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Original paper

Preliminary results coupling "Stochastic Mean Field" and "Boltzmann-Langevin One Body" models with Geant4

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ABSTRACT

Purpose: Monte Carlo (MC) simulations are widely used for medical applications and nuclear reaction models are fundamental for the simulation of the particle interactions with patients in ion therapy. Therefore, it is of utmost importance to have reliable models in MC simulations for such interactions. Geant4 is one of the most used toolkits for MC simulation. However, its models showed severe limitations in reproducing the yields measured in the interaction of ion beams below 100 MeV/u with thin targets. For this reason, we interfaced two models, SMF ("Stochastic Mean Field") and BLOB ("Boltzmann-Langevin One Body"), dedicated to simulate such reactions, with Geant4.

Methods: Both SMF and BLOB are semi-classical, one-body approaches to solve the Boltzmann-Langevin equation. They include an identical treatment of the mean-field propagation, on the basis of the same effective interaction, but they differ in the way fluctuations are included. Furthermore, we tested a correction to the excitation energy calculated for the light fragments emerging from the simulations and a simple coalescence model.

Results: While both SMF and BLOB have been developed to simulate heavy ion interactions, they show very good results in reproducing the experimental yields of light fragments, up to alpha particles, obtained in the interaction of ^{12}C with a thin carbon target at 62 MeV/u.

Conclusions: BLOB in particular gives promising results and this stresses the importance of integrating it into the Geant4 toolkit.

1. Introduction

Ion therapy is the treatment of tumours with protons (p), or heavier ions like carbon (C) and oxygen (O). Its clinical impact is constantly increasing, especially in the last ten years, as can be seen in Fig. 1. Nowadays 85 centres are active worldwide and almost 200 000 patients have been treated so far [1].

For such treatment, Monte Carlo (MC) simulations are essential since they are considered the gold standard for dosimetric calculations in ion therapy [2]. Moreover, MC codes are used to:

- generate input parameters, such as the depth-dose distribution in water for different ions, of the deterministic codes (pencil beam algorithms [3]) adopted to optimise the treatment planning in clinical practice [4];
- validate the dose calculation of the pencil beam algorithms, especially in cases with large tissue heterogeneities [5];
- estimate the risk of secondary cancer induction [6];
- estimate the production of beta emitters, such as ^{11}C and ^{15}O, which would allow for a non-invasive verification of the treatment via Positron Emission Tomography (PET) imaging during, or shortly after, the treatment itself. MC is needed in dose profiling because it interprets the observed spectra of the emitted radiation into delivered dose [7,8] and a large effort is ongoing to develop detectors to measure such emitted radiation, as for instance in references: [9–12].

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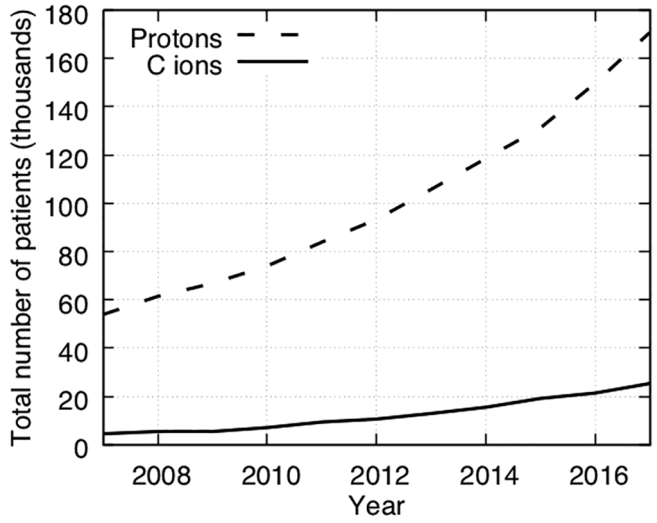

Fig. 1. Total number of patients treated with proton therapy (dashed line) and with carbon ion therapy (continuous line). Data from PTCOG [1].

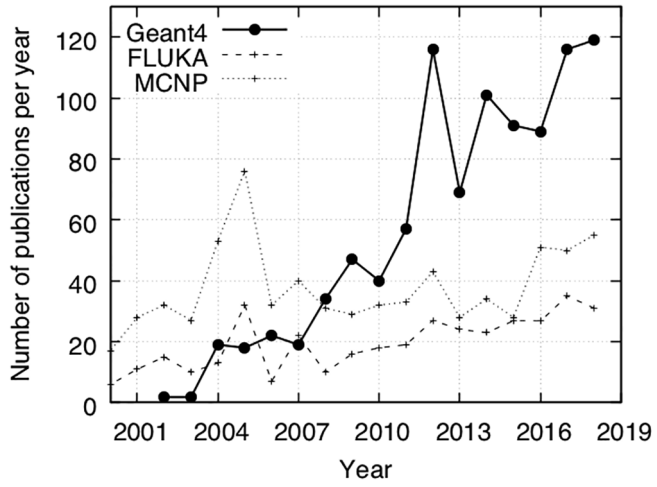

Fig. 2. Number of papers related to most-used MC codes found on PubMed per year.

MC codes are also used to compute the biological effects of radiation [13].

Therefore, having reliable nuclear fragmentation models in Monte Carlo (MC) simulation toolkits is of utmost importance for ion therapy [14].

Geant4 [15] is one of the most widely used MC toolkits, both in nuclear and particle physics and in medical applications. Geant4 is written in C++ and takes advantage of the object-oriented coding paradigm. Moreover, it is multithreaded, allowing an efficient use of modern CPUs. Finally, Geant4 is open source and developed by a large international collaboration.

Medical physicists began using Geant4 around the year 2000. A search on the PubMed citation database [16] finds almost 1000 medical physics publications related to Geant4. The first of them dates back to 2002 with a clearly increasing tendency, as can be seen in Fig. 2.

Geant4 simulates radiation transport and interaction with matter and has the capability to import the Computed Tomography (CT) scan of a patient in DICOM format [17], allowing the simulation of the interaction of the beam with a specific patient. Moreover, many programs specifically tailored to medical simulations have been developed using Geant4 as the physics engine, and -therefore- they use its nuclear reaction models. A Geant4 package dedicated to the simulation of early biological damage induced by ionising radiation at the DNA scale also exists: Geant4-DNA [18].

Despite the high impact of low energy nuclear reaction models and the wide usage of Geant4, recent literature has shown the limitations of the models implemented in Geant4 in reproducing the measured secondary yields of ion interactions below 100 MeV/u, in terms of production rates, angular and energy distributions. For example:

- Braunn et al. [19] have shown discrepancies up to one order of magnitude in ^{12}C fragmentation at 95 MeV/u on thick Polymethyl methacrylate (PMMA) target;
- De Napoli et al. [20] highlighted the limitations on the angular distribution of the secondaries emitted in the interaction of a 62 MeV/u ^{12}C beam with a thin carbon target. We updated such a benchmark [21] including the “Lige cascade model” (INCL++) [22,23], recently added in Geant4. To give the idea of the results obtained with the models available in Geant4, we show in Fig. 3 the results obtained for the emission of alpha particles. The complete benchmark can be found in [21];
- Dudouet et al. [24] found similar results with a 95 MeV/u ^{12}C beam on H, C, O, Al and Ti targets.

To improve the Geant4 capabilities in simulating nuclear reactions below 100 MeV/u, we interfaced it with two dedicated models for such reactions: SMF (“Stochastic Mean Field”) [28] and BLOB (“Boltzmann-Langevin One Body”) [29].

2. Material and methods

2.1. Nuclear interaction models

Nuclear collisions are generally described in two steps. The first step simulates the reaction dynamics, from the pre-equilibrium emission of the composite nuclear system up to the sharing of the available energy among the projectile and target nucleons, usually called “thermalisation”, and the production of excited nuclear fragments. The second step, the de-excitation phase, deals with the decays of such excited states after thermalisation.

SMF [28] and BLOB [29] are among the most advanced transport approaches used to handle the first stage of the collision process, where equilibrium approximations do not hold, at a few hundreds of MeV/u and below. Both are semi-classical, one-body approaches to solve the Boltzmann-Langevin equation and are based on the description of the time evolution of the nucleon phase space density distribution in a semi-classical way, i.e. taking into account the Pauli principle, as required for fermionic systems. The corresponding transport equation is solved numerically: SMF and BLOB sample the density distribution in phase space with test particles, typically from tens to hundreds per nucleon, depending on the size of the colliding nuclei. The test particles are evolved according to the action of an effective mean-field nuclear potential. For this work, we used 10^2 test particles per nucleon in SMF and $5{\cdot}10^2$ test particles per nucleon in BLOB.

Both SMF and BLOB include an identical treatment of the mean-field propagation, on the basis of the same effective interaction, but they differ in the way effects beyond the mean-field description, such as correlations and fluctuations, are included. In particular, while SMF employs a Boltzmann-Uehling-Uhlenbeck (BUU) collision term and considers only fluctuations of the spatial density, BLOB introduces fluctuations of the one-body density in full phase space through a modified collision term where nucleon-nucleon correlations are explicitly involved [30].

SMF and BLOB were designed and developed to simulate heavy ion interactions in the Fermi-energy regime. The improved treatment of the fluctuation dynamics in BLOB leads to a better description of multi-fragmentation reactions at Fermi energies [29]. Moreover BLOB has been recently applied to fragment production in spallation reactions [31]. We stress that the inclusion of fluctuations is essential to tackle

the description of multi-fragment production. In this respect, stochastic models, such as SMF and BLOB, represent an important improvement over standard BUU-like models. We already showed in preliminary work the potentialities of the two models in describing ^{12}C fragmentation, comparing their predicted relative total yields with experimental data using the SIMON [32] code for the de-excitation of the fragments [33] and the Geant4 statistical de-excitation model `G4ExcitationHandler` [21]. In this work, we present a more extended benchmark with the data-set of De Napoli et al. [20], i.e. experimentally measured double differential cross sections of fragment production from the interaction of a ^{12}C beam at 62 MeV/u with a thin ^{nat}C target. We coupled SMF and BLOB with Geant4 and its de-excitation phase, foreseeing their porting to Geant4.

2.2. Interface with Geant4

To couple SMF and BLOB with Geant4 we developed two "dummy" models in Geant4, `G4SMF` and `G4BLOB`, that is, we followed the Geant4 guidelines for developing models by inheriting from the Geant4 pure virtual class `G4VIntraNuclearTransportModel`. `G4SMF` and `G4BLOB` load the output from SMF and BLOB, respectively, and sample one of their final states. The reaction products are reconstructed by applying a clustering procedure to the one-body density $\rho(\mathbf{r})$ defining a "liquid" and a "gas" phase. The first one is associated with cells having density $\rho \geqslant 1/6 \cdot \rho_0$, being ρ_0 the saturation density, whereas the gas phase is composed by all the remaining test particles. Fragments are built connecting neighbouring cells of the liquid phase. Each liquid phase neighbourhood stands for a fragment. Once fragments are identified, from the knowledge of the one-body distribution function it is possible to calculate their mass, charge, and kinematical properties. For the interaction under consideration, there are typically two large fragments, each having real values of the mass ($\bar{A}$) and atomic number ($\bar{Z}$), as they result from the test particles clustering procedure which has been described before. Therefore, `G4SMF` and `G4BLOB` sample the number of neutrons (A − Z) and protons (Z) from $\bar{A}$ and $\bar{Z}$, converting $\bar{A}$ and $\bar{Z}$ to an integer (A and Z, respectively). This is done by using the fractional part of the real ($\bar{A} - \bar{Z}$ and $\bar{Z}$) as the probability that the number is rounded up or down.

The number of neutrons and protons are sampled independently for each fragment and then the number of nucleons emitted is sampled from the "gas" to match the total charge and barionic number of the initial state. Conservation of three-momentum is checked at the end; if it is not within 10%, the event is rejected and the sampling restarts.

Fragment excitation energies are calculated by subtracting the Fermi motion, evaluated in the local density approximation, from the fragment kinetic energy, taken in the fragment reference frame [34].

The number of test particles per nucleon used in BLOB is 500 to ensure an accurate phase space mapping. In SMF it is not recommended to increase the number of test particles per nucleon to more than 100 because the fluctuations in the interactions would be underestimated. BLOB does not suffer this problem because of its modified collision term.

The large fragments are then passed to the de-excitation model of Geant4, `G4ExcitationHandler`, for their statistical de-excitation. The Geant4 version used in this work is 10.5.p1, the most recent.

The results are then scaled by the total inelastic cross section and processed to reproduce the experimental angular resolution, geometrical acceptance and energy resolution. The total inelastic cross section used is the default in Geant4 for these reactions, the one calculated with the `G4ComponentGGNuclNuclXsc` class which uses the Glauber model with the Gribov correction calculated in the dipole approximation [35]. As can be seen in Table 1 all the models available in Geant4 for computing the inelastic cross sections in this energy domain give similar results.

The double differential cross sections obtained coupling SMF and BLOB with Geant4 are shown in Figs. 3–8, in all these plots we show

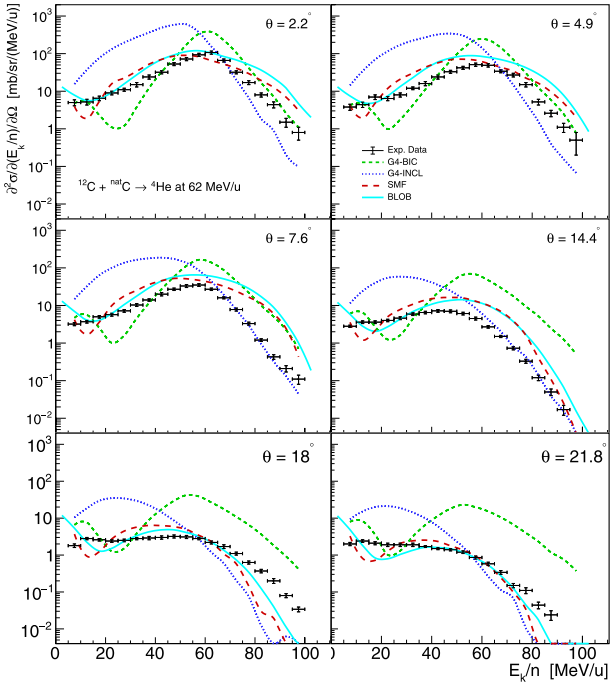

Fig. 3. Double differential cross sections of alpha particle production as a function of the kinetic energy of the produced fragment for different angles. Binary Intranuclear Cascade (BIC) [25] in green, and INCL++ [22,23] in blue "Stochastic Mean Field" (SMF) in red and "Boltzmann-Langevin One Body" (BLOB) in cyan. Another model, Quantum Molecular Dynamics (QMD) [26], is available for ion interactions in Geant4. However, it is not used by default below 100 MeV/u, where `G4IonQMDPhysics` calls BIC. A complete description of the benchmark of the models already available in Geant4, with QMD, can be found in [21]. This validation is included in the Geant4 validation system [27]. The experimental data are from De Napoli et al. [20] and were taken with a 62 MeV/u ^{12}C beam on a thin ^{nat}C target. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 1
Inelastic cross sections computed with the Geant4 models.

Model	Cross section (barn)	Reference
`G4ComponentGGNuclNuclXsc`	1.054	[35]
`G4IonsShenCrossSection`	1.0221	[36]
`G4IonsKoxCrossSection`	1.0083	[37]

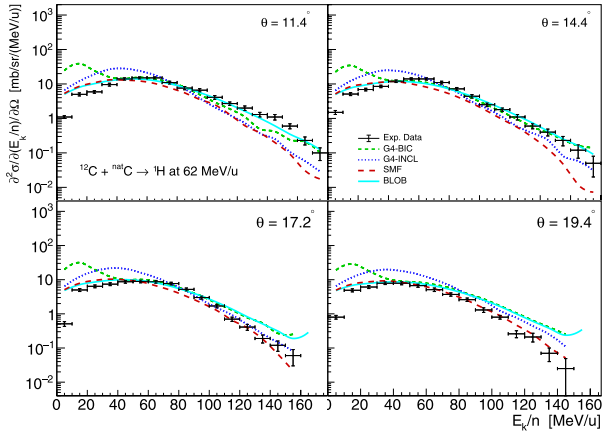

Fig. 4. Same as Fig. 3 but for protons.

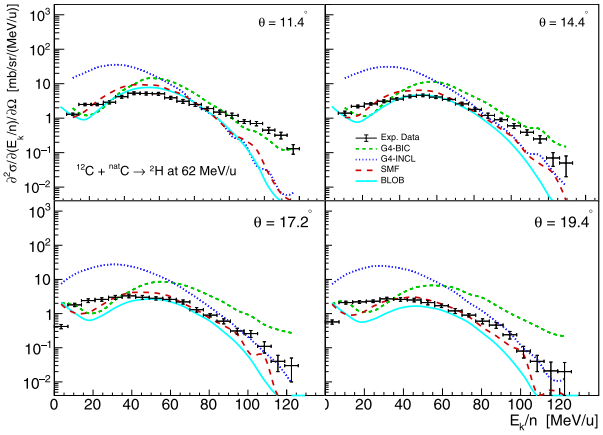

Fig. 5. Same as Fig. 3 but for deuterium.

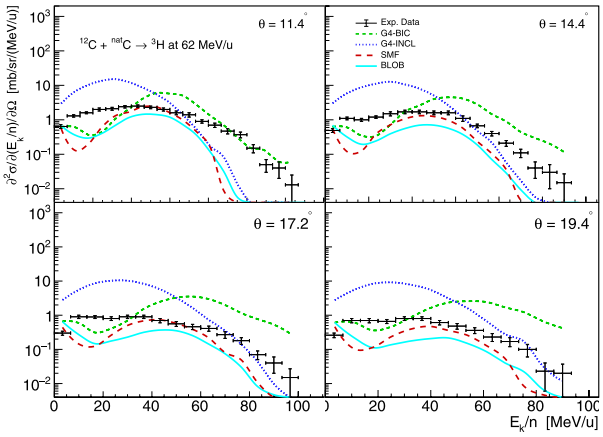

Fig. 6. Same as Fig. 3 but for tritium.

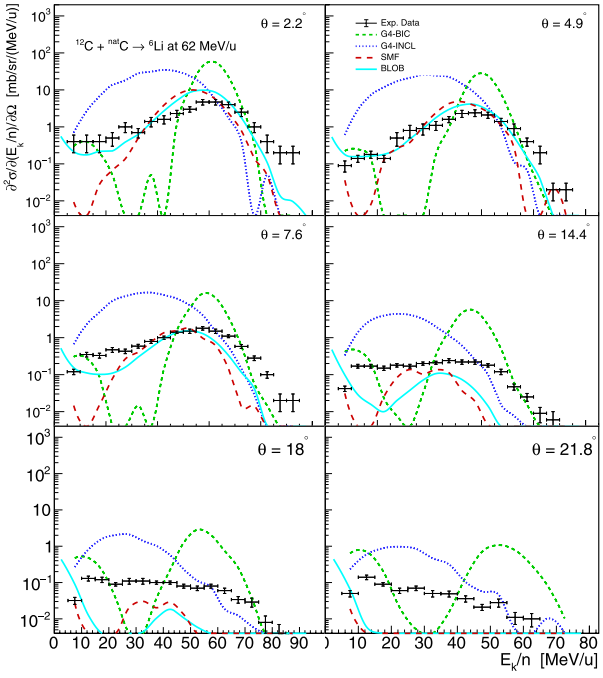

Fig. 7. Same as Fig. 3 but for ^{6}Li.

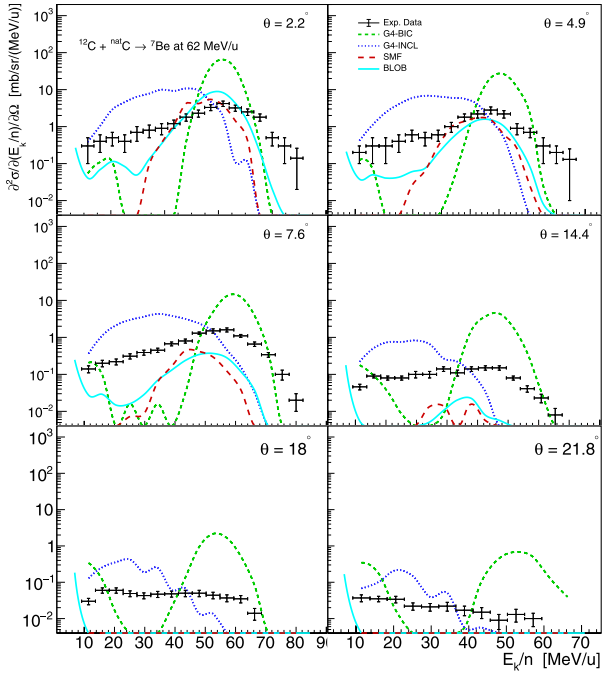

Fig. 8. Same as Fig. 3 but for ^{7}Be.

also the models already available in Geant4, to be taken as a reference.

2.3. Corrections

The clustering procedure discussed above provides reasonable results, for the description of the ground state and for excited primary fragment properties, in the case of medium-heavy nuclei. However, for light systems, such as the ones we are interested in, owing to numerical fluctuations of the phase space density, this procedure leads to an overestimation of the evaluated fragment excitation energies. The errors are larger in percentage when the fragment excitation energy is smaller, causing a spurious non-zero value even in the ground state. Hence, this problem affects to a large extent the results concerning the less central impact parameters. Indeed, the top plot of Fig. 9 does not show the expected fall-off with increasing impact parameter (b), as discussed above. To mitigate this effect, we applied a linear correction to the excitation energy for $b \geqslant b_0$, being $b_0 = 5.5$ fm, roughly twice the ^{12}C radius. Such a correction is linear with b and its maximum is 2.77 MeV/u. Such value corresponds to the average spurious ground state excitation energy associated with the fragments emerging from our calculations.

In addition, as already mentioned, in SMF and BLOB two-body interactions are explicitly treated as elastic collisions, of a stochastic nature, between test particles. Though the majority of the small fragments is produced during the de-excitation phase, some of them may emerge from the reaction dynamics, owing to correlations (two-body and even more than two-body correlations) which go beyond the stochastic two-body collision effects implemented in our procedure. These correlations may change the momentum distribution of the reaction products. To take into account these effects we developed a simple coalescence model for the nucleons sampled from the SMF and BLOB final state. In this simple model, if a proton and a neutron are closer than 6 fm and their momenta differ by less than 260 MeV/u, which roughly corresponds to the Fermi energy, they form a deuteron. This process is applied recursively to allow the formation of heavier ejectiles. The position of the coalesced fragment is the average of the fragments from which it was formed; its momentum, A and Z are sum of the coalescing fragments.

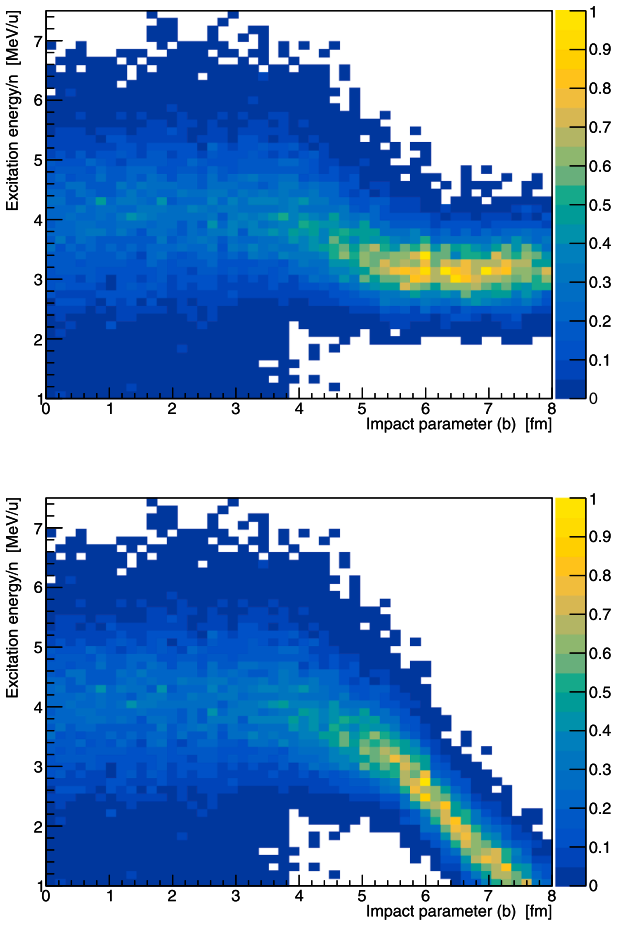

Fig. 9. Excitation energy of fragments with A > 1 output from BLOB as a function of the impact parameter *b*. The top plot shows the excitation energy before the correction and the bottom one after the correction described in the text. SMF results are not shown because they are similar.

The coalescence is applied up to the production of ^{4}He. Also the excitation energy correction has significant effects only on small ejectiles, up to ^{4}He. For this reason, we are showing their effects only on these fragments production in Figs. 10–13. As it can be noticed, the coalescence increases the production of ^{2}H and ^{3}H in all the spectra. Conversely, the coalescence lowers the spectrum of both H and ^{4}He, the former lowered in the whole range while the latter only below 40 MeV/u. The excitation energy correction has a significant impact only on increasing the ^{4}He production in the 62 MeV/u peak and decreasing the same spectrum in the higher energy region. This makes the shape of BLOB and SMF outputs closer to the experimental data. We show the effects of these two corrections only on BLOB, to keep the plots clear, but the effects on SMF are similar.

These corrections should not be considered as a final result but as an indication of the outcome that a better calculation of the fragments excitation energy and correlations effects implemented in BLOB could give.

3. Results and discussion

The obtained double differential cross sections are in reasonable agreement with experimental data for the small ejectiles, as can be seen in the plots from Figs. 3–7. BLOB shows better results than SMF, most probably because of the improved treatment of fluctuations and of the greater stability due to the larger number of test particles per nucleon used.

For larger fragments, such as ^{6}Li and ^{7}Be the agreement is poorer at large angles as shown in Figs. 7 and 8. This discrepancy is under investigation and could be due to the fact that the mean field is not strong enough to keep these fragments bound, or that their excitation energy is still over-estimated. In particular, the lack at large angle could be due to an under-estimate of the probability of formation of a neck between projectile and target. However, we already observed that BLOB gives better results than SMF, owing to the improved treatment of fluctuations. A detailed investigation of the neck dynamics in central events is in order.

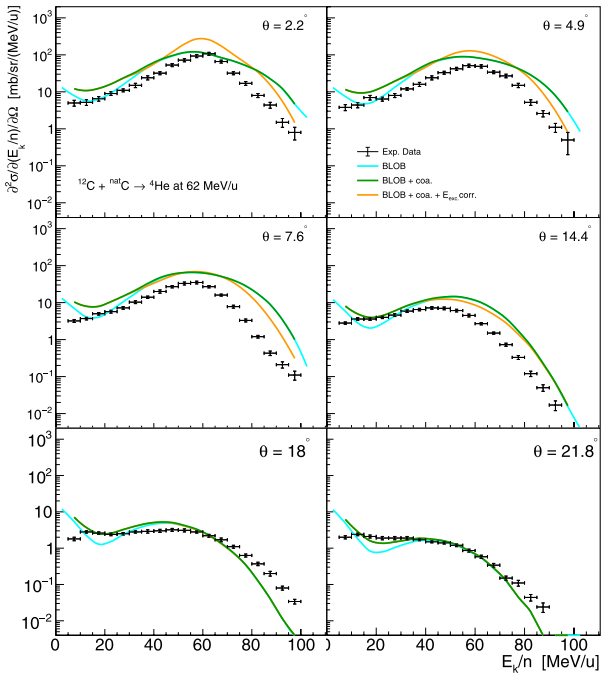

Fig. 10. Similar to Fig. 3 but besides the same BLOB results, still in cyan, we are showing the effects of the corrections described in the text: the coalescence, in green, and the coalescence and the excitation energy corrections together, in orange. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

4. Conclusions

In this paper we investigate the possibility to interface two low-energy reaction models (SMF and BLOB) with Geant4 and its de-excitation phase. Calculations have been performed to investigate light cluster and fragment production in ^{12}C on a thin Carbon target at 62 MeV/u. We observe that the double differential cross sections of the

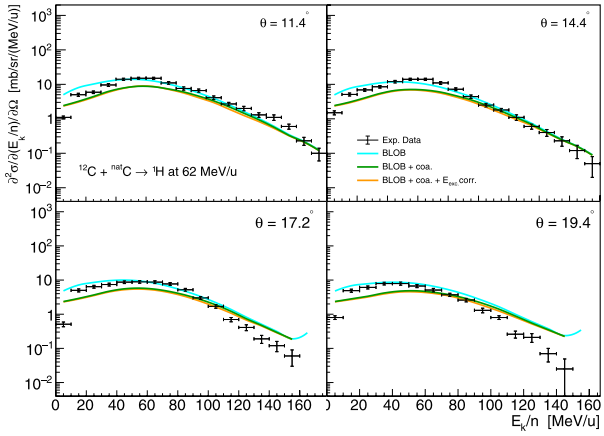

Fig. 11. Same as Fig. 10 but for protons.

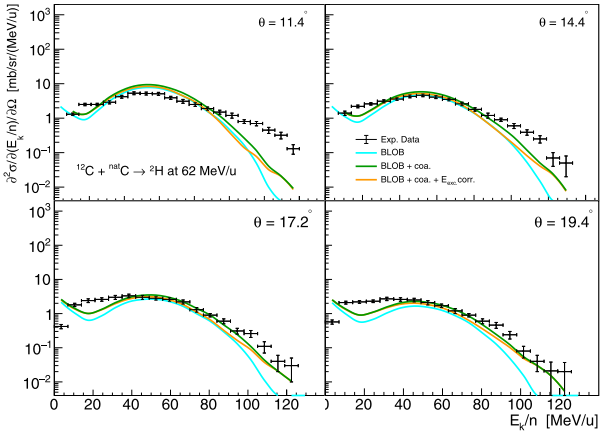

Fig. 12. Same as Fig. 10 but for deuterium.

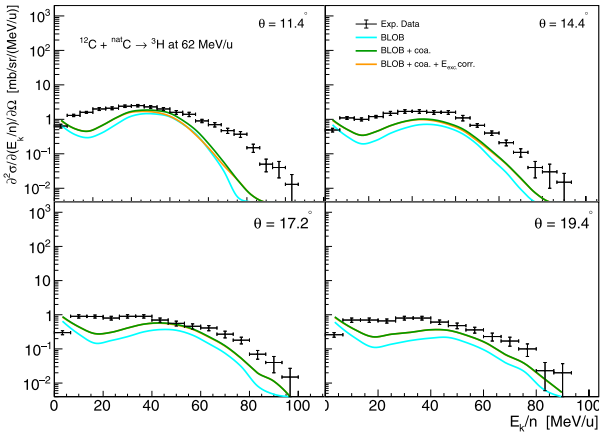

Fig. 13. Same as Fig. 10 but for tritium.

reaction products, as obtained in particular with BLOB, are, for almost all angles of emission, much closer to the experimental data than the predictions of models already available in Geant4 [21]. More specifically, a quite good agreement with experimental data is observed for light ejectiles, up to alpha particles while some problems remain at larger emission angles, where no model reproduce well the data.

The interplay between cluster emission of a dynamical nature, located mainly at mid-rapidity, and the statistical component, originating from the de-excitation of quasi-projectile and quasi-target sources, is well described by BLOB. Yet, this seems to be a major issue, at the beam energy considered, for the codes implemented in Geant4, as can be seen in Fig. 3 and more extensively in [21]. However, the BLOB calculations must be improved to reach a better reproduction of the mid-rapidity component of larger fragments, probably emerging from central reactions, thus needing an improved statistics of events.

Finally, the BLOB computation time is too large for its usage in medical applications. We are evaluating the possibility of porting it to the GPU, profiting from the fact that BLOB uses the test particle method. Thus, according to its computing scheme, BLOB could take advantage of the “single instruction on multiple data” approach of the GPU programming with a low thread divergency. In fact, we expect a speed up in the code by some orders of magnitude.

We are also investigating the possibility of training a Deep Learning algorithm, specifically a Variational Auto-Encoder (VAE), to emulate BLOB. Once trained, the VAE could produce a BLOB final state in a negligible time. The VAE training could be saved and distributed in binary compressed files with Geant4. Preliminary results are encouraging and a paper is in preparation [38].

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at https://doi.org/10.1016/j.ejmp.2019.10.026.

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