Recent Developments in Pre-equilibrium and De-excitation Models in Geant4

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The IAEA Benchmark on Spallation Reactions

- The benchmark was organized under the auspices of IAEA.
- To assess the prediction capabilities of the spallation models.
- To understand the reason for the success or deficiency of the models.
- To reach a consensus, if possible, on some of the physics ingredients.

Geant4 has participated with two cascade models:

- Binary Cascade
- Bertini cascade
Geant4 Low Energy Hadronic Models

- **Binary Cascade:**
  - a time-dependent model which depends as little as possible on parameterization and therefore can be expected to be more predictive
  - is an *in house* development, including its own precompound and evaporation models.

- **Bertini Cascade:**
  - it came from the INUCL code which was intended as an all-inclusive model
  - it came with its own pre-compound and de-excitation models, which are not very different in origin from those in Binary, but the implementations are different.

- **INCL/ABLA:**
  - IAEA benchmark

- **CHIPS (Chiral Invariant Phase Space)**

- **QMD (Quantum Molecular Dynamics Model)**
After Binary Cascade stage *native* pre-equilibrium follows

Native pre-equilibrium de-excitation model in Geant4 is a version of standard *exciton model*.

**Competitor processes:**

**Internal transition rates:**
- CEM (Cascade Exciton Model, Gudima et al). Default
- Blann-Machner's parameterization.

**Particle emission rates:**
- Nucleon emission in standard exciton formulation.
- Complex particle emission (d,t, $^3$He, $^4$He) from CEM.
Pre-equilibrium: new inverse reaction cross sections

**Key ingredient:** Inverse reaction cross sections play a mayor role in the calculation of (competing) emission probabilities.

**Theory driven old parameterization** (Dostrovski et al, 1959) (kept as option)

**NEW:** More realistic parameterization of reaction cross sections *(after release 9.2)*

- Chatterjee at al: Calculated with global optical model potentials, in turn fitted to reproduce available experimental data
- Kalbach's retuning (PRECO code)
- Wellisch's parameterization of proton reaction cross sections by direct fitting to experimental data
- **Default option** combines the best combination of inverse cross sections (Wellisch's parameterization for protons and Kalbach's one for the rest)
The transition from pre-equilibrium to equilibrium de-excitation should take place when:

\[ \lambda_+(p, h, E) = \lambda_-(p, h, E) \]  

(1)

Which can be roughly estimated as:

\[ n_{eq} = \sqrt{2gE^*} \]  

(2)

(Initially in G4PreCompoundModel)

NOW the more physically consistent condition (1) has been implemented by means of the appropriate algorithm.
Pre-equilibrium

G4BinaryCascade

G4PreCompoundModel::ApplyYourself

G4HadProjectile + G4Fragment

E_{inc} > 45 MeV

G4Fragment

G4BinaryCascade::ApplyYourself

G4BinaryCascade::Propagate

G4PreCompoundModel::DeExcite

A > 4

N_{excitons} < N_{equilibrium}

P_{emission} < P_{transition}

G4PreCompoundEmission::PerformEmission

G4PreCompoundTransition::PerformTransition

G4ExcitationHandler::BreakItUp

G4ReactionProductVector

G4HadFinalState
Equilibrium De-excitation

Five processes are considered:

**Alternates:**
- **Fermi Breakup**, for $Z<9$, $A<17$ (Botvina et al)
- **Statistical Multifragmentation**, for $E^*/A > 3$ MeV (Botvina et al)

**Competitors:**
- **Fission** (Bohr-Wheeler model + Amelin prescript.)

**Particle Evaporation:**
- Evaporation Model (Weisskopf-Ewing) : n, p, d, t, 3He, alphas)
- Generalized Evaporation Model (Furihata) : $Z<13$, $A<29$.

**Photon Evaporation:**
- Discrete (tabulated $E_1$, $M_1$, $E_2$)
- Continuum (GDR strength)
Equilibrium De-excitation

G4ExcitationHandler

G4Fragment

G4ExcitationHandler::BreakItUp

De-excitation first stage

A>4

A<Amax & Z<Zmax

G4FermiBreakUp::BreakItUp

G4Evaporation::BreakItUp

E*>Emin

G4StatMF::BreakItUp

De-excitation loop

A<5 || Nsec=1

Nsec>1

G4Evaporation::BreakItUp

E*>0

Nsec>1

G4FermiBreakUp::BreakItUp

Nsec=1

G4PhotonEvaporation::BreakItUp

A>1 & E*>0.1 eV

G4ReactionProductVector
Situation in AccApp'09 Conference

(related to geant4.9.2p01 official release results)

- No *ad hoc* tuning of level density parameter ratio $a_{\text{fis}}/a_{\text{evap}}$. (Preliminary trials show that it is critical, as reported in previous works).

- No *soft transition* from pre-equilibrium (i.e. increment of equilibrium at the expenses of pre-equilibrium).

- Very important: Parameters tuned in a "model suite" shouldn’t be assumed to work in a different *environment*, i.e. with different *coupled* models.

Ad hoc tuning of parameters was clearly necessary in order to reproduce fission data. *(Done in next release geant4.9.3)*
Progress after AccApp'09 Conference

(included in geant4.9.3 official release)

- Transition probabilities at pre-equilibrium (exciton model) have been calculated according to CEM

- **NEW**: Combined WE-GEM model has been implemented in de-excitation (allows description of IMF production)

- First retuning of parameters:
  - Tuning of level density parameter ratio $a_{fis}/a_{evap}$.
  - Tuning of the width of symmetric component of fission fragment distribution.
RESULTS

(geant4.9.3)
Neutron production at 65 MeV

Elastic scattering has been included

\( n + Fe \)
Neutron production at 1200 MeV

\( p + Pb \rightarrow n + X \) at 1200 MeV

E (MeV)

\( d\sigma / dE \) (mb/sr/MeV)
Proton production at 1200 MeV

$p + Ta \rightarrow p + X$ at 1200 MeV

$\theta = 30^\circ$

$\theta = 75^\circ$

$\theta = 100^\circ$

$\theta = 150^\circ$

$\frac{d\sigma}{d\Omega}/dE$ (mb/sr/MeV)

E (MeV)

BIC
BERT
Data
Underestimation at forward angles: evidence of direct processes
Deuteron production at 1200 MeV
Alpha production at 1200 MeV

\[ p + Au \rightarrow \alpha + X \text{ at 1200 MeV} \]
Isotopic distribution at 1 GeV

Fe+p @ 1GeV/A

after GEM inclusion

geant4.9.2p01

geant4.9.3

NOW
### Isotopic distribution at 1 GeV

<table>
<thead>
<tr>
<th>Isotope production (mb)</th>
<th>Pb + H → X at 1000 MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pb + p @ 1GeV/A</td>
<td>geant4.9.2p01</td>
</tr>
<tr>
<td>U + p @ 1GeV/A</td>
<td>geant4.9.2p01</td>
</tr>
</tbody>
</table>

#### Data vs. Simulation

- **geant4.9.2p01**: Pb+p @ 1GeV/A
- **geant4.9.3**: U+p @ 1GeV/A

**After GEM inclusion**

- **DATA**
- **BIN**
- **BIN1**
- **BERT**

**Isotopic distribution**

- **Pb+p @ 1GeV/A**
- **U+p @ 1GeV/A**

**Note**

- The data is compared with simulations using versions geant4.9.2p01 and geant4.9.3, showing the impact of GEM inclusion.
Isotopic distribution at 1 GeV

Pb+p @ 1 GeV/A

geant4.9.2p01

after GEM inclusion

geant4.9.3

NOW

U+p @ 1 GeV/A

geant4.9.2p01

after GEM inclusion

geant4.9.3

NOW
**Soft cut-off** transition from pre-equilibrium partially cures this problem, **but**, in our case, it worsens performance at fission and at pre-equilibrium

- A new version of the **soft cut-off** algorithm with $n_{eq}$ strictly calculated according to

  $$\lambda_+(p, h, E) = \lambda_-(p, h, E)$$

- The **diffusivity** of the transition has been drastically reduced

No chance for a **global set of parameters** (optimal for any combination of models)

- Different sets of fission parameters were fitted for each choice (with/without soft cut-off).
- "soft cut-off" ON
- Fission parameters have been fitted
- The situation at pre-equilibrium is quite the same
- CPU time increase (factor ~ 1.5)
Conclusions

- The review of the native pre-equilibrium and de-excitation models of Geant4 recently performed has led to an overall satisfactory reproduction of experimental data set of IAEA nuclear spallation reactions benchmark thanks to recently made improvements to:
  - Pre-equilibrium
  - Evaporation
  - Fission

- Additional development work is in progress:
  - Transition to de-excitation and fine parameter tuning (specific interest: spallation reactions)
  - Fermi Breakup and Photon Evaporation (specific interest: Hadrontherapy)
  - CPU performance and code cleanup (interest: all applications)
Thanks for your attention