Development and implementation of new Geant4 QMD model and its validation

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Geant4 Hadronic Physics Working Group Meeting,
Aug. 16th, 2023
Collaborators

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Osaka University

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University of Wollongong

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University of Wollongong

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The Australian National University
The QMD model is a quantum extension of the classical molecular-dynamics model and can describe hadronic processes, especially inelastic processes, in Geant4.

Collision between $^{12}\text{C}$
Development of more accurate QMD model

Introduction

1. Making nuclei
2. Setting
3. Propagation
4. Clustering

Three improvements

1. Skyrme interaction
2. $\alpha$-cluster structure
3. QMD model Parameter optimization

Three improvements

1. Skyrme interaction
2. $\alpha$-cluster structure
3. QMD model Parameter optimization

<table>
<thead>
<tr>
<th>Parameter</th>
<th>IQMD$^a$ (G4QMD)</th>
<th>SLy$^b$</th>
<th>SkM*</th>
<th>SII$^f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$ [MeV]</td>
<td>$-219.4$</td>
<td>$-297.82$</td>
<td>$-318$</td>
<td>$-122.921$</td>
</tr>
<tr>
<td>$J$ [MeV]</td>
<td>$165.3$</td>
<td>$219.21$</td>
<td>$249.5$</td>
<td>$55.543$</td>
</tr>
<tr>
<td>$g_1$ [MeV/mb]</td>
<td>$24.569$</td>
<td>$23.86$</td>
<td>$18.286$</td>
<td></td>
</tr>
<tr>
<td>$g_2$ [MeV/mb]</td>
<td>$97.66$</td>
<td>$90.857$</td>
<td>$6.439$</td>
<td></td>
</tr>
<tr>
<td>$C_1$ [MeV]</td>
<td>$25$</td>
<td>$32$</td>
<td>$32$</td>
<td>$32$</td>
</tr>
<tr>
<td>$\omega_1$ [fm$^{-1}$]</td>
<td>$0.08$</td>
<td>$0.08$</td>
<td>$0.08$</td>
<td></td>
</tr>
<tr>
<td>$\gamma$</td>
<td>$4/3$</td>
<td>$7/6$</td>
<td>$7/6$</td>
<td>$2$</td>
</tr>
<tr>
<td>$\delta$</td>
<td>$5/3$</td>
<td>$5/3$</td>
<td>$5/3$</td>
<td></td>
</tr>
<tr>
<td>$\Delta_{II} [fm^{-4}]$</td>
<td>$0.168$</td>
<td>$0.160$</td>
<td>$0.165$</td>
<td>$0.1452$</td>
</tr>
<tr>
<td>$E_0$ [MeV]</td>
<td>$-16.00$</td>
<td>$-15.97$</td>
<td>$-15.77$</td>
<td>$-15.83$</td>
</tr>
<tr>
<td>$K_0$ [MeV]</td>
<td>$237.8$</td>
<td>$230.2$</td>
<td>$216.8$</td>
<td>$355.9$</td>
</tr>
</tbody>
</table>

$\phi_i(r) \equiv \frac{1}{(2\pi L)^{3/4}} \exp\left(-\frac{(r - r_i)^2}{4L} + \frac{i}{\hbar} r \cdot \mathbf{p}_i\right)$
**Water Phantom**

### Materials and Methods

$^{12}\text{C}, 400\text{MeV/u} \rightarrow \text{Water}$


**Light Ion QMD (LIQMD)**
Angular distribution

Energy distribution

$^{12}\text{C}, 400\text{MeV/u} \rightarrow \text{Water}$
Implementation
# Implementation of LIQMD

## Materials and Methods

<table>
<thead>
<tr>
<th>qmd</th>
<th>Source code</th>
<th>light_ion_qmd</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>source/processes/hadronic/models/</td>
<td></td>
</tr>
<tr>
<td>G4QMDReaction</td>
<td>G4LightIonQMDReaction</td>
<td></td>
</tr>
<tr>
<td>G4QMDMeanField</td>
<td>G4LightIonQMDMeanField</td>
<td></td>
</tr>
<tr>
<td>G4QMDCollision</td>
<td>G4LightIonQMDCollision</td>
<td></td>
</tr>
<tr>
<td>G4QMDParameters</td>
<td>G4LightIonQMDParameters</td>
<td></td>
</tr>
<tr>
<td>G4QMDNucleus</td>
<td>G4LightIonQMDNucleus</td>
<td></td>
</tr>
<tr>
<td>G4QMDGroundStateNucleus</td>
<td>G4LightIonQMDGroundStateNucleus</td>
<td></td>
</tr>
<tr>
<td>G4QMDSystem</td>
<td>G4LightIonQMDSystem</td>
<td></td>
</tr>
<tr>
<td>G4QMDParticipant</td>
<td>G4LightIonQMDParticipant</td>
<td></td>
</tr>
</tbody>
</table>
Implementation of LIQMD

Materials and Methods

qmd

Source code
source/processes/hadronic/models/

use

Physics constructor
source/physics_lists/constructors/ions/

light_ion_qmd

G4IonLightIonQMDPhysics
(or G4LightIonQMDPhysics)
Implementation of LIQMD

Materials and Methods

qmd

Source code
source/processes/hadronic/models/

use

G4IonQMDPhysics

Physics constructor
source/physics_lists/constructors/ions/

use

Shielding

Physics list
source/physics_lists/lists/

light_ion_qmd

G4IonLightIonQMDPhysics
(or G4LightIonQMDPhysics)

Shielding, QGSP_BIC_AllHP
Add an option (G4bool useLightIonQMD)
Implementation of LIQMD

Materials and Methods

- qmd
  - Source code
    - source/processes/hadronic/models/
    - use
  - Physics constructor
    - source/physics_lists/constructors/ions/
    - use
  - Physics list
    - source/physics_lists/lists/
    - use
  - Example or test
    - examples/extended/medical/geant4-dev/tests/
    - use
  - G4IonLightIonQMDPhysics
    - (or G4LightIonQMDPhysics)
    - Shielding, QGSP_BIC_AllHP
    - Add an option (G4bool useLightIonQMD)
  - test61
    - Create new test or macro file for existing test

light_ion_qmd
Additional validation
Table I. Target characteristics.

<table>
<thead>
<tr>
<th>Target</th>
<th>Thickness (in µm)</th>
<th>Density (in g cm⁻²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C, CH₂</td>
<td>500</td>
<td>0.0411</td>
</tr>
<tr>
<td>Al 200</td>
<td>150</td>
<td>0.0540</td>
</tr>
<tr>
<td>Ti 125</td>
<td>200</td>
<td>0.0576</td>
</tr>
<tr>
<td>C 5</td>
<td>500</td>
<td>0.0642</td>
</tr>
</tbody>
</table>

The thicknesses of the silicon detectors were 20 cm, 21 cm, and 21 cm, respectively. To prevent interaction of the charged particles with the target, a 10 cm thick CsI(Tl) scintillator was placed behind the target.

Thin Targets

Targets: ¹H, ¹²C, ¹⁶O, ²⁷Al, ⁴⁸Ti

Materials and Methods

Fragments: ¹,²,³H, ³,⁴,⁶He, ⁶,⁷Li, ⁷,⁹,¹⁰Be, ⁸,¹⁰,¹¹B, ¹⁰,¹¹,¹²C

Beam: ¹²C, 94.6 ± 0.09 MeV/A


E600 experiment at the Grand Accelerateur National d’Ions Lourds (GANIL) facility.
\[ \frac{d\sigma}{d\theta} \text{ [b sr}^{-1}] \]

\[ \theta \text{ [deg]} \]

Target: \( ^1\text{H} \), \( ^{12}\text{C} \), \( ^{16}\text{O} \), \( ^{27}\text{Al} \), \( ^{48}\text{Ti} \)

\[ \text{Geant4 Version 11.1.1} \]
\[ \frac{d\sigma}{d\Omega} [\text{b sr}^{-1}] \]

**Target**

- $^1\text{H}$
- $^{12}\text{C}$
- $^{16}\text{O}$
- $^{27}\text{Al}$
- $^{48}\text{Ti}$

**Fragment**

- $^{10}\text{Be}$
- $^{10}\text{C}$
- $^{11}\text{C}$

**Graphs**

- $^{1\text{H}}(^{12}\text{C},^{10}\text{Be})$ vs $\theta$ [deg]
- $^{1\text{H}}(^{12}\text{C},^{10}\text{Be})$ vs $\theta$ [deg]
- $^{1\text{H}}(^{12}\text{C},^{10}\text{Be})$ vs $\theta$ [deg]
- $^{1\text{H}}(^{12}\text{C},^{10}\text{Be})$ vs $\theta$ [deg]
- $^{1\text{H}}(^{12}\text{C},^{10}\text{Be})$ vs $\theta$ [deg]

**Legend**

- **QMD**
- **LIQMD**
- **Exp.**

**Geant4 Version 11.1.1**
Depth-Dose Curve

Materials and Methods

- Recording the energy deposition to each voxel by Command-based scoring.

Simulation geometry (Unit : mm)

Positron-emitting nucleus Yield

Materials and Methods


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Simulation and analysis geometry (Unit : mm)

- Beam: 1730 mm
- Gelatin phantom: 380 mm
- Nozzle: 100 mm
- Proportional counter: 100 mm
- Ion beam path: 1.5 mm

Recording the number of decaying positron-emitting nuclei in each voxel at the initial time.

\[
Y_0(z) = f_{\text{Norm}} \frac{(G \ast \tilde{A}_0)(z)}{\lambda}
\]

Summary and Future plan

- We have verified the QMD especially for light ions and are considering to implement it as “Light Ion QMD” in Geant4.

- Currently, the final confirmation before the merge request is underway.

- We have verified the performance of Light Ion QMD with some experimental data and confirmed that it is as good as or better than the conventional QMD model, at least in light ion beams and targets.