Fission Reaction Event Yield Algorithm FREYA 2.0.2

J.M. Verbeke[a,*], J. Randrup[b], R. Vogt[a,c]

[a] *Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551, USA*
[b] *Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA*
[c] *University of California, Davis, One Shields Avenue, Davis, CA 95616, USA*

Abstract

FREYA (Fission Reaction Event Yield Algorithm) is a fission event generator which models complete fission events. As such, it automatically includes fluctuations as well as correlations between observables, resulting from conservation of energy and momentum. The purpose of this paper is to present the main differences between FREYA versions 1.0 and 2.0.2: additional fissionable isotopes, angular momentum conservation, Giant Dipole Resonance form factor for the statistical emission of photons, improved treatment of fission photon emission using RIPL database, and dependence on the incident neutron direction. FREYA 2.0.2 has been integrated into the LLNL Fission Library 2.0.2, which has itself been integrated into MCNP6.2, TRIPOLI-4.10, and can be called from Geant4.10.

New Version Program Summary:

Program title: FREYA 2.0.2

Catalogue identifier: TBD

Program summary URL: TBD

Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland

Licensing provisions: BSD 3-clause

*Corresponding author
Email address: verbeke2@llnl.gov (J.M. Verbeke)

No. of lines in distributed program, including test data, etc: TBD

No. of bytes in distributed program, including test data, etc: TBD

Distribution format: tar.gz

Programming language: Fortran 90, C++

Computer: any computer with a Fortran 90 and a C++ compiler, tested with (a) Intel 18-core Xeon E5-2695 v4 CPU, 2.1 GHz, 128 GB RAM, (b) Intel Core i7 CPU, 2.8 GHz, 16 GB RAM

Operating system: (a) Red Hat Enterprise Linux Server release 7.3 (GNU Fortran and g++ (GCC) 4.9.3), (b) MacBook Pro OS X 10.10.5 (GNU Fortran (GCC version 5.3.0) and C++ (Apple LLVM version 6.1.0))

Has the code been vectorized or parallelized? No

RAM: 6 GB

Classification: 17.8

External routines: None.

Journal Reference of previous version: J. M Verbeke, J. Randrup, R. Vogt, "Fission Reaction Yield Algorithm FREYA for Event-by-Event Simulation of Fission," Comp. Phys. Comm. 191, pp. 178-202; doi:10.1016/j.cpc.2015.02.002 (2015).

Does the new version supersede the previous version? Yes.

Reasons for the new version: New physics and more fissionable isotopes.

Summary of revisions: Additional fissionable isotopes, angular momentum conservation, Giant Dipole Resonance form factor for the statistical emission of photons, improved treatment of fission photon emission using `RIPL` database, and dependence on the incident neutron direction.

Nature of problem: Modeling of fission events.

Solution method: Simulation of complete fission events, production of secondary fission fragments, fission neutrons and photons.

Restrictions: Restricted to spontaneous fission of ^{238}U, ^{238}Pu, ^{240}Pu, ^{242}Pu, ^{244}Cm, ^{252}Cf; neutron-induced fission of ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, ^{241}Pu, for incident neutron energies less than 20 MeV.

Unusual features:

Running time: 8 s for 100,000 events

Keywords: fission, event-by-event Monte Carlo

1. Introduction

The computational model FREYA generates complete fission events, *i.e.* it provides the full kinematic information on the two product nuclei as well as all the emitted neutrons and photons. In its development, an emphasis had been put on speed, so large event samples can be generated fast, and FREYA therefore relies on experimental data supplemented by physics-based modeling.

This purpose of this update is to describe the physics changes that have been implemented into FREYA 2.0.2 since the last major release FREYA 1.0, documented in Ref. [1]. A complete manual [2] for this latest version is distributed with the software package and can be downloaded from the Computer Physics Communications Program Library http://www.cpc.cs.qub.ac.uk/overview.html or from http://nuclear.llnl.gov/simulations.

The stand-alone fission event generator FREYA 2.0.2 has been integrated into the LLNL Fission Library 2.0.2 [3], which in turn is an integral part of the transport codes MCNP6.2® [4], TRIPOLI-4.10® [5], and can be called from Geant4.10 [6].

The number of fission reactions that FREYA 2.0.2 implements has increased, it can currently handle spontaneous fissions of ^{238}U, ^{238}Pu, ^{240}Pu, ^{242}Pu, ^{244}Cm and ^{252}Cf. In addition to spontaneous fission, FREYA treats neutron-induced fission of ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, ^{241}Pu up to $E_n = 20\,\mathrm{MeV}$, and is sensitive to the direction of the incident neutron.

This update is divided into three parts to describe the physics behind the algorithms in FREYA. The system pre-fission is described in Sec. 2. Next, the scission process itself that results in binary fission with two excited fission fragments is treated in Sec. 3. Finally, de-excitation by post-fission radiation of neutrons and photons is described in Sec. 4.

2. Pre-fission radiation

There are two possible ways for neutrons to be emitted before fission occurs for sufficiently high incident neutron energies: pre-equilibrium neutron emission (which plays a role at the highest energies) and pre-fission neutron evaporation, referred to as multichance fission. `FREYA` handles both these possibilities.

Because there were no significant changes between `FREYA 1.0` and `FREYA 2.0.2` as far as pre-fission radiation, the reader is referred to Ref. [1] for details on pre-fission radiation.

3. Fission

After pre-fission radiation, the mass and charge of the initial compound nucleus are partitioned among the two fission fragments and the available energy is divided between the excitation of the two fragments and their relative kinetic energy. The selection of the fission fragment masses and charges has not substantially changed in `FREYA 2.0.2`.

Once the mass and charge of the two fragments have been selected, the linear and angular momenta of the two fragments and their internal excitations are sampled. `FREYA 2.0.2` takes the direction of the incident neutron into consideration for the emission of secondaries. The Q-value of the fission channel is the difference between the total mass of A_0 and the fragment ground-state masses,

$$Q_{LH} = M(A_0)c^2 - M_L c^2 - M_H c^2 \ . \tag{1}$$

Figures 1-2 show how the fission fragment energies are selected. `FREYA 1.0` was splitting the Q_{LH} value between the total kinetic energy and the statistical excitation energies of the fragments. `FREYA 2.0.2` now takes the rotational excitation into account as well. The Q_{LH} value is divided between the total kinetic energy (TKE), the total rotational and statistical excitations of the fragments. The average TKE is assumed to take the form

$$\overline{\mathrm{TKE}}(A_H, E_n) = \overline{\mathrm{TKE}}_{\mathrm{data}}(A_H) + d\mathrm{TKE}(E_n) \ . \tag{2}$$

The first term is extracted from data on thermal neutrons while the second is adjusted to the measured average neutron multiplicity, $\overline{\nu}$.

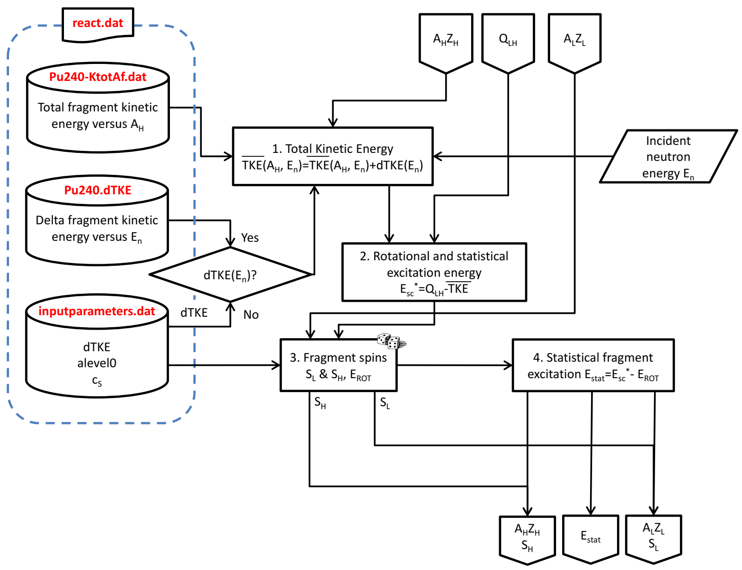

Figure 1: Selection of fission fragment rotational energies, new to `FREYA 2.0.2`, for the example of ^{239}Pu(n,f). Modified from Ref. [1].

After the average total fragment kinetic energy, $\overline{\mathrm{TKE}}$, has been calculated, the energy available for rotational and statistical excitation of the two fragments is then

$$E^*_{\mathrm{sc}} = Q - \overline{\mathrm{TKE}} \tag{3}$$

and the corresponding 'scission temperature' T_{sc} is obtained from

$$E^*_{\mathrm{sc}} = (A_0/e_0)T^2_{\mathrm{sc}}\,. \tag{4}$$

The inclusion of angular momentum in `FREYA` was described in Ref. [7]. The overall rigid rotation of the dinuclear configuration prior to scission, caused by the absorption of the incoming neutron and the recoil(s) from any evaporated neutron(s), dictates certain mean angular momenta in the two fragments. In addition, due to the statistical excitation of the scission complex, the fragments also acquire fluctuations around those mean values. `FREYA` includes fluctuations in the wriggling and bending modes (consisting of rotations in the same or opposite sense around an axis perpendicular to the dinuclear axis) but ignores

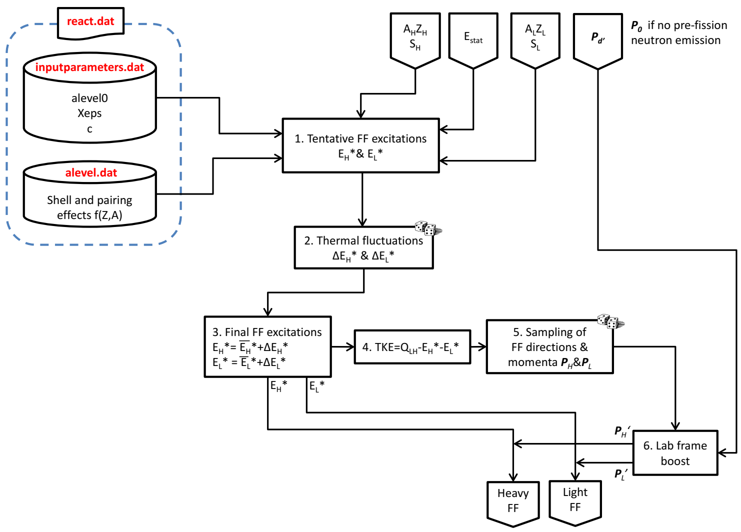

Figure 2: Selection of fission fragment excitations and momenta. Modified from Ref. [1]

tilting and twisting (in which the fragments rotate around the dinuclear axis). These dinuclear rotational modes are assumed to become statistically excited during scission and they are therefore described by Boltzmann distributions,

$$P_\pm(\boldsymbol{s}_\pm)\, ds_\pm^x ds_\pm^y \ \sim\ \mathrm{e}^{-s_\pm^2/2\mathcal{I}_\pm T_S} ds_\pm^x ds_\pm^y\,, \tag{5}$$

where $\boldsymbol{s}_\pm = (s_\pm^x, s_\pm^y, 0)$ is the spin of the normal modes with plus referring to the wriggling modes (having parallel rotations) and minus referring to the bending modes (having opposite rotations). The corresponding moments of inertia are denoted $\mathcal{I}_\pm$ [7, 8]. The degree of fluctuation is governed by the 'spin temperature'

$$T_S = c_S T_{\rm sc} \tag{6}$$

(see Eq. (6)) which can be adjusted by means of the parameter c_S. The fluctuations vanish for $c_S = 0$ so the fragments emerge with the angular momenta dictated by the overall rigid rotation of the scission configuration (which is usually very small for induced fission and entirely absent for spontaneous fission). The default value, $c_S = 1$, leads to $\overline{S}_L \sim 6.2\hbar$ and $\overline{S}_H \sim 7.6\hbar$ for ^{252}Cf(sf) and yields a reasonable agreement with the average energy of photons emitted in fission (see Ref. [7] for details).

After accounting for the total rotational energy of the two fragments, $E_{\rm rot}$, we are left with a total of

$$E_{\rm stat} = E^*_{\rm sc} - E_{\rm rot} \tag{7}$$

for statistical fragment excitation. It is partitioned between the two fragments as described in Ref. [1].

After the mean fragment excitation energies have been assigned as described above, `FREYA` considers the effect of thermal fluctuations. Whereas `FREYA 1.0` sampled an energy fluctuation δE^*_i from a normal distribution of variance $\sigma^2_{E_i} = 2\overline{E}^*_i T_i$ and adjusted the fragment excitations accordingly, arriving at

$$E^*_i \ = \ \overline{E}^*_i + \delta E^*_i \ , \ i = L, H \ , \tag{8}$$

`FREYA 2.0.2` samples an energy fluctuation δE^*_i from a normal distribution of variance

$$c^2 \sigma^2_{E_i} = 2c^2 \overline{E}^*_i T_i \ , \tag{9}$$

where the factor c multiplying the variance was introduced to explore the effect of the truncation of the normal distribution at the maximum available excitation. It can be adjusted for each fissile nucleus. Its value affects the neutron multiplicity distribution $P(\nu)$ [9]; previous work used the default value, $c = 1.0$.

Energy conservation is accounted for by making a compensating opposite fluctuation in the total kinetic energy [10],

$${\rm TKE} \ = \ \overline{\rm TKE} - \delta E^*_L - \delta E^*_H \ . \tag{10}$$

4. Post-fission radiation

As in `FREYA 1.0`, neutron evaporation occurs until the nuclear excitation energy of the fission fragments is below the threshold $S_n + Q_{\rm min}$, where S_n is the neutron separation energy and $Q_{\rm min} = 0.01$ MeV. Neutron evaporation continues as long as energetically possible. After neutron evaporation has ceased, the excited product nucleus will undergo sequential photon emission to rid itself of the remaining excitation energy. This energy is both statistical and rotational, see Fig. 1.

Photon emission is treated in several stages. Whereas `FREYA 1.0` only emitted statistical photons, `FREYA 2.0.2` now uses the `RIPL`-3 data library [11] for the discrete decays towards the end of the decay chain.

The first stage — common to `FREYA 1.0` and `FREYA 2.0.2` — is statistical radiation. These photons are emitted isotropically in the frame of the emitter nucleus with an energy that has been sampled from a black-body spectrum modulated by a giant-dipole resonance (GDR) form factor,

$$\frac{dN_\gamma}{dE_\gamma} \sim \frac{\Gamma_{\rm GDR}^2 E_\gamma^2}{(E_\gamma^2 - E_{\rm GDR}^2)^2 - \Gamma_{\rm GDR}^2 E_\gamma^2} \, E_\gamma^2 \, {\rm e}^{-E_\gamma/T} \,, \tag{11}$$

where T, the nuclear temperature prior to emission, is equal to the maximum possible temperature after emission. The position of the resonance is taken as $E_{\rm GDR}/{\rm MeV} = 31.2/A^{1/3} + 20.6/A^{1/6}$ [12], while its width is $\Gamma_{\rm GDR} = 5\,{\rm MeV}$. Each emission reduces the magnitude of the angular momentum by $dS = 1\,\hbar$. In the statistical radiation of photons, the GDR form factor

$$\frac{\Gamma_{\rm GDR}^2 E_\gamma^2}{(E_\gamma^2 - E_{\rm GDR}^2)^2 - \Gamma_{\rm GDR}^2 E_\gamma^2} \tag{12}$$

is new to `FREYA 2.0.2`.

In `FREYA 1.0`, the cascade was continued until the statistical excitation energy available for photon emission was exhausted and the photon energy was below a specified, detector-dependent threshold, $g_{\rm min}$, which is typically fixed at $g_{\rm min} = 100$ keV. `FREYA 2.0.2` instead splits the total excitation energy into statistical excitation and rotational energy. After the statistical excitation available for photon emission (when the statistical excitation energy is below the neutron separation energy) is exhausted, the rotational energy must still be disposed of. `FREYA 2.0.2` uses the discrete levels in the `RIPL-3` library [11] for photon transitions between levels when the photon cascade leads to an energy below any of the tabulated `RIPL-3` levels. The `RIPL-3` library tabulates discrete electromagnetic transitions for nuclei throughout the nuclear chart. While complete information is available for only relatively few of them, by invoking certain assumptions , it is possible to construct, for each product species, a table of the possible decays to the lowest discrete levels including the level energies ϵ_l, half lives t_l, and branching ratios. The discrete cascade continues either until the excitation energy is below $g_{\rm min}$, or the half-life t_l, exceeds a specified value $t_{\rm max}$, adjusted to reflect the detector response time . If the photon decay for a particular fragment is not in the `RIPL-3` tables, the fragment must still dispose of its rotational energy. In this case, photons are emitted along the yrast line as long as $S > 2$, after which the remaining energy is carried away by a single photon, as described in Ref. [8].

5. Acknowledgments

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and by Lawrence Berkeley National Laboratory under Contract DE-AC02-05CH11231. The authors wish to acknowledge the Office of Defense Nuclear Nonproliferation Research and Development in DOE/NNSA for their support.

If you download and use `FREYA 2.0.2`, we would be grateful if you could email freya@llnl.gov. For publications, please acknowledge `FREYA` by citing this article or Refs. [1, 2].

References

[1] J. Verbeke, J.Randrup, R.Vogt, Fission reaction yield algorithm `FREYA` for event-by-event simulation of fission, Comp. Phys. Comm. 191 (2015) 178–202. `doi:10.1016/j.cpc.2015.02.002`.

[2] J. Verbeke, J.Randrup, R.Vogt, Fission reaction yield algorithm `FREYA 2.0.2` user manual, Tech. Rep. LLNL-SM-705798, Lawrence Livermore National Laboratory (2016).

[3] J. Verbeke, C. Hagmann, D. Wright, Simulation of neutron and gamma-ray emission from fission and photofission. LLNL Fission Library 2.0.2, Tech. Rep. UCRL-AR-228518-REV-1, Lawrence Livermore National Laboratory (2016).

[4] T. Goorley, M. James, T. Booth, F. Brown, J. Bull, L. Cox, J. Durkee, J. Elson, M. Fensin, R. Forster, J. Hendricks, H. Hughes, R. Johns, B. Kiedrowski, R. Martz, S. Mashnik, G. McKinney, D. Pelowitz, R. Prael, J. Sweezy, L. Waters, T. Wilcox, T. Zukaitis, Initial MCNP6 release overview, Nuclear Technology 180 (2012) 298–315. doi:10.13182/NT11-135.

[5] TRIPOLI-4® Project Team, TRIPOLI-4 version 8 user guide, Tech. Rep. CEA-R-6316, Commissariat à l'énergie atomique et aux énergies alternatives (2013).

[6] J. Allison, K. Amako, J. Apostolakis, P. Arce, M. Asai, T. Aso, E. Bagli, A. Bagulya, S. Banerjee, G. Barrand, B. Beck, A. Bogdanov, D. Brandt, J. Brown, H. Burkhardt, D. Cano-Ott, S. Chauvie, K. Cho, G. Cirrone, G. Cooperman, M. Cortes-Giraldo, G. Cosmo, G. Cuttone, X. Dong, A. Dotti, V. Elvira, G. Folger, Z. Francis, A. Galoyan, L. Garnier, K. Genser, V. Grichine, S. Guatelli, P. Gueye, P. Gumplinger, A. Howard, I. Hrivnacova, S. Hwang, S. Incerti, A. Ivanchenko, V. Ivanchenko, F. Jones, S. Jun, P. Kaitaniemi, N. Karakatsanis, M. Karamitrosi, M. Kelsey, A. Kimura, T. Koi, H. Kurashige, A. Lechner, S. Lee, F. Longo, M. Maire, D. Mancusi, A. Mantero, E. Mendoza, B. Morgan, K. Murakami, T. Nikitina, L. Pandola, P. Paprocki, J. Perl, I. Petrovic, M. Pia, W. Pokorski, J. Quesada, M. Raine, M. Reis, A. Ribon, A. R. Fira, F. Romano, G. Russo, G. Santin, T. Sasaki, D. Sawkey, J. Shin, I. Strakovsky, A. Taborda, S. Tanaka, B. Tom, T. Toshito, N. Tran, P. Truscott, L. Urban, V. Uzhinsky, J. Verbeke, M. Verderi, B. Wendt, H. Wenzel, D. Wright, D. Wright, T. Yamashita, J. Yarba, H. Yoshida, Recent developments in Geant4, Nucl. Instr. Meth. A 835 (2016) 186–225. doi:10.1016/j.nima.2016.06.125.

[7] J. Randrup, R. Vogt, Refined treatment of angular momentum in the event-by-event fission model FREYA, Phys. Rev. C 89 (2014) 044601–1–6. doi:10.1103/PhysRevC.89.044601.

[8] R. Vogt, J. Randrup, Event-by-event study of photon observables in spontaneous and thermal fission, Phys. Rev. C 87 (2013) 044602–1–16. doi:10.1103/PhysRevC.87.044602.

[9] R. Vogt, J. Randrup, Neutron angular correlations in spontaneous and neutron-induced fission, Phys. Rev. C 90 (2014) 064623–1–7. doi:10.1103/PhysRevC.90.064623.

[10] R. Vogt, J. Randrup, D. Brown, M. Descalle, W. Ormand, Event-by-event evaluation of the prompt fission neutron spectrum from ^{239}Pu(n,f), Phys. Rev. C 85 (2012) 024608–1–18. doi:10.1103/PhysRevC.85.024608.

[11] R. Capote, M. Herman, P. Obložinský, P. Young, S. Goriely, T. Belgya, A. Ignatyuk, A. Koning, S. Hilaire, V. Plujko, M. Avrigeanu, O. Bersillon, M. Chadwick, T. Fukahori, Z. Ge, Y. Han, S. Kailas, J. Kopecky, V. Maslov, G. Reffo, M. Sin, E. Soukhovitskii, P. Talou, RIPL – reference input parameter library for calculation of nuclear reactions and nuclear data evaluations, Nucl. Data Sheets 110 (2009) 3107–3214. doi:10.1016/j.nds.2009.10.004.

[12] B. Berman, S. Fultz, Measurements of the giant dipole resonance with monoenergetic photons, Rev. Mod. Phys. 47 (1975) 713–760. doi:10.1103/RevModPhys.47.713.