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New native QMD code in Geant4

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Recently the number of hadron therapy facilities has been increasing rapidly. Some of them are designed for heavy ions and need a tool to simulate the passage of ions through matter. As well, the space engineering field requires good estimates of device damage caused by bombarding ions in cosmic rays. As a result, demands for detailed simulations of nucleus-nucleus interactions have increased. Quantum Molecular Dynamics (QMD) is the quantum extension of the classical molecular-dynamics model and is widely used to analyze various aspects of heavy ion reactions, especially for many-body processes, in particular the formation of complex fragments. A new C++ version of the QMD code has been developed for the Geant4 toolkit. Derivation of equations of motion and production of initial "ground state" nuclei are based on JQMD and R-JQMD. Recently proposed Lorentz covariant kinematics treatment in R-JQMD is also included. Final states of two-body collisions are calculated by the same scatter class which the Binary Cascade model uses. After the termination of the time evolution of QMD system, cluster identification carry out and identified clusters are regarded as a excited fragment nucleus and they are passed to excitation model in Geant4. Validation results represent a significant improvement over current Geant4 nucleus-nucleus collision models.

KEYWORDS: Quantum Molecular Dynamics, Monte Carlo, event generator

I. Introduction

Geant4[1)] is a software toolkit for the simulation of the passage of particles through matter. It is widely used in a variety of application domains, including high energy physics, nuclear physics, astrophysics, space engineering and medical physics. Some of these domains have a strong requirement of nucleus-nucleus interactions in their simulation. Geant4 provides Binary Light Ion Reaction model and Wilson Abrasion and Ablation models for those interactions. The former model is an extension of the Binary Cascade model[2)] in Geant4. The Wilson Abrasion model is a simplified macroscopic model based largely on geometric arguments at the cost of accuracy and nuclear ablation has been developed to provide a better approximation for the final nuclear fragment from an abrasion interaction. A further way to simulate ion transportation in Geant4 is to use an interface to well-established nucleus-nucleus reaction code[3)]. The adoption of object-oriented technology and following an iterative-incremental software process within Geant4 makes it easy to create such an interface. However the Binary Light Ion Reaction Model has a limitation for applicable nuclei and the prediction power of Wilson Abrasion and Ablation model does not always satisfy user requirements. The interfacing method forces additional effort to the user. The demand for a native Geant4 model which supports all types of nucleus with better prediction power was increased, and hence a new Quantum Molecular Dynamics (QMD) model[4)] model was developed for the Geant4 in response to these requests.

In this paper, we will explain the Binary Light Ion Reaction model. First several limitations of this approach will be discussed and then features of QMD model will be introduced in connection to these limitations. The validation plots of the new model will be shown in comparison to the results of Binary Light Ion Reaction model. Finally we will draw some conclusions.

II. Binary Light Ion Reaction Model in Geant4

This is an extension of Binary Cascade model for light ion reactions. The Binary Cascade model is a hybrid model between classical cascade code and the QMD description. In this model, a detailed 3-dimensional nucleus is created and participant particles will be transported inside the nucleus having exclusively binary scattering with internal nucleons. It is similar to QMD in that each participant particle is seen as Gaussian wave packet and the total wave function is assumed to be the direct product of the participants. The equations of motion are derived from the wave function and they have same structure as with classical Hamilton equations. However the Hamiltonian is calculated from the simple time-independent optical potential in the Binary Cascade. A participant particle of the Binary Cascade is either a primary particle including nucleons in the projectile nucleus or particles generated or scattered in the cascade and only the participant particles are propagated in the nucleus. Furthermore, scattering between participant particles is not taken into account. This is one of the reasons that using the model for a heavy ion reaction, is not recommended. Binary collisions of participant particles with the residual nucleus are checked by Pauli's exclusion principle and some of them will be therefore forbidden. Decays of the participating resonance are included and the principle also applied to them. The participant particle is tracked until a reaction, decay,

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escape from or capture by the nucleus occurs. After this cascading calculation, the residual nucleus is investigated and passed to the low energy models in Geant4 for further particle emissions. Completed information about the Binary Cascade model is available from the reference[2].

III. New Native QMD Model in Geant4

QMD is the quantum extension of the classical molecular dynamics model and is widely used to analyze various aspects of heavy ion reactions, especially for many-body processes, and in particular the formation of complex fragments. In the previous section, we mentioned several similar and dissimilar points between Binary Cascade and QMD. There are three major differences between them:
1) The definition of a participant particle, 2) The potential term in the Hamiltonian and 3) Participant-participant interactions.

At first, we will explain how they are each treated in QMD. The entire nucleons in the target and projectile nucleus are considered as participant particles in the QMD model. Therefore each nucleon has its own wave function, however the total wave function of a system is still assumed as the direct product of them. The potential terms of the Hamiltonian in QMD are calculated from the entire relation of particles in the system, in other words, it can be regarded as self-generating from the system configuration. On the contrary to Binary Cascade which tracks the participant particles sequentially, all particles in the system are tracked simultaneously in QMD. Along with the time evolution of the system, its potential is also dynamically changed. As there is no criterion between participant particle and others in QMD, participant-participant scatterings are naturally included. Therefore QMD accomplishes more detailed treatments of the above three points, however with a cost of computing performance.

The basic assumption of QMD is that each nucleon state is represented by a Gaussian wave function of width L,

$$\varphi_i(\mathbf{r}) \equiv \frac{1}{(2\pi L)^{3/4}} \exp\left(-\frac{(r-r_i)^2}{4L} + \frac{i}{\hbar} r \cdot p_i \right) \tag{1}$$

Where r_i and p_i represent the center values of position and momentum of the i^{th} particle. The total wave function is assumed to be a direct product of them,

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) \equiv \prod_i \varphi_i(r_i) \tag{2}$$

Equations of the motion of particle derived on the basis of the time dependent variation principal as

$$\dot{r}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial r_i} \tag{3}$$

where H is the Hamiltonian which consists particle energy including mass energy and the energy of the two-body interaction.

However, further details in the prescription of QMD differ from author to author and JAERI QMD (JQMD) [5] is selected as a basis for our model. In this model, the Hamiltonian is

$$H = \sum_i \sqrt{m_i^2 + p_i^2} + \hat{V} \tag{4}$$

A Skyrme type interaction**,** a Coulomb interaction, and a symmetry term are included in the effective Potential ($\hat{V}$**)**. The relativistic form of the energy expression is introduced in the Hamiltonian. The interaction term is a function of the squared spatial distance:

$$R_{ij} = (R_i - R_j)^2 \tag{5}$$

This is not a Lorentz scalar. In Relativistic QMD (RQMD) [6], they are replaced by the squared transverse four-dimensional distance,

$$-q_{Tij}^2 = -q_{ij}^2 + \frac{(q_{ij} \cdot p_{ij})^2}{p_{ij}^2} \tag{6}$$

q_{ij} is the four-dimensional distance and p_{ij} is the sum of the four momentum. In JQMD they change the argument by the squared distance in center of mass system of the two particles,

$$\tilde{R}_{ij}^2 = R_{ij}^2 + \gamma_{ij}^2 (R_{ij} \cdot \beta_{ij})^2 \tag{7}$$

with

$$\beta_{ij} = \frac{p_i + p_j}{E_i + E_j}, \quad \gamma_{ij} = \frac{1}{\sqrt{1-\beta_{ij}}} \tag{8}$$

As a result of this, the interaction term in (4) also depends on momentum.

Recently R-JQMD, the Lorentz covariant version of JQMD, has been proposed[7]. The covariant version of Hamiltonian (4) is

$$H_C = \sum_i \sqrt{p_i^2 + m_i^2 + 2m_i V_i} \tag{9}$$

where V_i is the effective potential felt by the i^{th} particle.
With on-mass-shell constraints and a simple form of the "time fixations" constraint, the entire particle has the same time coordinate. They justified the later assumption with the following argument "In high-energy reactions, two-body collisions are dominant; the purpose of the Lorentz-covariant formalism is only to describe relatively low energy phenomena between particles in a fast-moving medium".
From this assumption, they get following equation of motion together with a big improvement in CPU performance.

$$\dot{r}_i = \frac{p_i}{2p_i^0} + \sum_j \frac{2m_j}{2p_j^0} \frac{\tilde{V}_j}{\partial p_i} \tag{10}$$
$$= \frac{\partial}{\partial p_i} \sum_j \sqrt{p_j^2 + m_j^2 + 2m_j \tilde{V}}$$

$$\dot{p}_i = -\sum_j \frac{2m_j}{2p_j^0} \frac{\tilde{V}_j}{\partial r_i} \tag{11}$$
$$= \frac{\partial}{\partial r_i} \sum_j \sqrt{p_j^2 + m_j^2 + 2m_j \tilde{V}}$$

And the i^{th} particle has an effective mass of

$$m_i^* = \sqrt{m_i^2 + 2m_i V_i} \tag{12}$$

We follow their prescription and also use the same parameter values, such as the width of the Gaussian L = 2.0 fm^2 and so on.

For the case of two body collisions and resonance decay, we used the same codes which the Binary Cascade uses in Geant4. However for the relativistic covariant kinematic case, the effective mass of i^{th} particle (12) depends on the one-particle effective potential, V_i, which also depends on the momentum of the entire particle system. Therefore, in R-JQMD, all the effective masses are calculated iteratively for keeping energy conservation of the whole system. We track their treatment for this.

As already mentioned, the Binary cascade model creates detailed 3r+3p dimensional nucleus at the beginning of each reaction. However, we could not use them in our QMD code, because they are not stable enough in time evolution. Also, a real ground state as an energy minimum state of the nucleus is not available in the framework of QMD, because it does not have fermionic properties. However, a reasonably stable "ground state" nucleus is required for the initial phase space distribution of nucleons in the QMD calculation. JQMD succeeded to create such a "ground state" nucleus. We also follow their prescription of generating the ground state nucleus. And "ground state" nuclei for target and projectile will be Lorentz-boosted (construct) to the center-of-mass system between them. By this Lorentz transformation, additional instabilities are introduced into both nuclei in the case of the non-covariant version.

The time evolution of the QMD system will be calculated until a certain time, typically 100 fm/c. The delta T of the evolution is 1 fm/c. The user can modify both values from the Physics List of Geant4. After the termination of the time evolution, cluster identification is carried out in the phase space distribution of nucleons in the system. Each identified cluster is considered as a fragmented nucleus from the reaction and it usually has more energy than the ground state. Therefore, excitation energy of the nucleus is calculated and then the nucleus is passed on to other Geant4 models like Binary Cascade. However, unlike Binary Cascade which passes them to Precompound model and Excitation models by calling them inside of the model, the QMD model uses Excitation models directly. There are multiple choices of excitation model and one of them is the GEM model[8] which JQMD and RJQMD use. The default excitation model is currently this GEM model.

Figure 1 shows an example of time evolution of the reaction of 290MeV/n 56Fe ions bombarding a 208Pb target. Because of the small Lorentz factor (~1.3), the Lorentz contractions of both nuclei are not seen clearly.

IV. Cross Section of Nucleus-Nucleus Interaction

Nucleus-Nucleus (NN) cross section is not a fundamental component of either QMD or Binary Light Ions Cascade model. However without the cross section, no meaningful simulation beyond the study of the NN reaction itself can be done. In other words, Geant4 needs the cross section to decide where an NN reaction will happen in simulation geometry.

Many cross section formulae for NN collisions are included in Geant4, such as Tripathi[9] and Tripathi Light System[10], Shen[11], Kox[12] and Sihver[13]. These are empirical and parameterized formulae with theoretical insights and give total reaction cross section of wide variety of combination of projectile and target nucleus in fast. These cross sections are also used in the sampling of impact parameter in the QMD model.

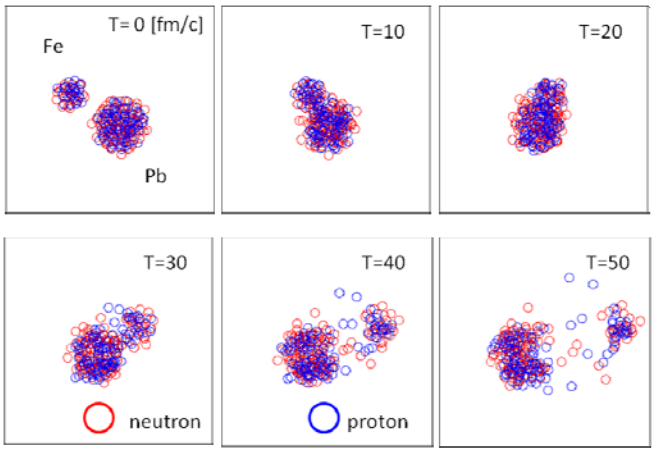

Fig. 1 Time evolution of reaction of 290 MeV/n Fe on Pb in position space. Red and Blue circle represents neutron and proton respectively. Full scale of each panel is 50 fm.

V. Comparison with Experiment

Some results produced with the new QMD model are presented in the following. **Figures 2 and 3** show the energy and angular differential neutron production from ions bombarding thin and thick targets. The results from the Binary Light Ion Reaction model are also plotted for comparison purposes. High energy tails in the neutron production above 60 degrees are reproduced much better in the new QMD for both thin and thick target.

Figure 4 shows the fragment particle production from 1GeV/n 56Fe ions bombarding an aluminum target. Results from Lorentz covariant (G4RQMD) and non covariant (G4QMD) versions are plotted with experimental data. As already mentioned, the Lorentz boost to the center-of-mass system of the projectile and target introduces large instabilities to the nuclei in the non covariant version. Nucleons easily evaporate from the projectile nucleus in the non covariant version. As the result of this, the number of fragmented particles of the non covariant version is larger than found by experiment. The fragmented particle production also depends on the excitation model which is used after the reaction phase of QMD. However in this comparison, both versions used the same excitation model in Geant4. The distribution of impact parameter of the collision

possibly effects the fragment production but the same sampling method is used in both calculations.

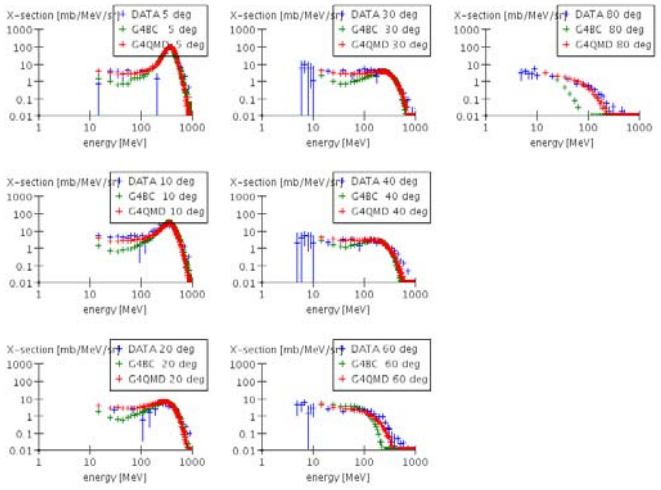

Fig. 2 Double-differential energy-angle neutron production from 290MeV/n 20Ne bombarding thin Carbon target. Data points come from Ref.[14]. G4BC and G4QMD represent the result from the Binary Light Ion Reaction model and this new QMD model in Geant4, respectively.

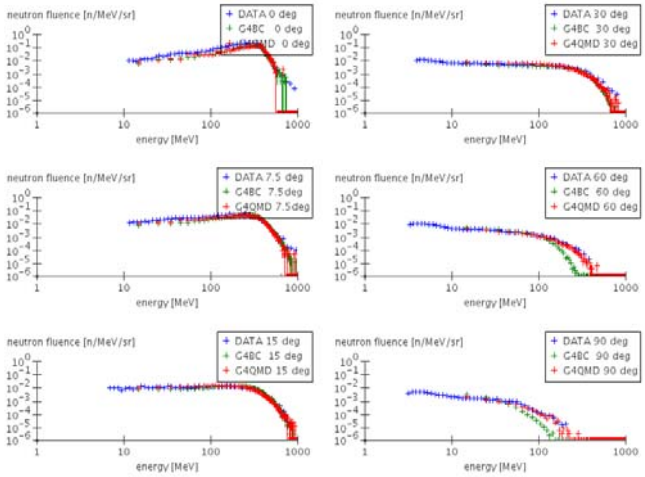

Fig. 3 Double-differential energy-angle neutron production from 400MeV/n 56Fe bombarding thick aluminum target. Data points come from Ref.[15]. G4BC and G4QMD represent the result from the Binary Light Ion Reaction model and this new QMD model in Geant4, respectively.

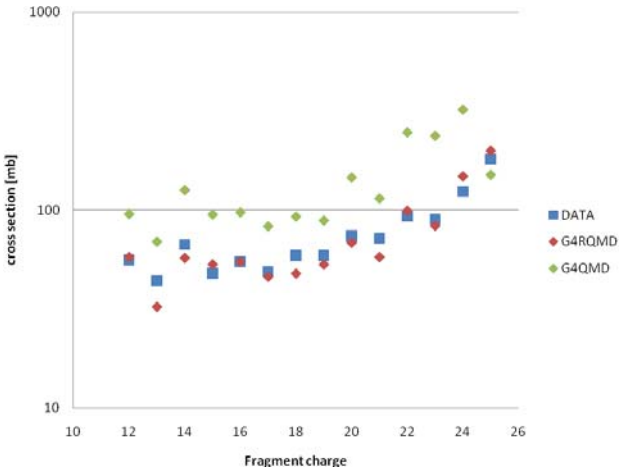

Fig. 4 Fragmentation cross sections for 1GeV/n 56Fe on Al. Data are taken from Ref. [16]. G4RQMD and G4QMD represents Lorentz covariant and non covariant version of this new QMD model in Geant4 respectively.

VI. Conclusion

A new C++ native version of QMD model is successfully developed in Geant4. The deviations of equations of motion, two-body effective interactions and construction of a "ground state" nucleus are based on JQMD. Final states of two body collision and decays of strong resonances are calculated by the same codes which Binary Cascade uses in Geant4. After the termination of time evolution of the QMD system, cluster identifications are carried out on the phase space distribution of nucleons in the system. Identified clusters are regarded as an excited fragmented nucleus and they are passed into excitation models in Geant4 for further particle emissions.

Not many validation plots are shown in this paper but they show significantly improved results compared to previous Geant4 models.

Only event generator like validations are presented in this paper. However the QMD model is already included in the Geant4 distribution and validations of the model with the fully integrated geometries, such as Bragg peak simulation for ion therapy facilities, single event upsets in semiconductor devices in space vehicles have already been done by users of Geant4 with or without the collaboration of us.

We also include Lorentz covariant kinematics which have been recently proposed by the authors of JQMD. Validation of the fragmented particle production from 1GeV/n 56Fe on aluminum shows the improved results over the non covariant version. We would like to confirm by comparing the elastic ratio and the time evolution of direct transverse momentum in the future.

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