Modeling fission in FIFRELIN

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P(ND)_2-2 Perspectives on Nuclear Data for the Next Decade,
14-17 October, 2014, BIII, France
Context

Models in FIFRELIN

Fission observables: comparison with experiments

Beyond common observables

Perspectives
**Codes for simulating fission fragment de-excitation**

- **Madland-Nix** model @ LANL, USA *(neutrons / PFNS + Nubar)* 1982
- **Point-by-Point** model @ Bucharest Univ., Romania (extended MN+) ~2000
- **GEF** code @ CENBG, France *(from CN to Fiss. Obs.)* ~2010
- **CGMF** code @ LANL, USA *(Fiss. Obs. / -W or -HF model)* ~2005
- **FREYA** code @ LLNL, USA *(Fiss. Obs. / -W model)* ~2010
- **FIFRELIN** code @ CEA, France *(Fiss. Obs. / -W or -HF model)* ~2010


Main contributions of Monte Carlo codes

- Distributions, correlations between fission observables,
- Complete and consistent set of calculated fission observables: neutron spectra and multiplicities as well as gamma spectra and multiplicities in addition of prompt energy release, post neutron yields, ...

**Context**

**CGM/F**

**FIFRELIN**

**GEF**

**Point by Point**

**FREYA**
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Perspectives
Definitions

- Prompt emission: before $\beta^-$ decay
- Prediction: By establishing the ‘as better as possible’ calculation scheme (models, model parameters, hypothesis…) we can reproduce some given ‘target observables’ (global quantities, e.g. $\bar{v}_L$, $\bar{v}_H$) and then look at other ones (predicting them):
  
  \[ P(\nu) , P(\nu \gamma), \bar{v}(TKE) , \ldots \]

Hypothesis

- Binary Fission
- $n/\gamma/e^-$ emission after FF full acceleration (fragments have recovered their gs deformation)
- NEDA (A. Matsumoto et al., J. of Nucl. Sc. and Tech. 49, 782 (2012)) not accounted for.
1. Mass ($A$)
2. Kinetic Energy ($KE$)
3. Nuclear Charge ($Z$)
4. Spin, Parity ($J^\pi$)
5. Excitation Energy ($E^*$)

Fission Fragment characteristics sampling

Pre-neutron mass yields from experiment or fission modes

Pre-neutron kinetic energy distributions as function of mass from experiment or fission modes

Nuclear Charge as a function of mass (Wahl model)

Spin distribution from models

Models in FIFRELIN

Pre-neutron kinetic energy distributions as function of mass from experiment or fission modes

Nuclear Charge Polarization as a function of mass from experiment

P(Z) gaussian + EOZ, EON factors

Spin distribution from models

$P(J) = \frac{(2J+1)}{2\sigma^2} \exp \left(-\frac{(J+1/2)^2}{2\sigma^2}\right)$
Excitation energy sharing between fragments

At scission:

intrinsic excitation energy
+ deformation energy + collective excitation

\[ TXE = a_{sc} T_{sc}^2 + E_{def} + E_{coll} \]

After full acceleration:

the rotational energy is not included in the intrinsic excitation energy

\[ TXE = a_L T_L^2 + a_H T_H^2 + E_{rot}^L + E_{rot}^H \]

A part of excitation energy at scission is converted in rotational energy (collective excitation)

Rotating deformed Liquid Drop model

\[ E_{rot} = \frac{\hbar^2 J(J+1)}{2\Xi} \]

only the intrinsic excitation energy corresponding to

\[ TXE - (E_{rot}^L + E_{rot}^H) \]

is partitioned through

\[ E_{L,H}^* = a_{L,H} T_{L,H}^2 \]
∀ L, H \quad E^* = a \quad T^2

R_T(A) = T_L/T_H

A_L = A_{\text{CN}} - 132 \quad A_H = 132

\begin{align*}
A_L &= A_{\text{H}} = A_{\text{CN}} / 2 \\
R_T^\text{max} &= 1.0
\end{align*}

\begin{align*}
A_L &= 78 \quad A_H = A_{\text{CN}} - 78
\end{align*}

\begin{align*}
A_{\text{CN}} / 2 &\quad 132 &\quad A_{\text{CN}} - 78
\end{align*}

\begin{align*}
\text{Ignatuyk prescription} \\
a = \overline{a} \left( 1 + \delta W \frac{1 - e^{-U^*}}{U^*} \right)
\end{align*}

\begin{align*}
\text{Shell corrections, pairing, …}
\end{align*}

\begin{align*}
\text{Max } R_T(A_{\text{H}}=130) ? \\
\text{R}_T(Z) ? \\
R_T^m
\end{align*}

\begin{align*}
R_T(A) \text{ succesfully tested by Talou et al., Phys. Rev. C 83, 064612 (2011)}
\end{align*}
Weisskopf evaporation theory for neutron emission

+ DICEBOX like MC scheme for gamma emission (‘Nuclear Realization’)

- Residual nuclear temperature $T(A-1,Z,E^*)$

- Step by step temperature dependent neutron spectrum

- Neutron emission down to $S_n(J) = S_n + E_{rot}(J)$

- Gamma emission:
  - Level densities
    - CGCM,CTM,HFB-tabulated
  - Strength functions
    - SLO,EGLO, QRPA (from HFB or HF+BCS)
  - Experimental level schemes from RIPL-3
\[ P_n = \frac{\Gamma_n}{\Gamma_\gamma + \Gamma_n} \]

\[ P_\gamma = \frac{\Gamma_\gamma}{\Gamma_\gamma + \Gamma_n} \]

**‘Hauser-Feshbach’ statistical theory for n/\gamma emission**

- Neutron transmission coefficients from:
  - Talys/Ecis code (Koning-Delaroche, Jeukenne-Lejeune-Mahaux OMP from RIPL-3)

- Gamma transmission coefficients (as previously described)
  - **Level densities**
    - CGCM,CTM,HFB-tabulated
  - **Strength functions**
    - SLO,EGLO, QRPA (from HFB or HF+BCS)
  - **Experimental nuclear level schemes**

**NB:** Experimental nuclear level schemes taken from RIPL-3 are completed with models from \( E_{\text{cut-off}} \) up to an energy \( E_{\text{bin}} \) corresponding to a given level density (default: \( 5.10^4 \) MeV\(^{-1} \)).

\( E_{\text{bin}} \) is the starting point for bin description.
Free parameters of the simulation (the big 5!)

- **Fraction (k)** of the rigid spheroid moment of inertia $J$ involved in the rotational energy formula $E_{rot} = \hbar^2 J (J + 1) / (2k)$

  - Rigid spheroid: $J = k \times J_{\text{rig}} = k \times 2/5 \ AMR^2 (1 + 0.31\beta_2 + \cdots)$
  - Hydrodynamical system: $J = k \times J_{\text{fluid}} = k \times (9/8\pi) \ AMR^2 \beta_2^2$

- **Initial fission fragment total angular momenta** $P(J) = \frac{(J + 1/2)}{\sigma^2} \exp \left( -\frac{(J + 1/2)^2}{\sigma^2} \right)$

  - $\sigma^2 \sim J \ T / \hbar^2$ [used in previous studies: Litaize et al., Phys. Proc. 31, 51 (2012)]
  - $<\sigma_L>, <\sigma_H>$
  - $<J>(A) \rightarrow \sigma(A)$
  - $<J>(A,E^*) \rightarrow \sigma(A,E^*)$

- **Extrema values of the temperature ratio** $R_{T}(A) \quad R_{T}^{\text{min}}, \ R_{T}^{\text{max}}$
(1) Calculated values may change a little from a presentation to another due to releases of the code

- Context
- Models in FIFRELIN
- Fission observables: comparison with experiments
- Beyond common observables
- Perspectives
Average prompt neutron multiplicity as a function of pre-neutron mass

Fission Observables: comparison with experiment

Average prompt neutron energy in CM as a function of pre-neutron mass

252Cf (sf)

Fission Observables: comparison with experiment

$^{252}\text{Cf (sf)}$

Average prompt gamma multiplicity as a function of pre-neutron mass

$N_{\gamma}(E)$

Prompt fission gamma spectrum

$M_{\gamma} / \text{MeV}$

$A$

$\gamma$ multiplicity

mass number $A$

$0,0$  $0,1$  $0,2$  $0,3$  $0,4$  $0,5$  $0,6$  $0,7$  $0,8$  $0,9$  $1,0$  $1,1$  $1,2$  $1,3$  $1,4$  $1,5$

$1E-4$  $1E-3$  $0,01$  $0,1$  $1$  $10$

$\bullet$ Billnert 2012 (100keV, 3ns)

$\bigcirc$ Verbinsky 1973 (140 keV, 10ns)

$\bigcirc$ FIFRELIN (100 keV, 3ns)

$\bigcirc$ Chyzh 2012 'Bayesian'

$\bigcirc$ Chyzh 2012 'SVD'

$\bullet$ Schmidt-Fabian 1988

$\bigcirc$ FIFRELIN

$\bigcirc$ Verbinsky 1973

$\bigcirc$ Billnert 2012

$\bullet$ Chyzh 2012 'Bayesian'

$\bullet$ Chyzh 2012 'SVD'

Average prompt gamma multiplicity as a function of pre-neutron mass

$0,0$  $0,1$  $0,2$  $0,3$  $0,4$  $0,5$  $0,6$  $0,7$  $0,8$  $0,9$  $1,0$  $1,1$  $1,2$  $1,3$  $1,4$  $1,5$

$0$  $1$  $2$  $3$  $4$  $5$  $6$  $7$  $8$  $9$  $10$  $11$  $12$  $13$  $14$  $15$

$M_{\gamma} / \text{MeV}$

$A$

$0$  $1$  $2$  $3$  $4$  $5$  $6$  $7$  $8$  $9$  $10$  $11$  $12$  $13$  $14$  $15$

$\gamma$ multiplicity

mass number $A$
Fission Observables: comparison with experiment

Average prompt neutron multiplicity as a function of pre-neutron fragment mass

\[ \overline{\nu}(A) \]

Average prompt gamma multiplicity as a function of pre-neutron fragment mass

\[ \overline{M}_\gamma(A) \]

Neutron average quantities

<table>
<thead>
<tr>
<th></th>
<th>( \overline{\nu}_L )</th>
<th>( \overline{\nu}_H )</th>
<th>( \overline{\nu} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nishio 2004</td>
<td>1.42</td>
<td>1.01</td>
<td>2.43 ± 0.03</td>
</tr>
<tr>
<td>FIFRELIN</td>
<td>1.41 ± 0.001</td>
<td>1.02 ± 0.001</td>
<td>2.43 ± 0.001</td>
</tr>
</tbody>
</table>

Gamma average quantities

<table>
<thead>
<tr>
<th></th>
<th>Threshold</th>
<th>( \Delta T )</th>
<th>( \langle \gamma/f \rangle )</th>
<th>( \langle E_{\gamma,\text{tot}} \rangle ) (MeV)</th>
<th>( \langle \varepsilon_\gamma \rangle ) (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oberstedt 2013</td>
<td>100 keV</td>
<td>5 ns</td>
<td>8.19 ± 0.11</td>
<td>6.92 ± 0.09</td>
<td>0.85 ± 0.02</td>
</tr>
<tr>
<td>FIFRELIN</td>
<td>100 keV</td>
<td>5 ns</td>
<td>8.04 ± 0.01</td>
<td>7.02 ± 0.01</td>
<td>0.875 ± 0.001</td>
</tr>
</tbody>
</table>

\( 235^U(n_{\text{th}},f) \)
Fission Observables: comparison with experiment

**Prompt fission neutron spectrum**

\[ N_y(E) \]

\[ ^{235}\text{U}(n_{th}, f) \]

<table>
<thead>
<tr>
<th><strong>FIFRELIN</strong></th>
<th>(\langle E \rangle)</th>
<th>(\langle V \rangle)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-HF (LDM)</td>
<td>2.102(2)</td>
<td>2.424(2)</td>
</tr>
<tr>
<td>(CGCM)</td>
<td>1.891(1)</td>
<td>2.444(1)</td>
</tr>
<tr>
<td>(CTM)</td>
<td>2.079(2)</td>
<td>2.397(2)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>FIFRELIN -W</strong></th>
<th>(\langle E \rangle)</th>
<th>(\langle V \rangle)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1.945(2)</td>
<td>2.430(3)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>JEFF-3.2</strong></th>
<th>(\langle E \rangle)</th>
<th>(\langle V \rangle)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2.03</td>
<td>2.42</td>
</tr>
</tbody>
</table>

- Micro data 1.974(2)
- Macro data 2.03

Ratio to Maxwellian (T=1.32 MeV)

- Hambsch 2010
- Starostov 1983
- Nefedov 1983
- Lajtai 1985
- JEFF-3.2
- CGCM/EGLO/KD
- CTM/EGLO/KD
- HFB/EGLO
- -W

O. LITAIZE  P(ND)^2-2 Perspectives on Nuclear Data for the Next Decade, 14-17 October, 2014, BIII, France
Fission Observables: comparison with experiment

Position of the structures at low energy is reproduced by the calculation

$^{235}\text{U}(n_{\text{th}},f)$

Prompt fission gamma spectrum

Lower strength in the calculation above 6 MeV?
Fission Observables: comparison with experiment

Average prompt gamma multiplicity as a function of pre-neutron fragment mass

\[ 239\text{Pu} \ (n_{\text{th}}, f) \]

\[ M_\gamma(A) \]

\[ N_\gamma(E) \]

<table>
<thead>
<tr>
<th></th>
<th>Threshold [keV]</th>
<th>( \Delta T ) [ns]</th>
<th>( M_\gamma ) [( \gamma/f )]</th>
<th>( \langle E^\text{tot} \rangle ) [MeV]</th>
<th>( \langle \epsilon_\gamma \rangle ) [MeV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Verbinski 1973</td>
<td>140</td>
<td>10</td>
<td>7.23</td>
<td>6.81 ± 0.03</td>
<td>0.94</td>
</tr>
<tr>
<td>FIFRELIN</td>
<td>140</td>
<td>10</td>
<td>7.19</td>
<td>6.81</td>
<td>0.95</td>
</tr>
</tbody>
</table>

**Prompt fission gamma spectrum**

O. Serot, O. Litaize, D. Regnier, Workshop Gamma-2, 24-26 sept. 2013

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Context

Models in FIFRELIN

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Beyond common observables

Perspectives
Beyond common observables

Resolution below 1.4 MeV: 5 keV

Gamma spectra
- per mass
- per charge
- per emitting fragment
- per multipolarity

$\gamma(E | A, Z, XL)$

$^{235}\text{U}(n_{th}, f)$
Influence of the maximum half life considered in the simulation

Useful for comparison with experiments (coincidence time window)

E_{level} = 266.83 keV
T_{1/2} = 2.0 ns

93\text{Rb}

Importance of the data available from nuclear structure
Sensibility of the PFGS to the initial spin distribution

- Increasing the initial spin of FF increases the PFGS in the low energy range (below 1 MeV).

\[ {}^{235}\text{U}(n_{\text{th}},f) \]

\[ <J>_L = 6 \hbar \]
\[ <J>_L = 9 \hbar \]
Beyond common observables

Noticeable difference observed between two models (among others) below 200 keV…

\(^{235}\text{U}(n_{th},f)\)

Differential spectra & multiplicities

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The responsible could have a mass around 93

The responsible could be Kr, Rb or Sr ...

Remember that due to neutron emission, the mass shown here is not the mass of the γ-emitter
Beyond common observables

- **This guy may be potentially guilty**
- **Experiment could help to choose between those two models.**
- **Theory could explain why.**

- **Not this one!**

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Isotopic yields $Y(A,Z)$

Beyond common observables

Around 400 nuclei calculated
Introduction

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Beyond common observables

Perspectives
Ongoing work

- Fission modes,
- Excitation energy sharing at scission,
- Multiple chance fission,
- Scission neutrons,

- Level Density, spin cut-off,
- Photon strength functions,
- Neutron transmission coefficients, ...

- Weisskopf / Hauser-Feshbach deexcitation models,
- Parallel computing
- Coupling codes, extended application area (detection, transport in reactors, heating, …)
**Isomeric ratio calculations**

152\textsuperscript{Eu} after thermal neutron capture

→ CIRENE measurements
→ Calculation: \( I_{\text{th}} = 0.21\% \)

- Experimental precision not sufficient. What about new facilities?
- Less sensitive to PSF
- Sensitive to LD

---

### 152\textsuperscript{Eu} (\( J^\pi = 3^+ \))

- FIFRELIN
- [1] \( \langle I_{\text{res}} \rangle = (36.4 \pm 3.7)\% \)
- [1] \( \langle I_{\text{th}} \rangle = 35.9\% \)

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![Graph showing isomeric ratio calculations for 152\textsuperscript{Eu} after thermal neutron capture.](image-url)

- EGLO
- SLO
- HF BCS + QRPA
- HFB + QRPA

---

\( \langle I_{\text{R}} \rangle = 37.0 \)

\( \langle I_{\text{R}} \rangle = 36.5 \)

\( \langle I_{\text{R}} \rangle = 36.6 \)

\( \langle I_{\text{R}} \rangle = 36.9 \)
Calculate a matrix of isomeric ratio in a \([ J, E^*, \pi]\) ensemble.

Simulation of fission gives Spin distribution after neutron emission \(P(J)\) and excitation energy after neutron emission \(P(E^*)\).

- Could be used to estimate isomeric ratio in fission and to select the optimal distribution.
- Find the best spin distribution that allows to reproduce ‘fine’ observables:
  - Yields of specific fragment pairs (Kr-Ba, …),
  - Population of well known 2\(^+\) states of even even nuclei (from EXILL campaign and FIPPS in a near future).

CEA/DEN - CEA/DSM – CNRS/LPSC collaboration
Improve Modeling

- Using tabulated ‘microscopic’ ingredients
  - HFB +QRPA compared to SLO, EGLO, MLO … a clash of clans ? … not sure.

- Accounting for energy partition at scission from microscopic calculations provided by SPY code (PES + HFB D1S) to estimate the energy available for particle emission

<table>
<thead>
<tr>
<th>Input / Output</th>
<th>Today</th>
<th>Next decade ?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass and Kinetic Energy distributions before neutron emission</td>
<td>• Reconstructed from experimental post neutron distributions, • Calculated from fission mode parameters</td>
<td>• HFB calculations (CEA/DAM), • Langevin equations (LANL, LLNL), • Provided by GEF code (CENBG), • New experimental facilities</td>
</tr>
<tr>
<td>Charge distribution</td>
<td>• UCD+ΔZ+EOZ+EON.</td>
<td>• New experimental facilities (FALSTAFF, FIPPS, SOFIA, SPIDER…)</td>
</tr>
<tr>
<td>Spin distribution</td>
<td>• Various spin cut-off formula • Check with PFGS, PFGM</td>
<td>• Check with isomeric ratio • Check with yields of specific fragment pairs (EXILL)</td>
</tr>
<tr>
<td>Excitation energy sharing</td>
<td>• $R_T(A)$</td>
<td>• HFB from SPY code (CEA/DAM/DSM) • Influence of scission neutrons</td>
</tr>
<tr>
<td>De-excitation process</td>
<td>• CGCM-CTM/EGLO-SLO/KD</td>
<td>• CGCM-CTM/EGLO-SLO/KD + HFB/QRPA, deformed OMP, …</td>
</tr>
<tr>
<td>Observables</td>
<td>• Yield, spectrum, multiplicity from estimators</td>
<td>• Same + other from ‘root tree’, angular correlations, …</td>
</tr>
</tbody>
</table>