Improvements and developments of physics models in PHITS for radiotherapy and space applications

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1. PHITS - Short Introduction

2. PHITS - Improved Models
   2.1 A-A Total Reaction Cross Sections
   2.2 Kurotama Hybrid $\sigma_R$ Model
   2.3 Intra-Nuclear Cascade Code with Distorted Wave Born Approximation
   2.3 Relativistic JAERI Quantum Molecular Dynamics (JQMD-2)
   2.4 Statistical Multi-Fragmentation Model (SMM)

3. Summary
What is PHITS?

Particle and Heavy Ion Transport code System

**Capability**

Transport and collision of all particles over wide energy range

- Transport in 3D phase space with magnetic field & gravity
- Collision of neutron, proton, meson, baryon, electron, photon, heavy ions
- Energy range: $10^{-5}$ eV to 100 GeV/u

**All-in-one-Package**

All contents of PHITS (source files, binary, data libraries, graphic utility, etc.) are fully integrated in one package

- OECD/NEA Databank (Europe)
- RSICC (USA, Canada)
- RIST (Japan)

**Applications**

- Accelerator Design
- Radiation Therapy & Protection
- Space & Geoscience
**Map of Models used in PHITS**

<table>
<thead>
<tr>
<th>Neutron</th>
<th>Proton, Pion (other hadrons)</th>
<th>Nucleus</th>
<th>Muon</th>
<th>e⁻ / e⁺</th>
<th>Photon</th>
</tr>
</thead>
<tbody>
<tr>
<td>200 GeV</td>
<td>Intra-nuclear cascade (JAM) + Evaporation (GEM)</td>
<td>100 GeV/n</td>
<td>100 GeV</td>
<td>100 GeV</td>
<td>100 GeV</td>
</tr>
<tr>
<td>3.0 GeV</td>
<td>Intra-nuclear cascade (INCL4.6) + Evaporation (GEM)</td>
<td>Quantum Molecular Dynamics (JQMD-2) + Virtual Photonic Nuclear Data Library (JENDL-4.0)</td>
<td>Atomic Data Library (EEDL / ITS3.0 / EPDL97) or Atomic Data Library JENDL-4.0 / EPDL97 or EGS5</td>
<td>Atomic Data Library JENDL-4.0 / EPDL97 or EGS5</td>
<td>Atomic Data Library JENDL-4.0 / EPDL97 or EGS5</td>
</tr>
<tr>
<td>20 MeV</td>
<td>Nuclear Data Library (JENDL-4.0)</td>
<td>Ionization SPAR or ATIMA</td>
<td>200 MeV</td>
<td>1 keV</td>
<td>2 MeV</td>
</tr>
<tr>
<td>10⁻⁵ eV</td>
<td>1 MeV</td>
<td>10 MeV/n</td>
<td>100 MeV</td>
<td>1 keV</td>
<td>1 keV</td>
</tr>
</tbody>
</table>

**Event generator mode:**
Specify all secondary charged particles produced from low-energy neutron interaction

Switching energies can be changed in the input file of PHITS
The $\sigma_R$ decides the collision distance $d$?

Where will the reaction occur?
When the energy increases, Coulomb shielding decreases
-> cross section increases to be larger than the geometrical model
When the energy increases even more, the cross section decreases until it is $\sim \pi r_o^2 (R_p + R_t)^2$ assuming a simple geometrical model with spherical nucleus.
Above the threshold of $\pi$ production, the inelastic channels are open for the nucleon-nucleon interactions, which lead to a slight increase of the cross section.
After the resonances, the cross section are roughly independent of the projectile energy.
The "Kurotama*" $\sigma_R$ is a "black sphere*,**" formula for the reaction cross section for protons on stable nuclei, as a function of $A$ and $E_p$:

$$\sigma_R = \pi a_0^2 \left( 1 + \frac{\Delta a}{a_0} \right)^2$$

$a = "black sphere radius", which is determined from $2pa \sin(\theta_M/2)$, where:

- $p =$ proton incident momentum in the center-of-mass frame
- $\theta_M =$ first peak angle for the measured diffraction in proton–nucleus elastic scattering

$a_0 = "the black sphere radius"$ at $E_p = 800$ MeV

$\Delta a$ is the deviation of $a$ from $a_0$ at given $E_p$ above 100 MeV

This formula can easily be extended to nucleus-nucleus reactions by using $\pi (a_P + a_T)^2$, where $a_P (a_T)$ denotes the BS radius of a projectile (target).

"Hybride Kurotama" $\sigma_R$ model


Hybrid Kurotama: the BS model was connected to the parameterization developed by Tripathi et al. at 400 MeV/nucleon for $p + \text{He/He} + p$, $\text{He} + \text{nucleus}$ reactions and at 115 MeV/nucleon for all other reactions.
"Hybride Kurotama" $\sigma_R$ model


Included in PHITS !!!
New INC models can consider the production of high-energy light fragments.

Double differential cross sections of Pb($p,n$) and Fe($p,d$) reactions calculated using PHITS employing JAM, INCL4.6, or INC-ELF.

INCL4.6 is selected as the default model for simulating not only nucleon-induced but also $d$, $t$, $^3$He and $\alpha$-induced nuclear reactions.
For the design of radiation shielding, it is important to adequately describe the reaction processes induced by neutrons as well as deuterons.

A new method for nuclear reaction modeling that combines INCL with DWBA has therefore been developed.

Using a combination of INCL and DWBA is based on the assumption that the nuclear reaction processes from each model can be distinguished spatially.

The “direct process” described by DWBA occurs at the surface of the target nucleus, whereas the cascade processes by INCL generally occur inside the nucleus.
DWBA of two transfer reactions with the deuteron incident, (d, n) and (d, p) is performed using the TWO-FNR code.

The direct process is a coherent process, while the cascade processes are basically incoherent.

The neutrons issued from the first process generally have a higher energy than the incident energy, whereas a large majority of the neutrons generated by the cascade have lower energies than the incident energy.

In a PHITS simulation, the occurrence of a DWBA event is randomly determined according to the ratio of the DWBA cross section ($\sigma_{\text{DWBA}}$) to the $\sigma_R$. The $\sigma_{\text{DWBA}}$ is calculated by integrating over emitted angles and summing over reaction channels of angular differential cross sections (ADXs).
Therefore, we have developed a new method for nuclear reaction modeling that combines INCL [3,33,34] with DWBA [6]. Using a combination of INCL and DWBA is based on the assumption that the nuclear reaction processes from each model can be distinguished spatially. The "direct process" described by DWBA occurs at the surface of the target nucleus, whereas the cascade processes by INCL generally occur inside the nucleus. The direct process is a coherent process, while the cascade processes are basically incoherent. The neutrons issued from the first process generally have a higher energy than the incident energy, whereas a large majority of the neutrons generated by the cascade have lower energies than the incident energy.

Angular dependence of double differential cross sections of emitted neutrons from 10 MeV $^9\text{Be}(d,xn)$
Solid red lines - calculated by the combined method
Closed circles - experimental data* measured with a 0.015 mm thin target.

JAERI Quantum Molecular Dynamics (JQMD-2)

JQMD

Nucleus was unstable $\rightarrow$ Spurious decay and true reactions were mixed

Decay during time evolution

Decay by frame transform

Peripheral collision

JQMD-2

Reject unstable states

"ground state" screening

Interaction corrected for frame

Interaction

Spurious decay is excluded

Peripheral collision

Inhibition of spurious decay $\rightarrow$ New version can consider peripheral collisions
Statistical Multi-fragmentation Model (SMM)

Intra-Nuclear Cascade (JAM / INCL4.6 / JQMD-2) → Excited Nucleus ($\leq 2$ MeV/u) → Evaporation GEM → Fission

Simulation Procedure of Nuclear Reaction in PHITS

Production cross sections of $^{24}$Na and $^{75}$Se from Pb bombarded by C ions

(A) $^{24}$Na

(B) $^{75}$Se

Ogawa et al.
Simulation Procedure of Nuclear Reaction in PHITS

Intra-Nuclear Cascade
JAM / INCL4.6 / JQMD-2

Excited Nucleus (> 2 MeV/u)

Evaporation
GEM

Production cross sections of $^{24}$Na and $^{75}$Se from Pb bombarded by C ions.

Accuracy of the estimation of intermediate-mass-fragment yields are improved!

Ratio of simulated fragmentation cross sections for the reactions of $^{12}\text{C} + \text{Pb}$ to measured cross sections*, averaged over 50–100 MeV/u

* T. Ogawa et al. NIM A 723 (2013) 36.
Statistical Multi-fragmentation Model (SMM)

The graph shows the ratio of simulated fragmentation cross sections for the reactions of $^{nat}$Pb($^{12}$C,x) to measured cross sections*, averaged over 100-400 MeV/u.

* T. Ogawa et al. NIM A 723 (2013) 36.
• **Nuclear data libraries** are necessary for simulating low-energy neutrons
• Cross sections of low-energy neutron significantly depend on shell structure

• PHITS Readable Format of nuclear data: **ACE format** (same as MCNP)
• Libraries: JENDL-4.0
• ENDF, LA150, JENDL-HE file (optional)

Neutron reaction cross sections of $^{112}$Cd and $^{113}$Cd taken from JENDL4.0
1. Total reaction cross section model and the mean free paths of the transported particles have been improved.
   - Kurotama Hybrid $\sigma_R$ model

2. Production of nucleon and d, t, $^3$He and $^4$He induced reactions have been improved by inclusion of two new Intra-Nuclear Cascade models.
   - Intra-Nuclear Cascade of Liège
   - INC-ELF, developed at Kyushu university

3. To better reproduce production of light fragments from high multiplicity events a combination of
   - JQMD-2/INCL, SMM and the evaporation model GEM

has been included in PHITS.
4. A new approach to describe the n spectra of deuteron-induced reactions in the Monte Carlo simulations has been developed.

- INCL + DWBA

5. An ENSDF-based de-excitation model EBITEM is included.

6. Photo-nuclear reactions up to 1 GeV are included.

7. Statistical uncertainty estimation has been modified, nuclear and data libraries revised, and a tally to interface PHITS with the radioactivity estimator DCHAIN-SP has been established.

8. The electromagnetic transport algorithm has also been improved and user-defined tally functions introduced.
Thank you very much for your attention!!