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Improved integrated nucleus-nucleus inelastic cross sections for light nuclides in Geant4

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Abstract

We propose a new root-mean-square radius parameterization for light nuclei $A \leq 30$ suitable for use in Geant4 calculations of nucleus-nucleus total hadronic inelastic scattering cross sections. The new approach takes into account the proton-neutron asymmetry of the reactants, and was fit to 360 measured total inelastic cross sections from the EXFOR database. Measured nuclear radii are better described in the new approach than the current Geant4 implementation, particularly for unstable nuclides, and there is better agreement with measured cross sections for both stable and unstable nuclides. The improved parameterization should help in carbon-ion therapy applications in particular.

Keywords: Nucleus-Nucleus cross section, Geant4, Nuclear radii

The Monte Carlo simulation toolkit Geant4 [1, 2] models particle transport in matter, and is used in a wide range of research fields including space science, radiation protection, and medical physics. One key factor in simulations of ion transport is the total inelastic (or reaction) cross section. For example, in hadron therapy applications, at energies of 400 MeV/nucleon, up to 70% of ^{12}C beam nuclei may undergo some nuclear reaction before reaching the tumour site [3]. Precise treatment planning therefore requires reliable predictions for inelastic cross sections of ^{12}C, and any lighter (possibly unstable) secondary fragments, interacting with any isotopes found in the body.

Geant4 uses a model based on the Glauber approximation [4] to calculate integrated inelastic cross sections for nucleus-nucleus interactions (GG model) [5, 6]. The approach assumes the colliding nuclei have Gaussian shaped density distributions, allowing analytic evaluation of the density convolutions required. A Gribov screening correction is included [7], as well as a phenomenological Coulomb repulsion correction, which reduces the cross section at low energies. Nuclear radii enter as a key parameter in the model. In the current Geant4 implementation, the radii are parameterized in terms of the mass number A. However, it takes no account of the proton-neutron asymmetry of the nuclides, making it unreliable for unstable nuclei.

In this paper, we propose an improved radius model for use with the Geant4 GG cross sections. Our primary aim is to improve the predictive power of the model for hadron therapy and space radiation applications, and we therefore focus on light nuclides with $A \leq 30$. The model includes a term dependent on the proton-neutron asymmetry, designed to improve predictions for unstable isotopes. The new radius model is fit to reproduce measured inelastic cross sections from the EXFOR database [8], and then is compared to the existing Geant4 implementation (Throughout the present work, we compare to Geant4 version 10.5.) and experimental measurements of radii [9, 10, 11, 12, 13]. The cross sections from the GG model, using the new radii, are then compared to experimental data [14, 15, 16, 17, 18, 19, 20] from the EXFOR database [8].

We first briefly present the Glauber-Gribov model that is implemented (and widely used) within Geant4. Several publications by Grichine provide more detail on the Geant4 implementation [21, 22, 23]. The model assumes the two colliding nuclei have Gaussian shaped density distributions, with radius parameters R_p and R_t. The corre-

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sponding inelastic cross section is then given as:

$$\sigma_R = \frac{\beta\pi(R_p^2+R_t^2)}{\gamma}\ln\left[1+\frac{\gamma A_p A_t \overline{\sigma}}{\beta\pi(R_p^2+R_t^2)}\right]\left[1-\frac{V_B}{T_{cm}}\right], \tag{1}$$

where $\beta = 2.0$ and $\gamma = 2.4$. The cross sections are phenomenologically corrected for Coulomb repulsion with the term of $[1 - V_B/T_{cm}]$ where $V_B = Z_p Z_t e^2/2(R_p + R_t)$ is the approximate Coulomb barrier. Here, Z_p (Z_t) is the number of protons in the projectile (target), T_{cm} is the center of mass kinetic energy, and e is the electron charge. $\overline{\sigma}$ is the isospin-averaged nucleon-nucleon cross section for the collision,

$$A_p A_t \overline{\sigma} = (Z_p Z_t + N_p N_t)\sigma_{pp} + (Z_p N_t + N_p Z_t)\sigma_{np}, \tag{2}$$

where σ_{pp} is the total proton-proton cross section, with the assumption that $\sigma_{nn} = \sigma_{pp}$, and σ_{np} is the total proton-neutron cross section.

In Geant4 v10.5, the radii R_p and R_t are parameterized in terms of the atomic mass number A of each reactant, with different forms for different mass ranges:

$$R(A) = \begin{cases} r_0(1 - A^{-2/3})A^{1/3} & (10 < A \leq 30) \\ r_0 A^{1/3} & (30 < A < 50) \\ r_0 A^{0.27} & (A \geq 50). \end{cases} \tag{3}$$

The values of the parameter r_0 have been chosen for each range as 1.26 ($10 < A \leq 15$), 1.19 ($15 < A \leq 20$), 1.12 ($20 < A \leq 30$), 1.10 ($30 < A < 50$) and 1.00 ($A \geq 50$). For light stable nuclides with $A < 10$, the radii are taken from electron scattering measurements of charge radii. Specific values are given for $^{1-3}$H and $^{3-4}$He, and a single value is used for all Lithium isotopes (2.4 fm), and all Beryllium isotopes (2.51 fm). Other isotopes with $A < 10$ (^{6}He, ^{8}He, and ^{8}B) default to the $30 < A < 50$ parameterization ($1.1A^{1/3}$).

The primary limitation of the present approach is that the radii are dependent only on the mass number A and not the relative numbers of protons and neutrons. Unstable nuclides, with asymmetric numbers of protons and neutrons, can have dramatically different nuclear radii from those at stability, even where A is the same. To address this deficiency, we propose an alternative form, given by:

$$R(A,Z) = c_1 A^{1/3} + c_2/A^{1/3} + c_3\Delta(A,Z)^2. \tag{4}$$

The first and second terms account for the gross mass number dependence, and match the forms from the current Geant4 model. The third term accounts for the proton-neutron asymmetry of the nuclides, with respect to the valley of β-stability, and is defined as follows. We assume that the number of neutrons $N = A - Z$ for nuclides at stability follows approximately:

$$N_v(A) = 0.5A + (0.028A)^2 - (0.011A)^3. \tag{5}$$

Table 1: Parameters of the new radius model.

c_1 [fm]	c_2 [fm]	c_3 [fm]
0.77330	1.3821	30.283

Δ characterises the neutron excess (or deficit) for the isotope in question, and is defined as

$$\Delta(A,Z) = \frac{N_v(A) - N}{A}. \tag{6}$$

The new expression for $R(A,Z)$ replaces those in Eq. 3 for $A \leq 30$. The parameters c_{1-3} were fit to 360 measured inelastic cross sections extracted from the EXFOR database [8]. This data set encompass a wide range of nucleus-nucleus reactions, with the constraint that $A_p \leq 30$ and $A_t \leq 30$, with $E > 10$ MeV/nucleon. The fitted parameters c_{1-3} can be found in Table 1. Since the light (stable) nuclides with $A < 10$ exhibit strong clustering which can influence their radii, we have retained the explicit radius values taken from electron scattering measurements. However, we have updated the values used to include explicit values for ^{6,7}Li and ^{9}Be. The other Lithium and Beryllium isotopes use the expression for $R(A,Z)$ above.

We emphasise that since the fit was made to inelastic cross sections, $R(A,Z)$ should be considered an effective radius, i.e. that required for Gaussian density distributions to reproduce inelastic cross sections in the GG model. For light nuclides, where the density distributions are approximately Gaussian, a direct comparison may be made to measurements, but for heavier nuclides this may not be the case.

We now compare results using the new radius parameterization to that from Geant4, both to radii measurements and inelastic cross sections. Figure 1 shows the nuclear radii models as a function of number of neutrons for light elements, compared to experimental values. In the current Geant4 model, a fixed radius is applied for Li (2.4 fm) and Be (2.51 fm). Above Z=4, the Geant4 model shows good agreement with the experimental radii in the region of stable isotopes, but typically underestimates the radii for neutron-rich isotopes. In addition, the Geant4 model has discontinuities at $A = 15$ and 20 where the paramerization used changes. The alternative model proposed here has good agreement in a whole number of neutrons range across B to F. It should be noted that the majority of the experimental values shown are actually derived from inelastic cross section measurements, and so the agreement with the alternative radius model ought to be good. However, the comparison illustrates that the new expression encapsulates the broad trends with proton-neutron asymmetry.

The dependence of the GG cross sections on the radius model were studied by comparing the cross sections of several projectile-target pairs, shown in Figure 2. For stable nuclides, we consider ^{12}C+^{12}C and ^{12}C+^{27}Al, as shown in left two figures of Figure 2, where there are extensive sets of data available. For ^{12}C+^{12}C both models agree reasonably well. For ^{12}C+^{27}Al, the alternative model is considerably better, with the GG version exhibiting a significant systematic overestimation of the data. Though our new model is specifically focused on improving the results for unstable situations, the ^{27}Al results suggest that more careful benchmarking of stable systems is urgently required. The other reactions, ^{14}C+^{12}C, ^{19}O+^{28}Si, and ^{16}N+^{28}Si, highlight the sparsity of experimental data for unstable systems, but the data are generally better described with the new radius model.

In summary, we have proposed an improved radius model suitable for calculations of nuclear inelastic cross sections of light nuclides with $A \leq 30$. The model shows better agreement with the experimental measurements of radii, particularly for unstable light isotopes when compared to the current model used in Geant4. As a result, there is improved agreement with experimental inelastic cross sections. The disagreement between the existing Geant4 model and the data for ^{12}C+^{27}Al indicate more comprehensive benchmarking is required.

A number of further improvements may be made. The expression used for the barrier energy V_B could be improved by careful analysis of available low-energy inelastic cross sections (see e.g., [24]) including comparisons for unstable nuclides where available. The parameterizations of σ_{pp} and σ_{np} could also be improved to remove the slight discontinuities near 300 and 500 MeV/nucleon. Though not the focus of this paper, improvements must also be made for heavier systems. This will require a different approach to the one taken here, since very little experimental data is available, and the density distributions for $A > 30$ nuclides are non-Gaussian.

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References

[1] S. Agostinelli *et al.*, Nucl. Instrum. Meth. A, 2003; 506: 250-303.
[2] J. Allison *et al.*, Nucl. Instrum. Meth. A, 2016; 835: 186-225.
[3] E Haettner, H. Iwase and D. Schardt, Rad. Prot. Dos., 2006; 122: 485-487.
[4] R. J. Glauber, In Lectures in Theoretical Physics, ed. WE Brittin and LG Dunham, New York: Interscience, 1959; 1 :315.
[5] B. Z. Kopeliovich, Phys. Rev. C, 2003; 68: 044906.
[6] M. L. Miller *et al.*, Annu. Rev. Nucl. Part. Sci., 2007; 57: 205–43.
[7] V. N. Gribov, Yad. Fiz., 1969; 9: 640 [Sov. J. Nucl. Phys., 1969; 9: 369].
[8] V.V.Zerkin *et al.*, Nucl. Instrum. Meth. A, 2018; 888: 31.
[9] A.Ozawa *et al.*, Nucl. Phys. A, 2001; 691: 599–617.
[10] E. Liatard *et al.*, Euro Phys. Letts., 1990; 13: 401.
[11] L. Chulkov *et al.*, Nucl. Phys. A, 1998; 603: 219.
[12] A. Ozawa *et al.*, Nucl. Phys. A,1996; 608:63
[13] I. Tanihata *et al.*, in: W.D. Myers, J.M. Nitschke, E.B. Norman (Eds.), Proc. 1st Int. Conf. on Radioactive Nuclear Beams, World Scientific, Singapore, 1990, p. 429.
[14] Kox *et al.*, Phys. Lett. B, 1985; 159(1): 15–18.
[15] Kox *et al.*, Nucl. Phys. A, 1984; 420(1): 162–172.
[16] Takechi *et al.*, Phys. Rev. C, 2009; 79: 061601.
[17] Zhang *et al.*, Nucl. Phys. A, 2002; 707(3–4): 303–324.
[18] Fang *et al.*, Phys. Rev. C, 2004; 69: 034613.
[19] A.C.C.Villari *et al.*, Phys. Lett. B, 1991; 268(3–4): 345–350.
[20] A.Khouaja *et al.*, 2006; 780(1–2): 1–12.
[21] V. M. Grichine, Europ. Phys. J. C, 2009; 62(2): 399–404.
[22] V. M. Grichine, Nucl. Instrum. Meth B, 2009; 267(14): 2460–2462.
[23] V. M. Grichine, Nucl. Instrum. Meth B, 2018; 427: 60–62.
[24] S. Kox *et al.*, Phys. Rev. C 35, 1678 (1987).

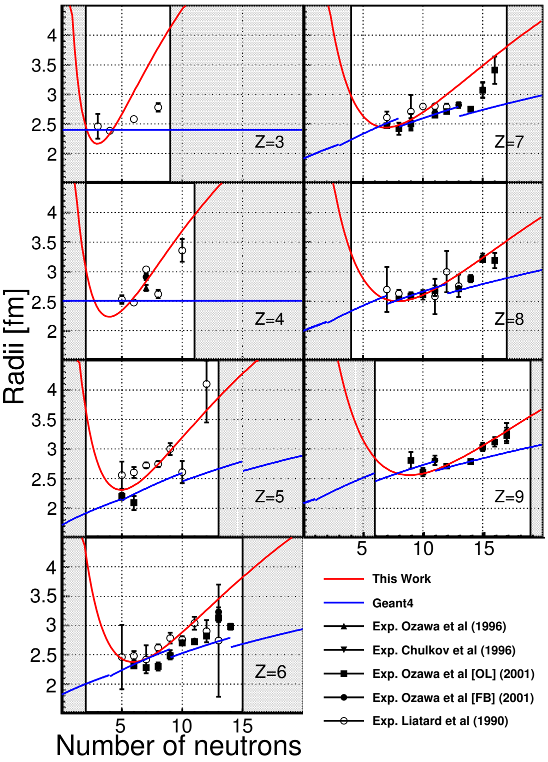

Figure 1: Nuclear radii as a function of number of neutrons for different light elements. The grey bands indicate the proton (left) and neutron (right) driplines where the nuclides are no longer bound.

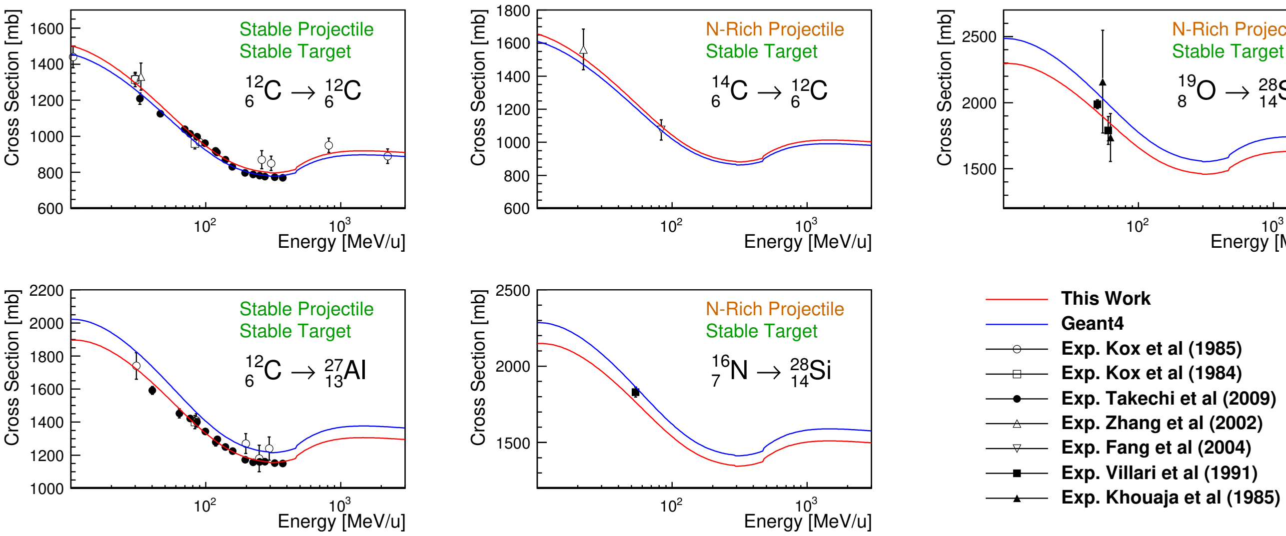

Figure 2: Integrated GG cross sections as a function of kinetic energy of the projectile. The existing GG model is shown in blue, and the version presented here shown in red.