```

defines the path to the data libraries used for the Hauser-Feshbach calculations and for the initial fission fragment yields. This directory contains the RIPL-3 library of discrete levels available for many nuclei, and level density parameter systematics that are needed for fragments with unknown nuclear structure. This path should be changed by the user to reflect his/her own local data structure.:

```
const double ENERGY_BIN = 0.05;  // 50 keV
```

This constant defines the width of the energy-bin (in MeV) used in the continuum representation of the nuclear levels. A smaller value would provide a finer energy grid for the gamma-ray transitions in the continuum. For instance, if this quantity is set to 50 keV, then the minimum energy for the gamma transitions in the continuum would be 50 keV as well. Reducing this value will provide a continuum photon spectrum for energies below 50 keV, but could dramatically increase the computation time. A larger value would significantly speed up the calculations, but would cut the lower-energy part of the photon spectrum.:

```
const double CONTINUUM_LOWER_CUT = 0.02;
```

A problem inherent to all Hauser-Feshbach-type codes is the matching between the continuum and the discrete level regions describing the structure of a nucleus. The continuum region is defined by an ensemble of energy bins and a level density distribution $\rho(U_{bin}, J, \pi)$ for each energy bin. On the other hand, at lower energies, the nucleus is assumed to be fully characterized by a set of discrete levels with specific energies, spins and parities. In the course of following the decay of an excited nucleus, one sometimes populates a certain continuum energy-bin at low excitation energy, but with a high spin. The decay to this continuum state to a lower discrete level with much lower spin is strongly hampered, and can lead to an artificial series of low-energy $E1$ transitions in the continuum until a more probable low-spin transfer transition becomes available. This result is not physical. To reduce the impact of this effect, we have introduced the quantity `CONTINUUM_LOWER_CUT` to eliminate any transition below this energy.

We do not encourage users to modify this quantity, unless they know exactly what they are doing. We are working on a better solution to this problem.

```
const bool INCLUDE_INTERNAL_CONVERSION = true;
```

This boolean is set to TRUE if one wants to include the internal conversion transitions into the decay of the fragments.

```
const bool RANDOM_SEED_BY_TIME = true;
```

This boolean can be set to FALSE if one wants to fix the initial seed of the pseudo-random number generator used for the Monte Carlo samplings. This is useful in testing the reproducibility of the results, but should be set to TRUE in actual calculations.

```
const double EXPERIMENTAL_TIME_WINDOW = 1.0e-8; // 10 ns
```

This value should correspond to the experimental time coincidence window used to define the prompt fission data recorded in coincidence with a fission event. In the example above, this value is set to 10 ns. The probability of continuing a gamma cascade from an isomeric state will then depend on the value of the time window and the half-life of this isomeric state. By default, this constant is set to a negative value so that all cascades are followed until they reach the ground-state of a fission product.

config-ff.h

The `config-ff.h` is an additional configuration file, specific to fission fragment decay calculations.

```
#define MPIRUN
// #undef MPIRUN
```

CGMF can be run using MPI parallel instructions on a multi-processor machine. This can be done by commenting out the `#define MPIRUN` directive and recompiling the code. Using `#undef MPIRUN` instead would generate a non-MPI executable that is suitable to a one-processor machine.

What follows is a set of constants that define the sizes of arrays used throughout the code:

```
const int    NUMA   =  300; // number of masses A
const int    NUMZ   =  100; // number of charges Z
const int    NUMTKE =  300; // number of Total Kinetic Energy values

const int      NUME =  401; // number of energies in level density tables;
                            // dE=0.25 MeV; up to Emax=100 MeV
const double deltaE = 0.25; // energy-bin size used in level density tables

const int    NUMdZ  =   21; // [-dZ:+dZ] if dZ=10 for charge distribution
                            // around most probable Zp[A]
```

```
const int   NUMMULT =   50; // number of multiplicities

const int NUMANGLES =   73; // number of angles in angular distribution
const double dTheta =  2.5; // angular bins (degrees)

const int MAX_NUMBER_PARTICLES = 50; // max. number of particles (n or g)
                                     // emitted per fragment in a fission event

const int NUMBER_SPECTRUM_ENERGY_GRID = 641; //551;
```

Note that **none of those settings should be changed**, except by an informed user.

4.2 Important Classes & Methods

Note: This section needs to be updated to include the incident neutron energy dependence up to 20 MeV.

4.2.1 Class `FissionFragments.cpp`

This class provides all the methods and variables needed to produce the initial fission fragment yields, prior to neutron emission, characterized by a mass A, a charge Z, a kinetic energy KE, an excitation energy U, a spin J, and a parity π. The constructor is declared as:

```
FissionFragments::FissionFragments (int ZAID, float Einc, double alphaSpin);
```

In input, the user has to provide:

- the `ZAID` of the fissioning nucleus, i.e., $1000 \times Z + A$ that uniquely identifies a nucleus,
- the energy of the incident neutron, `Einc`, which should be given in MeV. In the case of spontaneous fission, 0.0 should be given.
- `alphaSpin`, which is a multiplying factor entering in the initial spin distribution of the fission fragments. Default is 1.0, which means that the original level density spin distribution for the fragments is used.

The constructor then calls the methods `setOptions()` and `init()`. The first method sets options that completely characterize the fission fragment yields $Y(A, Z, TKE)$ from partial experimental data and some systematics. It also defines the type of energy sorting mechanism allowed by the code.

Note: Below the threshold for the 2nd-chance fission, only one set of fission fragment yields have to be constructed at a particular excitation energy. At higher energies, the situation is much more complicated, as the pre-fission neutron spectrum, which includes evaporation and pre-equilibrium components, has to be sampled, leading to a residual nucleus $(A_c - \nu, Z_c, E_{res})$ that can then fission. The yields are therefore constructed "on-the-fly" while generating fission events.

The `init()` method then creates the fission fragments as:

```
fragments = new Nucleus[2];
```

where `Nucleus` is a class that fully describes a nucleus. In particular, it constructs the nuclear structure defined by a set of known low-lying discrete levels, read from the RIPL-3 database, and produces a continuum of energy bins above a certain matching energy. It also reads in nuclear masses, ground-state deformations, and individual decay transitions that are present in the database.

4.2.2 Class FissionEvents.cpp

The class FissionEvents.cpp provides objects and methods to read and analyze the Monte Carlo histories produced by **CGMF**. The constructor:

```
FissionEvents::FissionEvents (int maxNumberEvents) { init(maxNumberEvents); }
```

simply calls an initialization method with the maximum number of events to read and analyze. The init() method initializes several objects and variables: it first instantiates the objects:

```
lightFragments = new fragmentEventType [maxNumberEvents];
heavyFragments = new fragmentEventType [maxNumberEvents];
```

with the size of maxNumberEvents.

A fragmentEventType is a structure that fully characterizes a fission fragment event:

```
struct fragmentEventType {
  int    A, Z;
  double KE;  // kinetic energy (MeV)
  double Ui;  // initial excitation energy (MeV)
  int    Pi;  // initial parity
  double Ji;  // initial spin
  emissionType emissions[3]; // neutrons [0], gammas [1] and internal conversion [2]
};
```

where the emissionType objects are themselves defined as:

```
struct emissionType {
  int multiplicity;
  double cmEnergies   [MAX_NUMBER_PARTICLES];
  double labEnergies  [MAX_NUMBER_PARTICLES];
  double cmAngles     [MAX_NUMBER_PARTICLES];
  double labAngles    [MAX_NUMBER_PARTICLES];
  int transitionTypes [MAX_NUMBER_PARTICLES];
};
```

and fully defines a particular emission in energy, angle in both the center-of-mass and laboratory frames, and type of emission, e.g., neutron, gamma or internal conversion.

The lightFragments and heavyFragments objects are then used to store all fission event data for the total number of events (maxNumberEvents).

The initialization subroutine also defines the outgoing energy grid used to report the particle energy spectra. It finally initializes several storage arrays.

The following method:

```
void FissionEvents::addFragments (fissionFragmentType lf, fissionFragmentType hf) {...};
```

is used to save all the data pertaining to the fission fragments (A, Z, KE, U, J, π) in a fission event, for both complementary fragments.

The decay of the fission fragments is handled by the routine specMCMain() (described below). Once all Monte Carlo samplings have been performed, the results are then saved into a history file by:

```
void FissionEvents::writeHistories (string outputFilename) {...};
```

This routine simply takes an filename in input, opens the file for writing, and writes all the Monte Carlo histories onto it. The resulting file can later be read and analyzed using the method:

```
void FissionEvents::readHistories (string inputFilename, int numberEvents) {...};
```

The next step is to analyze the results. This is done through:

```
void FissionEvents::analyzeResults (void) {...};
```

This routine loops over all fission events, and fills out many variables and arrays, such as `particles->lfEcm`, which records the center-of-mass energies of the emitted neutrons and photons coming from the light fragment, `particles->nuTKE[iTKE]`, which records the average particle multiplicity as a function of the total kinetic energy, `gammaMultiplicityNu[]`, which records the gamma-ray multiplicity versus neutron multiplicity correlations, etc.

Note that if **CGMF** is run with MPI parallel instructions, then `MPI_Reduce()` calls are made here.

Another routine:

```
void FissionEvents::computeFinalResults (emittedParticleType * particles) {...};
```

is used to finalize the results by transforming histograms into spectra, renormalizing yields, calculate different average quantities as a function of fragment properties, etc. Those two last routines may be merged in a future (cleaner) version of the code.

Finally, results can be saved in a format that is custom-readable by GNUPLOT scripts through:

```
void FissionEvents::saveResultsToGnuplot () {...};
```

4.2.3 Method `specMCMain()`

This method is at the core of **CGM/F** calculations. It performs Monte Carlo samplings of emission probabilities for all open channels following the Hauser-Feshbach *[Hauser-Feshbach:1952]* statistical formalism of nuclear reactions. For every initial configuration of a compound nucleus (A, Z) in excitation energy U, spin J and parity π, it prepares the nucleus by reading its known low-lying structure from the RIPL-3 database, prepares its continuum energy-bins, and compute the neutron and photon transmission coefficients. It does this for a certain number of nuclei that can be produced in multiple neutron emissions.

The method then samples the emission probability distributions, and choses one particular decay path. It records the Monte Carlo histories through `recordEmittedParticles()` for further reading and analysis by **CGMF**.

CHAPTER

FIVE

INSTALLATION

5.1 Obtaining the code

At this time, **CGMF** is under LANL Copyrights, and can only be obtained through direct communication with the authors (please send us an email at <talou@lanl.gov>). We are hoping that future releases of the code will be made available under an **open source** license.

5.2 Configuration files

CGMF package is available as a compressed archive file, `.tar.gz`. It contains all the source files, auxiliary data files, as well as this documentation. Once uncompressed and unarchived with the instruction `tar -czvf`, the director structure shows:

- `examples/`
- `src/`
- `data/`
- `doc/`
- `README`

All source files are under the `src/` directory. The `data/` directory contains all data files required by **CGMF**, such as level density parameterizations, nuclear structure data files, and initial fission fragment yields.

The `doc/` directory contains this user manual in both *HTML* and *PDF* formats.

Prior to executing **CGMF**, the user will need to follow these steps:

1. mv `src/`
2. Edit configuration file `config.h`, and modify `DATADIR` to specify the main data directory (installation-dependent) as well as `WORKDIR` to decide where output results should be written
3. Edit `Makefile` to specify C/C++ compilers (gcc/g++ by default)
4. Type: `make`

It will create the executable `CGMF.x`, which can be used on the command terminal with the user options as described in this manual.

5.3 Compilers

The compilation of **CGMF** has been successfully tested on several machines and compilers, including:

- GCC v.4.2.1, Mac OS X 10.8.4, MacBook Pro Intel Core 2 Duo
- GCC v.4.2.1, Mac OS X 10.7.5, MacPro Dual-Core Intel Xeon
- GCC v.4.1.2, Red Hat 4.1.2-52, Linux Cluster 4x32 nodes (MPI-parallelized version)

CHAPTER

SIX

USAGE

6.1 Command Line Options

The **CGMF** code is executed as:

```
./CGMF.x [-ie] [-nr]
```

where the arguments ('ie' options are **required**) are as follows:

```
-i ZAIDt
```

where `ZAIDt` is 1000*Z+A for the target nucleus in the case of neutron-induced fission, and for the fissioning nucleus in the case of spontaneous fission;

```
-e Einc
```

where `Einc` is the incident neutron energy in MeV (0.0 in the case of spontaneous fission).

The number of Monte Carlo fission events to be computed is specified by:

```
-n nevents
```

where `nevents` is the number of Monte Carlo fission events to run or to be read. If `nevents` is negative, it produces initial fission fragments yields Y(A,Z,KE,U,J,p). This argument is optional. Its default value is set to one million events.

The user can opt to read a Monte Carlo history file, previously produced by **CGMF**, by using:

```
-r historyFile
```

`historyFile` is the name of the file (absolute path) containing calculated Monte Carlo histories. It can be combined with the `-n` option to read only parts of the history file. If the number of events is not specified, a default of up to 1,000,000 events will be read. If the number of events saved in the history file is less than one million, then of course only that (smaller) number of events will be read.

6.2 Output Files

CGMF produces the following output files:

- **summary.CGMF**: Summary of results for both prompt neutrons and photons
- **results.CGMF**: Results related to fission fragment data
- **neutrons.CGMF**: Results on prompt fission neutrons
- **gammas.CGMF**: Results on prompt fission gamma rays

- **histories.CGMF**: List mode of Monte Carlo fission events

The **summary.CGMF** file provides the results for average quantities such as the average prompt neutron multiplicities $\overline{\nu}_{T,L,H}$, the average kinetic energy of the prompt neutrons in the center-of-mass frame, $\langle E_{cm}^{T,L,H} \rangle$, the average kinetic energy of the prompt neutrons in the laboratory frame, $\langle E_{lab}^{T,L,H} \rangle$, and similar quantities for the prompt fission photons. In these expressions, the subscripts T, L, H designate the total, light fragment, and heavy fragment, respectively. This file also provides basic information on the fission fragment average masses, charges and kinetic energies.

The **results.CGMF** file contains general results pertaining to the distribution of the fission fragments in mass, charge, kinetic energy, initial excitation energy and spin distributions, and correlations between average total quantities such as neutron multiplicity versus gamma multiplicity.

The **neutrons.CGMF** and **gammas.CGMF** contain results specific to the prompt fission neutrons and gammas: average spectra in the center-of-mass and laboratory frames, exclusive spectra for 1, 2, etc particles out, particle multiplicity distributions, mass-dependent average multiplicity, etc. Those two files are created identically and therefore share the same structure and format.

Finally, the **histories.CGMF** file contains all Monte Carlo histories produced by **CGMF**. Here is an example of the first fission event recorded in the case of Cf-252 spontaneous fission:

```
112 44 18.712 9.0 -1 108.416 2 4 0 0 0 2 3 3 3
1.839 1.335 3.431 0.792 1.060 1.898 1.374 0.982
2.737 0.000 2.737 0.000 0.712 0.000 0.712 0.000 0.423 0.000 0.423 0.000 0.241 0.000 0.241 0.000
140 54 10.788 4.0 1 86.733 2 0 0 0 0
0.965 1.870 2.040 2.424 0.669 1.988 1.806 2.552
```

The first line corresponds to the light fragment ($A = 112, Z = 44$), with an initial excitation energy of 18.712 MeV, a spin of 9.0, a negative parity (-1), and an initial kinetic energy of 108.416 MeV. The next three integers indicate the number of neutrons emitted (here, 2), the number of gamma rays (here, 4) and the number of internal conversions (here, 0). The following numbers (here, 002333) indicate the nature of the transitions. If a neutron is emitted, this number is 0; if this is a gamma ray, then it is 1 for a continuum-to-continuum transition, 2 for a continuum-to-discrete, and 3 for a discrete-to-discrete transition. This classification is useful for debugging purposes, as well as physics to determine the nature of the transitions and perform slices on the large dataset produced by the code.

The second line describes the characteristics of the emitted neutrons: $\{\epsilon_{cm}, \theta_{cm}, E_{lab}, \theta_{lab}\}$, for each emitted neutron (here, 2). The third line describes the characteristics of the emitted photons, following the same format as for the neutrons.

The final two lines correspond to the same information as above, except for the complementary heavy fragment ($A = 140, Z = 54$).

This sequence is repeated for a number of times corresponding to the number of fission events provided by the user.

6.3 Running with MPI

CGMF can be used on parallel machines using the MPI library. To create an MPI-ready executable, the file `config-ff.h` needs to be edited by replacing:

```
#undef MPIRUN
```

with:

```
#define MPIRUN
```

Also, the compiler option needs to be modified in the Makefile to use an MPI wrapper, e.g., `mpipp`, `mpi++`.

CHAPTER

SEVEN

TEST CASES

7.1 Test #1: Computing Initial Fission Fragment Yields $Y(A, Z, KE, U, J, \pi)$

This test case produces pre-neutron fission fragment yields for neutron-induced fission on Pu-239 for incident neutron energies ranging from thermal up to 20 MeV. The calculations were made using the systematics described in the Physics Section.

Numerical results are saved in files:

```
Yields.94239.[energy]MeV.CGMF
```

Some results are also shown in the following figures.

7.2 Test #2: Reading and Analyzing a Monte Carlo History File

CGMF provides an option to read a history file of fission events previously generated. It is useful to analyze the results without having to run again a large number of events. Combined with the `-n` command line option, it also lets the user read a smaller number of events than saved in the file, potentially saving a lot of time when analyzing averaged quantities.

This test case #2 reads a history file of Monte Carlo fission events for the thermal neutron-induced fission of Pu-239, reading only 100,000 events:

```
CGMF.x -i 94239 -e 2.53e-8 -r histories.CGMF.test2 -n 100000
```

and generates the following default **CGMF** output files:

- summary.CGMF: a summary of the main average results for the fission fragments, neutrons and gamma rays.
- results.CGMF: some distributions as a function of mass, charge and kinetic energy of the fragments.
- neutrons.CGMF: neutron data (spectra, distributions, averages)
- gammas.CGMF: gamma-ray data (spectra, distributions, averages)

The output file **summary.CGMF** is given here:

```
-------------------------------------------------------
                      User Input
-------------------------------------------------------
 ZAID Target                        = 94239
 Incident Neutron Energy (MeV)      = 2.5300e-08
 Spin distribution factor (alphaI)  = 0.0000e+00
 Number of Monte Carlo events       = 1000000
```

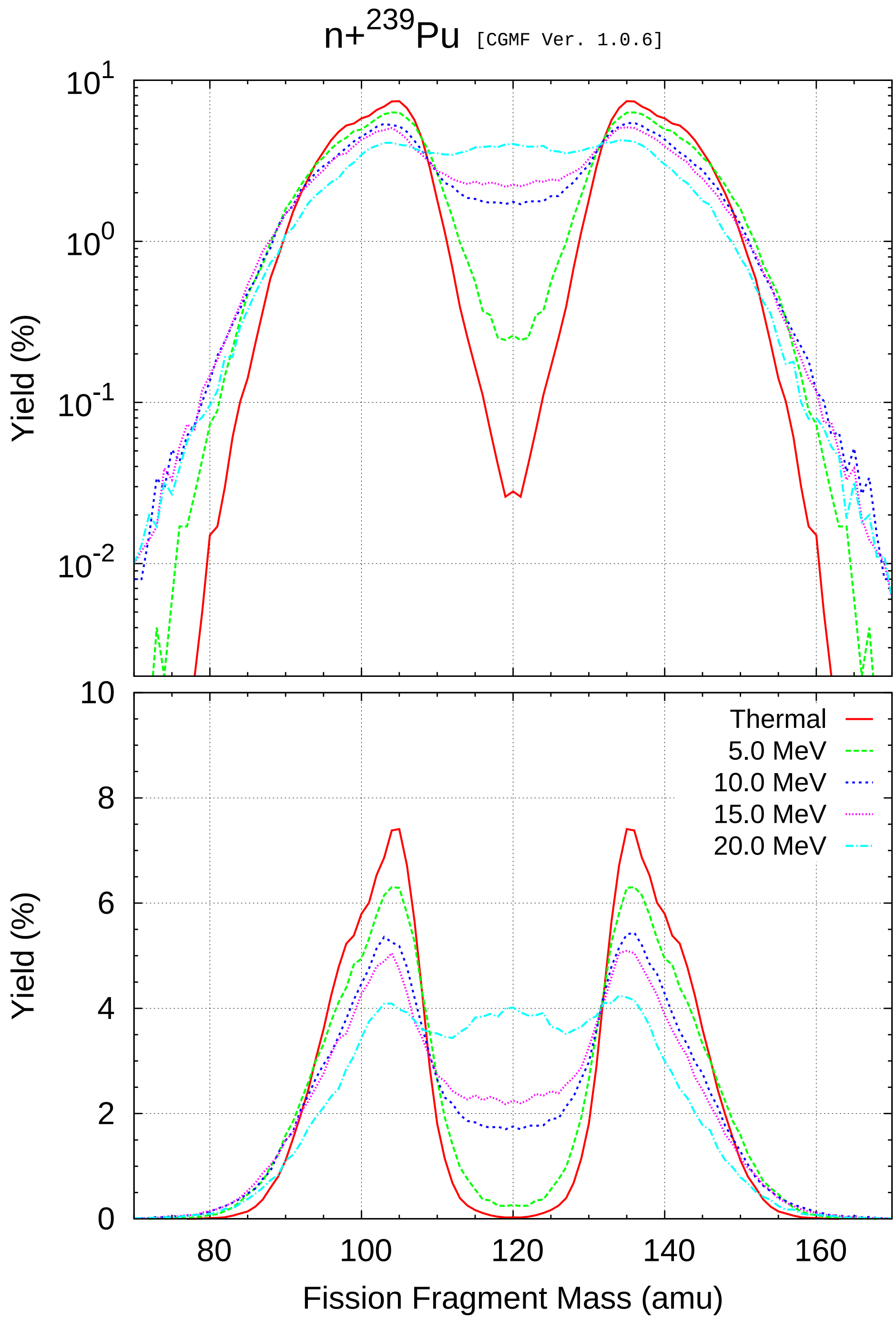


Fig. 7.1: Pre-neutron fission fragment yields produced by **CGMF** in the case of neutron-induced fission reaction on Pu-239 for incident energies from thermal up to 20 MeV.

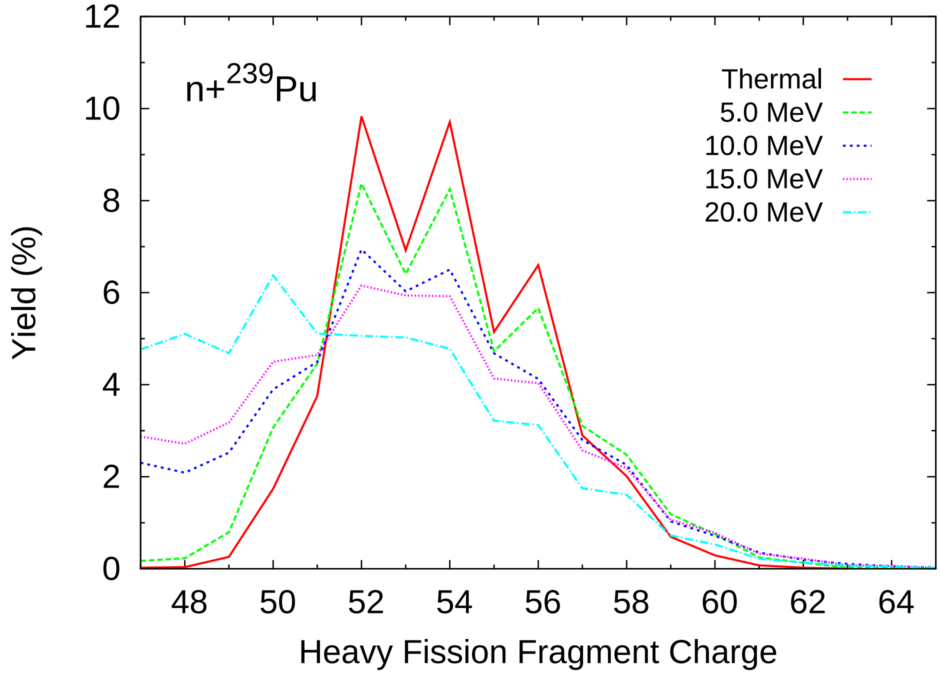


Fig. 7.2: Heavy fission fragment charge distributions as a function of the incident neutron energy.

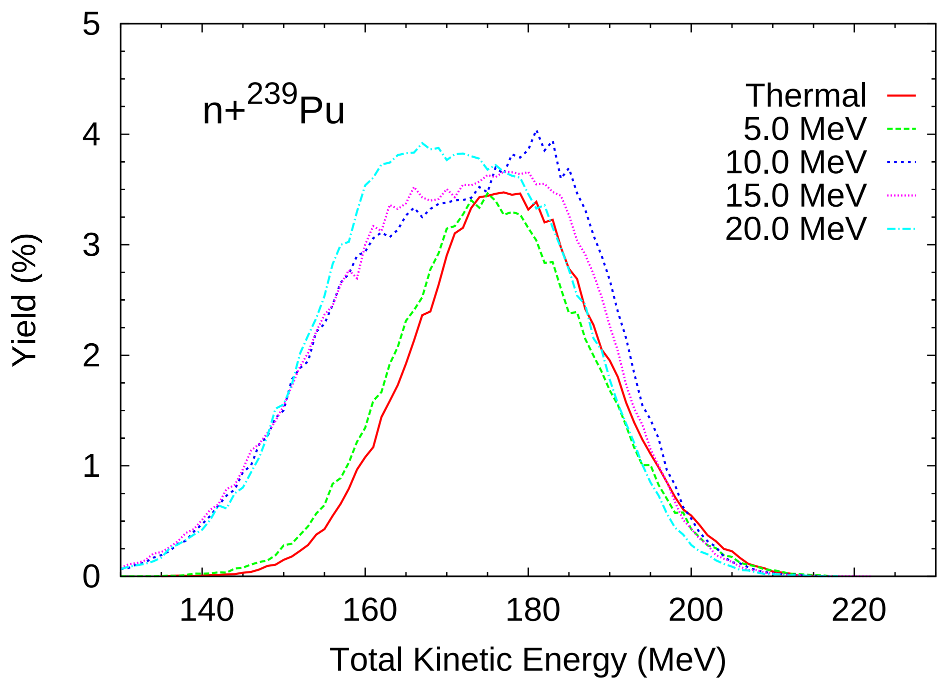


Fig. 7.3: Incident neutron energy dependence of the total kinetic energy yields.

```
-------------------------------------------------------

*******************************************************
                C G M F  Summary of Results
*******************************************************
                n ( 2.5300e-08 MeV ) + 94239
*******************************************************


------------------------------------------------------------------------------------------
|              | All Fragments | Light Fragments | Heavy Fragments | Pre-Fission | Total |
------------------------------------------------------------------------------------------
|      A       |   119.999     |     100.307      |     139.692      |
|      Z       |    47.000     |      39.714      |      54.285      |
| TKE/KE (MeV) |   176.948     |     102.582      |      73.869      |
--------------------------------------------------------------------

 << Neutrons >>

--------------------------------------------------------------------
|    < nu >    |     2.977     |       1.588      |       1.389      |
|    < Ecm >   |     1.274     |       1.265      |       1.284      |
|    < Elab >  |     2.030     |       2.250      |       1.778      |
--------------------------------------------------------------------

 << Gamma Rays >>

--------------------------------------------------------------------
|    < nu >    |     9.184     |       4.616      |       4.569      |
|    < Ecm >   |     0.774     |       0.760      |       0.787      |
|    < Elab >  |     0.774     |       0.760      |       0.787      |
--------------------------------------------------------------------
```

7.3 Test #3: Cf-252 Spontaneous Fission

This test performs a default calculation in the case of Cf-252 spontaneous fission.

> **Warning:** TO REVIEW.

Run **CGMF** by typing:

```
./CGMF.x -i 98252 -e 0.0 -n 100000
```

It will produce several `.CGMF` output files. Among them, `summary.CGMF` gives a summary of results for both prompt neutrons and gamma rays, as well as the average light and heavy fragments mass, charge, and kinetic energy:

```
-------------------------------------------------------
                      User Input
-------------------------------------------------------
 ZAID Target                         = 98252
 Incident Neutron Energy (MeV)       = 0.0000e+00
 Spin distribution factor (alphaI) = 1.7000e+00
 Number of Monte Carlo events        = 640000
-------------------------------------------------------


*******************************************************
```

```
                C G M F  Summary of Results
*******************************************************
               Spontaneous fission of 98252
*******************************************************


------------------------------------------------------------------------------------------------
|              | All Fragments | Light Fragments | Heavy Fragments | Pre-Fission |     Total     |
------------------------------------------------------------------------------------------------
|      A       |   126.000     |    108.407      |    143.593      |
|      Z       |    49.000     |     42.540      |     55.460      |
| TKE/KE (MeV) |   185.284     |    105.091      |     79.694      |
------------------------------------------------------------------------------------------------

 << Neutrons >>

------------------------------------------------------------------------------------------------
|    < nu >    |     3.755     |      2.108      |      1.648      |
|    < Ecm >   |     1.319     |      1.400      |      1.215      |
|    < Elab >  |     2.083     |      2.344      |      1.748      |
------------------------------------------------------------------------------------------------

 << Gamma Rays >>

------------------------------------------------------------------------------------------------
|    < nu >    |     9.475     |      4.810      |      4.665      |
|    < Ecm >   |     0.717     |      0.732      |      0.701      |
|    < Elab >  |     0.717     |      0.732      |      0.701      |
------------------------------------------------------------------------------------------------
```

Processed results are stored in `neutrons.CGMF` for prompt neutrons and in `gammas.CGMF` for prompt gammas. Results are saved as:

```
#
# CGMF Results
#
# [gnuplot #0] lab spec, cm spec, LF lab spec, LF cm spec, HF lab spec, HF cm spec
#
# [gnuplot #1] c.m. spectrum
# Energy     Total        nu=1       nu=2       nu=3        nu=4       nu=5
#  (MeV)      (1/MeV)
# ...
# [gnuplot #2] P(nu) P_LF(nu) P_HF(nu)
# ...
# [gnuplot #3] A  Y(A)    <nu>(A)   <Ecm>(A)  <Ecm>(A)|cut  <Elab>(A)
# ...
# [gnuplot #4] Theta   n-LF    n-n
#       (deg)    (arb. u.)    (arb. u.)
# ...
# [gnuplot #5] TKE   Y(TKE)   <nu>  <Ecm>  <Elab>
#             (MeV)    (n/f)  (MeV)   (MeV)    (MeV)
# ...
# [gnuplot #6] Einc, <nu>, <nu_l>, <nu_h>, <Ecm>, <Ecm_l>, <Ecm_h>, <Elab>, <Elab_l>, <Elab_h>
```

This structure is meant to be used very easily with plotting programs such as `gnuplot`. Examples of plots and results are shown below for Cf-252 (sf):

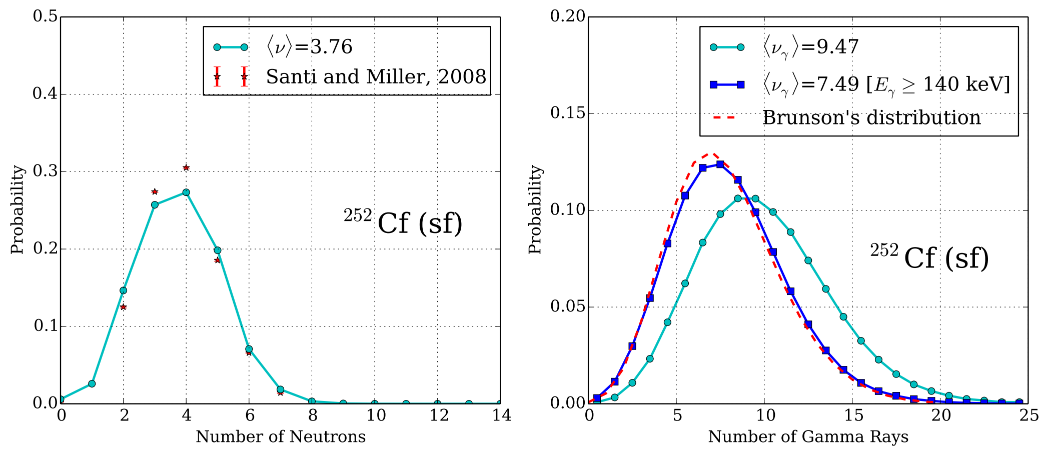


Fig. 7.4: Prompt fission neutron and gamma multiplicity distribution $P(\nu)$ calculated by **CGMF** in the case of Cf-252 spontaneous fission.

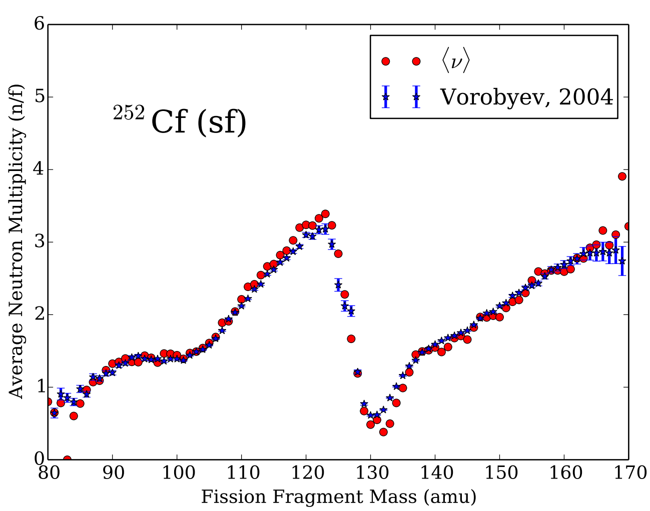


Fig. 7.5: Average prompt fission neutron multiplicity calculated as a function of the fission fragment mass in the case of Cf-252 spontaneous fission, and compared to two recent experimental data sets.

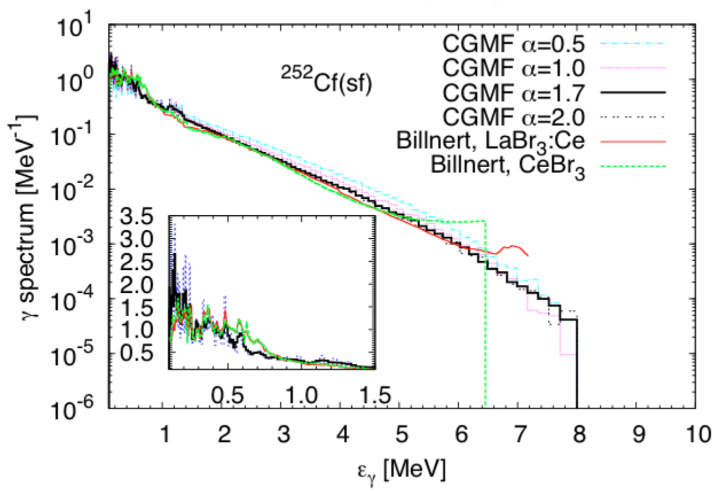


Fig. 7.6: Average prompt fission gamma-ray spectrum calculated in the case of Cf-252 spontaneous fission, using different values of the α parameter to modify the initial spin distribution. The experimental data are from Billnert, 2013.

7.4 Test #4: n+Pu-239 at En=10.0 MeV

Here, 10 MeV neutrons are incident on Pu-239. The command line is as follows:

```
CGMF.x -i 94239 -e 10.0 -n 100000
```

Actually, the results shown here were obtained on a Linux cluster running MPI for better statistics. A total of 640,000 fission events were generated.

7.5 Test #5: Time-Gate on Cf-252 (sf) Calculated Gamma-Ray Spectrum

In this test case, a time coincidence window is applied to the calculation of the prompt fission gamma spectrum. There is no command line option to set the time coincidence window. Instead, it is set in the file `config.h`. In this particular test case, the Cf-252 (sf) was studied and the gamma spectrum coming for the fragment Te-134 was studied with time gates Δt =10, 30, 50 and 100 ns. The result is shown in Fig. *fig-Cf252-timegates*.

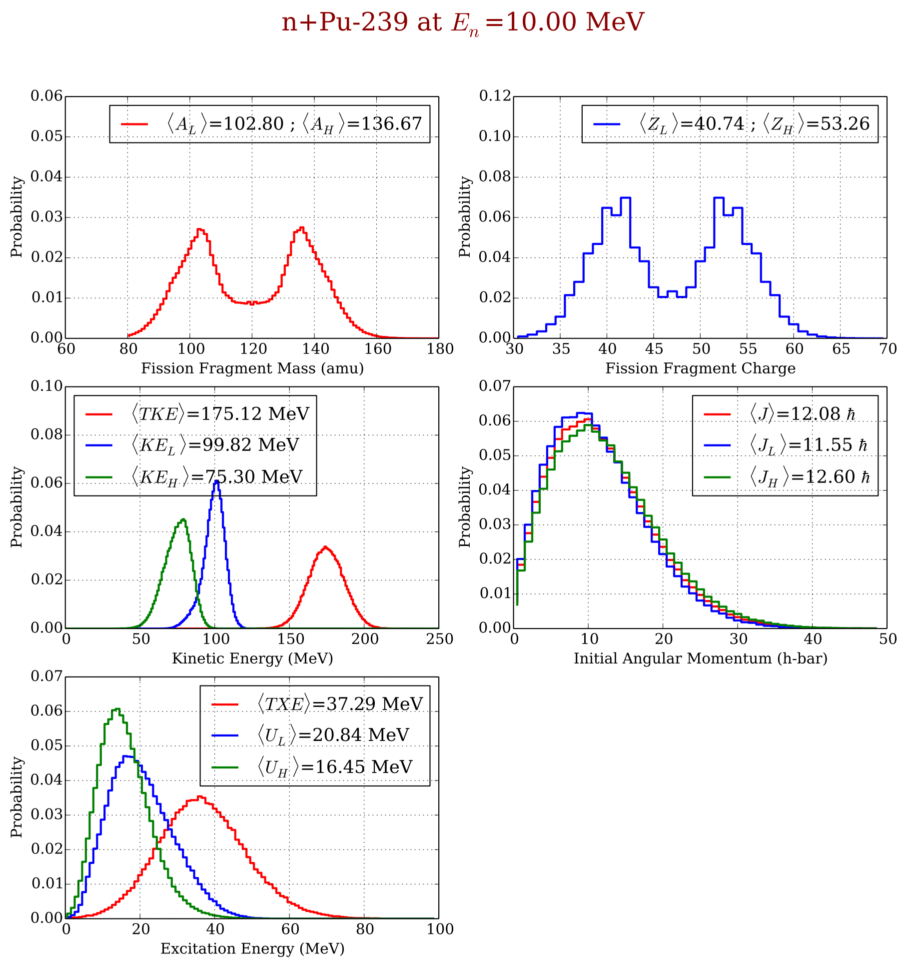


Fig. 7.7: Initial fission fragment yields reconstructed in the 10.0 MeV neutron-induced fission reaction on Pu-239.

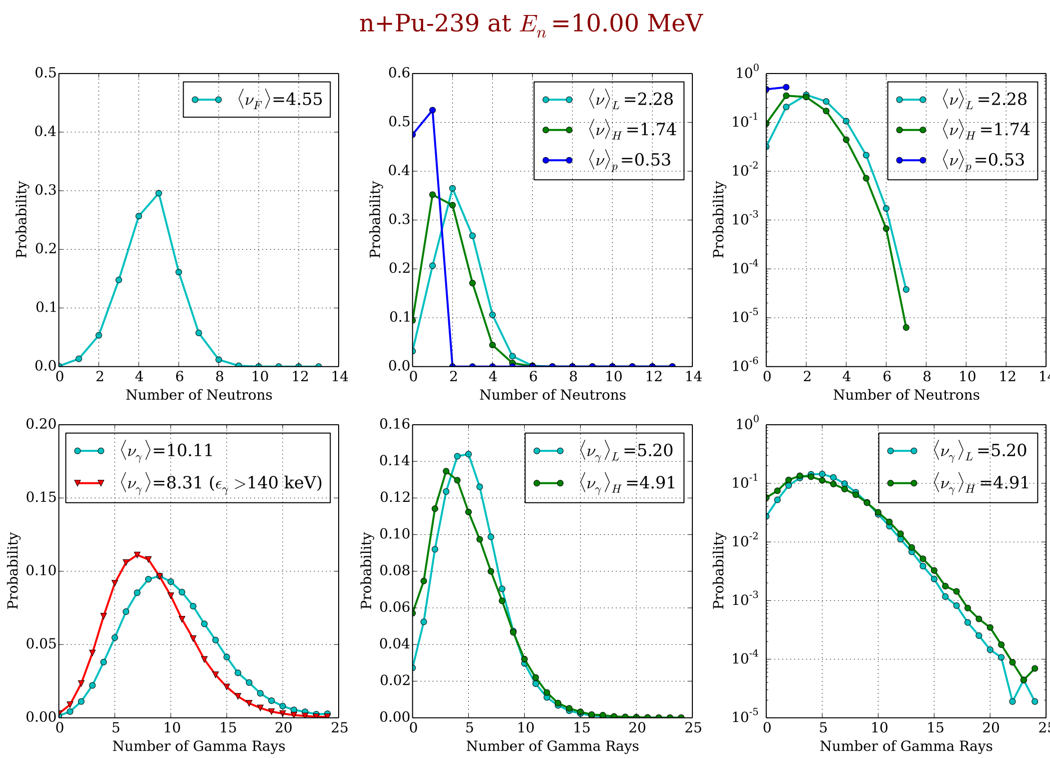


Fig. 7.8: Prompt fission neutron and gamma multiplicity distributions for 10.0 MeV neutron incident on Pu-239. At 10.0 MeV, there is already a contribution from the second-chance fission process, and the calculated average number of pre-fission neutrons emitted in this case is 0.53 (blue points).

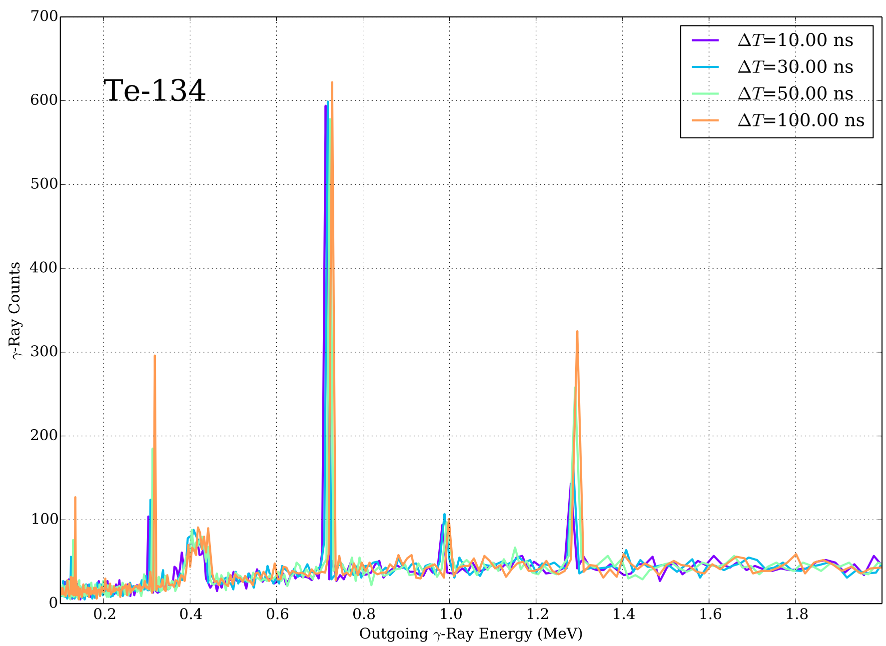


Fig. 7.9: Different time coincidence windows have been applied to the gamma-ray spectrum from the Te-134 fission fragment.

CHAPTER

EIGHT

REFERENCES

8.1 Journal Publications

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- "Advanced Monte Carlo Modeling of Prompt Fission Neutrons for Thermal and Fast Neutron-Induced Fission Reaction on Pu-239," P. Talou, B. Becker, T. Kawano, M. B. Chadwick, and Y. Danon, Phys. Rev. C 83, 064612 (2011).
- "Monte Carlo Hauser-Feshbach Predictions of Prompt Fission Gamma Rays- Application to $n_{\mathrm{th}}+$ U-235, $n_{\mathrm{th}}+$ Pu-239 and Cf-252 (sf)," B.Becker, P. Talou, T. Kawano, Y. Danon, and I. Stetcu, Phys. Rev. C 87, 014617 (2013).
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- "Properties of prompt fission gamma rays," I. Stetcu, P. Talou, T. Kawano, and M. Jandel, Phys. Rev. C 90, 024617 (2014).

8.2 Conference Proceedings

- "Prompt Fission Neutrons and Gamma Rays," P. Talou, T. Kawano, and I. Stetcu, to appear in proceedings of the International Conference on Nuclear Data for Science and Technology, ND2013, New York, NY, March 4-8, 2013.
- "Monte Carlo Hauser-Feshbach Calculations of Prompt Fission Neutrons and Gamma Rays," P. Talou, T. Kawano and I. Stetcu, in proceedings of the Fifth International Conference on Fission and Properties of Neutron-Rich Nuclei, Sanibel Island, Florida, USA, Nov. 4-10, 2012, p.581, Eds. J. H. Hamilton, A. V. Ramayya, World Scientific, 2014.

CHAPTER

NINE

CONCLUSIONS & FUTURE WORK

This document describes the **CGMF** Monte Carlo code, which computes the decay of excited fission fragments through the evaporation of prompt fission neutrons and photons. It provides a brief overview of the physics implemented in the code, as well as a description of the main code algorithm and details on the most important routines. A description of the input options available to the user is provided, as well as a suite of test cases.

In the future, we plan to work on the following extensions of the present version (1.0.6) of the code, namely:

- The excitation energy partitioning is performed following an empirical approach that provides the correct average number of prompt neutrons emitted from the light versus the heavy fragment. It can be explained qualitatively by the role of collective deformations and shell effects in each fragment. A more sound and quantitative approach is being worked out now.
- It is assumed that no correlation exists between the angular momenta of the two complementary fragments. This is a strong assumption that should be revisited.
- The role played by the optical model potential used in **CGMF** should be revisited. Preliminary calculations indicate that the choice of the OMP is particularly important to describe parts of the average neutron spectrum. It is particularly important since most OMPs have been developed for nuclei near the valley of stability, while fission fragments are very neutron-rich.
- In **CGMF** as in all Hauser-Feshbach codes, the problem of populating high-spin states near the transition between the continuum and the discrete regions of a nucleus produces some spurious low-energy gamma transitions that limit the predictions of the prompt fission gamma spectrum at the lowest energies. The current version of the code handles this problem by placing a low-energy cut-off, but this solution remains unsatisfactory.

CHAPTER TEN

REVISIONS HISTORY

10.1 Version 1.1.0

Revision committed on: **NOT YET COMMITTED**

To be released by the end of CY2015. It should include the following capabilities:

- Extension to higher incident neutron energies up to 20 MeV
- Systematics for a few more actinides
- Test cases
- Improved speed
- Clear documentation

This version should be the basis for an open-source version to be released later in 2016, but before the end of the project. Could it make it to GEANT4, TRIPOLI, etc.?

10.2 Version 1.0.6

Revision committed on: **Aug. 28, 2015**

This is a major revision that extends the capabilities of the code to higher incident neutron energies, from thermal up to 20 MeV. It accounts for the multi-chance fission processes as well as pre-equilibrium neutrons prior to fission. Systematics of pre-neutron emission fission fragment yields have been implemented for Pu-239 up to 20 MeV. Systematics for more isotopes are being developed for the next release of the code.

10.3 Version 1.0.5

Revision committed on: **Nov. 17, 2014**

The option to include the experimental time coincidence window to measure "prompt" fission data has been added. If a time window is set in the config.h file, the half-lives of isomeric states are used to determine wether or not a gamma cascade should continue to the ground-state.

10.4 Version 1.0.4

Revision committed on: **Apr. 22, 2014**

Added option to read Y(A,Z,TKE) file directly. This file contains all non-zero initial fission fragment yields, in a format used in the framework of the IAEA CRP on "Prompt Fission Neutron Spectra of Actinides".

10.5 Version 1.0.3

Revision committed on: **Nov. 20, 2013**

Fixed bug on following fission event counter in the case of symmetric fission.

10.6 Version 1.0.2

Revision committed on: **Nov. 5, 2013**

Removed main input file. Only command-line options are now available.

10.7 Version 1.0.1

Revision committed on: **Sep. 9, 2013**

Added reading history file option. Once a history file has been produced, it can be read directly from `CGMF` without having to re-do the calculations once more. The number of events read in can also be set as a user option.

10.8 Version 1.0

Version committed on: **May 31, 2013**

First official version. It corresponds to the LANL code release **LA-CC-13-063**.

Requested Capabilities <requests> # Glossary <glossary>

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