Study on Transport Properties of Charged Particles in Plasmas Based on GEANT4 and the Modified LP Theory

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Abstract

For controlled nuclear fusion, it is of significance to develop a comprehensive simulation environment for Inertial Confinement Fusion(ICF) . This environment must accurately calculate the energy loss of charged particles in high-temperature, high-density plasma, and simulate the physical parameters of fusion reactions and products. This study presents a novel implementation of a modified Li-Petrasso (MLP) energy loss theory within the Geant4 framework, to address the critical challenge of simulating charged particle transport in high-temperature, high-density plasma for ICF research. The modified theory integrates binary collision terms, collective plasma effects, and quantum degeneracy corrections, enabling accurate calculations of stopping power, mean collision path, and energy transfer dynamics for particles such as recoil alpha particles, deuterons, and tritons under extreme plasma conditions. This work provides a detailed introduction to how to embed and calculate this process within Geant4 and verifies the correctness of the embedded model. Full simulation of the fusion process is also conducted. The results demonstrate that the improved Geant4 can effectively handle the energy loss of charged particles in such environments, calculate important fusion parameters like neutron energy spectrum and energy transfer ratios, and observe the production of ultra-high-energy neutrons. Comparisons with experimental fusion data show significant improvements in consistency, validating the improved Geant4's validity and accuracy. This work has, for the first time, achieved full simulation of charged particle energy loss and secondary neutron spectrum of ICF using Geant4, providing valuable insights into ICF characteristics and aiding in the development of more accurate fusion simulations.

Full Text

Study on Transport Properties of Charged Particles in Plasmas Based on Geant4 and the Modified LP Theory∗

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For controlled nuclear fusion, it is crucial to develop a comprehensive simulation environment for Inertial Confinement Fusion (ICF) that can accurately calculate the energy loss of charged particles in high-temperature, high-density plasmas and simulate the physical parameters of fusion reactions and products. This study presents a novel implementation of a modified Li-Petrasso (MLP) energy loss theory within the Geant4 framework to address the critical challenge of simulating charged particle transport in high-temperature, high-density plasmas for ICF research. The modified theory integrates binary collision terms, collective plasma effects, and quantum degeneracy corrections, enabling accurate calculations of stopping power, mean collision path, and energy transfer dynamics for particles such as recoil alpha particles, deuterons, and tritons under extreme plasma conditions. This work provides a detailed introduction to the embedding and calculation of this process within Geant4 and verifies the correctness of the embedded model. A full simulation of the fusion process is also conducted. The results demonstrate that the improved Geant4 can effectively handle the energy loss of charged particles in such environments, calculate important fusion parameters like neutron energy spectrum and energy transfer ratios, and observe the production of ultra-high-energy neutrons. Comparisons with experimental fusion data show significant improvements in consistency, validating the validity and accuracy of the improved Geant4. This work has, for the first time, achieved a full simulation of charged particle energy loss and secondary neutron spectrum in ICF using Geant4, providing valuable insights into ICF characteristics and aiding in the development of more accurate fusion simulations.

Keywords: ICF; Monte Carlo; Geant4; Energy Loss; Li-Petrasso Theory

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INTRODUCTION

Controlled nuclear fusion is a promising solution to the future energy crisis and one of the key scientific challenges to overcome. There are two main approaches to controlled nuclear fusion: Magnetic Confinement Fusion (MCF) and Inertial Confinement Fusion (ICF) [1, 2].

ICF is a method of achieving nuclear fusion by utilizing the inertia of the fuel itself. Its core principle involves rapidly heating and compressing the fuel with high-energy laser or particle beams, bringing the fuel to a state of high temperature and high density within an extremely short period of time, thereby triggering nuclear fusion reactions [3, 4]. ICF typically uses deuterium-tritium (D-T) fuel, which is encapsulated within a small target capsule. The outer shell of the target capsule is usually made of appropriate materials (such as plastic or metal) to ensure uniform ablation under high-energy irradiation. The two approaches for target implosion are shown in Figure 1 [Figure 1: see original paper].

These D-T fuel pellets are driven by external energy pulses to be heated and compressed into a high-temperature, high-density plasma state. In this state, deuterium and tritium can overcome Coulomb repulsion and undergo nuclear fusion reactions [5, 6]. Various fusion reactions can occur, such as D-D fusion, D-T fusion, T-T fusion, and other secondary reactions. Among them, the fusion reaction with the largest reaction cross-section and the most energy release is D-T fusion, as shown in Eq. (1).

$$D + T \to \alpha(3.54\,\mathrm{MeV}) + n(14.1\,\mathrm{MeV})$$

Theoretically, this reaction releases 17.59 MeV of energy, producing an alpha particle with an energy of 3.54 MeV and a neutron with an energy of 14.1 MeV. After these high-energy neutrons and alpha particles are emitted, they will be slowed down in the material, transferring their energy to the surrounding deuterons and tritons. This process leaves the ions in a relatively high-energy state when they participate in subsequent fusion reactions. As the energy of the deuteron and triton involved in the reaction increases, ultra-high-energy neutrons with energies greater than 15 MeV can be produced. Frenje et al. [7] have elucidated the process of generating ultra-high-energy neutrons, as shown in Figure 2 [Figure 2: see original paper]. In 2020, Hayes et al. [8] conducted advanced experiments on ultra-high-energy neutrons with NIF.

Currently, many large-scale laser ICF facilities are in operation around the world, such as the NIF in the United States [9], the LMJ in France [10], and the SG-III in China [11]. The NIF, located at Lawrence Livermore National Laboratory in the United States, can deliver 192 laser beams with a total energy of 2.05 MJ at a wavelength of 351 nm [12]. LMJ is located in France and can output 178 laser beams with a total energy of 1.4 MJ at a wavelength of 351 nm [13]. China's ICF research began in the 1970s with a proposal by Mr. Wang Ganchang to use lasers to drive nuclear fusion. SG-III is a high-performance, high-power neodymium glass laser facility developed under the leadership of the China Academy of Engineering Physics. It is the largest laser fusion facility in

Asia and the second-largest laser driver in the world, which can output 48 laser beams with a total energy of 180 kJ.

In laser ICF research, the study of transport properties of charged particles in high-temperature, high-density plasma has always been an important and challenging issue [14]. By characterizing the transport properties of charged particles in high-temperature, high-density plasma, it is possible to obtain information on energy deposition and charge exchange of ion beams in plasma. This, in turn, can help address key issues in controlled nuclear fusion, such as self-sustained burning and ion-driven ignition in ICF [15, 16]. However, despite relatively in-depth research on ion energy loss in conventional materials [17], studying the transport of charged particles in such high-temperature and high-density environments (with temperatures typically ranging from 1 to 30 keV and electron densities from $1 \times 10^{25}\,\mathrm{cm}^{-3}$ to $1 \times 10^{27}\,\mathrm{cm}^{-3}$) is extremely challenging. Currently, the focus of global research in this area is concentrated on studying ion energy deposition in plasma through theoretical analysis and numerical computation [18]. For example, the early Bethe theory (based on Coulomb collision theory) is capable of calculating the contributions of bound electrons and free electrons in plasma [19]. In 1993, Chi-Kang Li and Petrasso [20] proposed the Li-Petrasso (LP) theory based on the Fokker-Planck equation and Boltzmann equation, which includes both close-collision terms and long-range collective effect terms. In 2005, Brown et al. [21] introduced the Brown-Preston-Singleton (BPS) theory, which not only includes short-range Coulomb collision terms and long-range collective effect terms but also incorporates quantum degeneracy corrections. In 2017, Cayzac et al. [22] compared experimental data with computational results from LP and BPS theories, and the results showed that LP theory overestimated ion energy loss near the Bragg peak but performed well in the high-energy region. In 2019, Frenje et al. [23] conducted similar work using experimental data, indicating that BPS theory underestimated ion energy loss in the low-speed region, while both LP and BPS theories performed well in the high-speed region. At the same time, Zylstra [24] made improvements to LP theory by revising the velocity ratio parameter, refining the Coulomb logarithm, correcting the relative velocity calculations, and incorporating the treatment of electron degeneracy effects. These modifications enhanced the model's performance in the high-speed region, making it suitable for calculating the energy loss of charged particles in ICF, especially in diagnostics and self-heating modeling. In April 2025, Archubi and Arista proposed a semi-classical dielectric function model combining quantum electronic and classical ionic contributions and derived expressions for energy-loss moments [25]. In recent years, some experiments have been conducted successively. Based on the work of Malko et al. [26], Figure 3 [Figure 3: see original paper] presents some of the reported experiments.

It is evident from the figure that the majority of ion energy loss experiments are conducted under ideal plasma conditions, where the velocity of the incident particles exceeds the electron thermal velocity.

Geant4 is a Monte Carlo simulation software for particle transport developed by CERN, based on the C++ language, which has been updated to v11.3.1 [27], and this study is based on v11.3.1. Geant4 is widely used in various aspects ranging from medical physics to particle physics [28–30]. Compared with MCNP, a Monte Carlo simulation software developed by LANL, Geant4 supports more complex geometries and more detailed physical modeling [31, 32]. Both support transport calculations of many types of particles, including muons, mesons, and ions. However, licensing of MCNP is limited. In recent years, scholars have been exploring comparisons of Geant4 and MCNP for related calculations [33, 34].

Since conducting actual ICF experiments is extremely difficult and experimental data is extremely valuable, it is of great importance to explore a suitable energy loss model using limited available existing data. In recent years, many researchers have attempted to utilize Geant4 to conduct work in the field of fusion [35–38]. In 2022, Mohtashami et al. [39] explored fusion simulations using Geant4, but their study focused on non-extreme plasma conditions. Regarding the transport of charged particles in high-temperature and high-density plasma, if Geant4 can be used to achieve high-fidelity and accurate calculations, it will play an important role in promoting the academic community's understanding and verification of the properties of high-temperature plasma and will help humanity achieve controlled nuclear fusion sooner.

However, Geant4 has not yet implemented this functionality. The reason is that Geant4 is designed for cold calculations and does not include energy loss models for particles in high-temperature, high-density plasmas [40, 41].

To break through the challenge mentioned above, this work implements a charged particle transport module for high-temperature, high-density plasma within Geant4, based on a modified Li-Petrasso (MLP) theory. First, this work provides a detailed introduction to the MLP used in this work and discusses calculations and applicability of plasma environments. Second, the computational logic of Geant4 and the detailed implementation process of MLP within Geant4 are introduced. Correctness verification of the improved Geant4 is also implemented. Finally, the energy loss of recoil deuteron and triton, as well as the energy transfer distribution, mean collision path, energy spectrum, and output angle of fusion neutrons are calculated. These results are compared and analyzed with both experimental data and the original Geant4 calculation data, which proves the correctness and accuracy of this work.

INTRODUCTION TO THE MODIFIED LP THEORY

As mentioned in the introduction, the theoretical model used in this work is the modified LP theory proposed by Zylstra [24]. This section is divided into two parts. The first part briefly introduces the fundamental plasma parameters used in the calculations, while the second part provides a detailed explanation of the modified theory.

A. Fundamental Characteristics of Plasma

Plasma is a quasi-neutral gas composed of charged particles and neutral particles. Some important plasma parameters relevant to the calculations are introduced below [42].

(1) **Debye Shielding Effect**: Plasma has the characteristic of shielding external electric potentials, which is known as Debye shielding. It is this property that endows plasma with its electrical neutrality. The Debye shielding length for electrons is given by $\lambda_D = (cid : 113)\epsilon_0 T_f/(n_f e^2)$, where e_f is the field particle charge, n_f is the electron number density of the plasma, and T_f is the electron temperature in units of eV.

(2) **Plasma Frequency**: When a plasma in equilibrium is disturbed, the internal electric field induces collective motion to restore the quasi-neutral state. These collective motions can be described by the plasma frequency $\omega_{tf} = (cid : 113)f/m_f\epsilon_0$, where m_f is the mass of field particle, and $n_f e^2 n_f$ is the particle number density.

(3) **Coupling Effect**: The coupling effect coefficient characterizes the interaction intensity between particles within the plasma as well as between incident particles and field particles. The coupling coefficient within the plasma is given by $\Gamma_{ij} = Z_i e Z_j e^2/(4\pi\epsilon_0 r_0 T)$, where $Z_i e$ and $Z_j e$ are charge numbers of particle species i and j in the plasma, and r_0 is the Wigner-Seitz radius of the electrons. Plasma with a coupling coefficient much less than 1 is called ideal and weakly collisional plasma and can be described using linear theory.

(4) **Electron Degeneracy**: The electron degeneracy parameter is a physical quantity that determines whether electrons in a plasma are in a degenerate state. It is defined as the ratio of electron temperature T_e to Fermi energy E_F, which is $\Theta = k_B T_e$. When the electron degeneracy parameter is much greater than 1, the plasma is in a non-degenerate state, and effects of electron degeneracy can be neglected.

Plasmas are commonly classified in two ways. The first classification is based on density and temperature, dividing plasma into relativistic, non-relativistic, and quantum degenerate plasma. Among them, plasma with temperatures $T > 551$ keV is classified as relativistic plasma. The second classification is based on the strength of interactions, distinguishing between ideal and non-ideal plasma. The common classifications of natural and laboratory plasma are shown in Figure 4 [Figure 4: see original paper].

B. Modified LP Theory

The core equation of the MLP is given in Eq. (2), and the overall stopping power is composed of both binary collision term and collective effect term.

$$(cid:19)^2(cid:18)Z_{pe}(cid:26)G(x_{p/f})\ln\Lambda_b+(cid:19)(cid:18)\omega_{pf}\lambda_D(cid:19)(cid:18)\omega_{pf}\lambda_D(cid:19)(cid:$$

where Z_p is the charge number of incident particle, v_p is the velocity of incident particle, $G(x_{p/f})$ is the modified Chandrasekhar function, $x_{p/f}$ equals v_f^2, $\ln\Lambda_b$ is the Coulomb logarithm and K_0 and K_1 are the irregular modified cylindrical Bessel function of the zeroth and first order, respectively, describing the contribution of collective plasma effects.

For binary collision term, $G(x_{p/f})\ln\Lambda_b$ describes energy loss due to Coulomb collisions between incident particles and field particles (including electrons and ions) expressed as Eq. (3)(4)

$$G(x_{t/f}) = \mu(x_{t/f})-(cid:26)\frac{d\mu(x_{t/f})}{dx_{t/f}}\ln\Lambda_b(cid:20)\mu(x_{t/f})+(cid:21)(cid:27)\frac{d\mu(x_{t/f})}{dx_{t/f}}$$

$$\mu(x_{t/f}) = (cid:112)x_{t/f}) - (cid:112)x_{t/f}e^{-x_{t/f}}\mathrm{erf}($$

For collective effect term, $(\omega_{pf}\lambda_D)K_{0K}1$ quantifies the energy loss due to collective plasma oscillations. This term degenerates into a logarithmic form in the high-speed limit ($v_p \gg \omega_{pf}\lambda_D$); however, at low or moderate speeds, the complete Bessel function expression is required.

The modified Coulomb logarithm is expressed as Eq. (5)(6)

$$\ln\Lambda_b = \ln[1 + ((cid:115)p_{\min} = (cid:18)\hbar(cid:19)^2$$

where $p_{\min}$ represents the minimum collision parameter, and $L = Z_p e_f/m_r\mu^2$ represents the classical minimum collision parameter, where u is the relative velocity and m_r is the reduced mass of incident and field particles.

Here u is expressed as Eq. (7).

$$(cid:115)2k_BT_fm_fv^2 2k_BT_f+v_p(cid:18)(cid:19)m_fv^2(cid:32)(cid:115)(cid:33)m_fv^2 2k_BT_f$$

when $v_p \ll v_f$, $u \approx (cid:112)8k_BT_f/\pi m_f$, while if $v_p \gg v_f$, $u \approx v_p$.

And in degenerate regimes where the Fermi energy can be comparable to the thermal temperature, the theory introduces an effective temperature expressed as Eq. (8).

$$T_{\mathrm{eff}} = T_e\frac{F_{3/2}(\mu_e/k_BT_e)}{F_{1/2}(\mu_e/k_BT_e)}$$

where F_j is the Fermi integral and μ_e is the chemical potential. For more details, please refer to the reference.

This theory unifies the contributions of binary collisions and collective effects to energy loss, and is applicable to a wide range of conditions, from classical to quantum, and from weakly coupled to strongly coupled plasma. Moreover, the modified parameters such as the Coulomb logarithm, relative velocity, and effective temperature have significantly enhanced the model's accuracy in both high-speed and low-speed limits.

IMPLEMENTATION OF MLP IN GEANT4

Regarding the usage of Geant4, CERN has already provided detailed documentation. This section mainly focuses on the source code coupling related to the MLP and verification of its correctness. The nuclear data libraries used in this work are the default libraries of Geant4, such as ENDF/B-VIII.0, JEFF-3.3, and ENSDF, etc.

A. Construction of Calculation Module of MLP

An overview of the process is shown in Figure 5 [Figure 5: see original paper]. Within the Geant4 kernel, three essential classes must be registered: DetectorConstruction, PhysicsList, and PrimaryGeneratorAction. G4-MT is also used for accelerating computation. First, modeling plasma materials involves specifying key information such as material density, temperature, and geometry in DetectorConstruction. Second, in PrimaryGeneratorAction, key information of incident particles, such as position, emission direction, energy, and type, is defined. Finally, the PhysicsList class is responsible for registering the physical processes involved in the simulation. G4-MT cross-thread mode is employed for parallel computing, which greatly improves the efficiency of Monte Carlo simulations. In this work, the stopping power process model for incident particles is replaced with MLP. Additionally, elastic and inelastic collision models are registered to ensure proper functioning of fusion reactions. The calculation of stopping power includes three parts: electron stopping (dE_e/dx), ion stopping (dE_i/dx), and collective effect stopping (dE_c/dx).

In summary, the physics list used in this work is presented in Table 1 . This work has created two calculation models, G4ionLPStopping and G4eLPStopping. The electron stopping power is calculated in G4eLPStopping, while ion stopping power and the contribution from collective effects are computed in G4ionLPStopping. Other physical processes continue to use the default models of Geant4. Pseudo-code for the calculation of electron stopping power, ion stopping power, and stopping power due to collective effects is shown in Table 2 . This computational procedure aligns with the theoretical framework described in Section II B.

After embedding the model, UserSteppingAction is employed to tally the energy loss of incident particles at each step and the occurrence of fusion reaction. It can also tally the energy released by various reactions, as well as the yield, energy spectrum, and emission angles of secondary particles generated. The results are stored as histograms in a ROOT-format file. Pseudo-code for this part is shown in Table 3 .

B. Correctness Verification of MLP in Geant4

To verify the correctness of the coupled model, this section constructs a fusion scenario to calculate the energy loss of alpha particles with an initial energy of 3.54 MeV. The physical modeling in Geant4 is shown in Figure 6 [Figure 6: see original paper], with high-temperature, high-density D-T plasma as the background environment. The particle source is placed at the center of the material and emits isotropically, and in each simulation, 5 million particles are emitted. In this section, following the simulation environment of reference [24], only energy loss due to electromagnetic processes is considered, without taking elastic, inelastic, and other processes into account, as shown in Figure 6 A. The reason for conducting this simulation is to facilitate the comparison of the calculation results with those in the reference literature, as the reference literature only considered the electromagnetic energy loss process during the calculations. However, in Section V and Section IV, all the complete physical processes are taken into consideration, as shown in Figure 6 B.

Figure 7 [Figure 7: see original paper] shows the stopping power results of the LP theory and the BPS theory from the reference, and the MLP from the present work with α particles as the incident particles. It should be noted that in the figures of this paper, S_e is used to represent the electron stopping power, while S_i is used to represent the stopping power due to ion stopping. Near the Bragg peak, the calculation results are about 30% - 60% higher than those of the BPS theory, which is also the main drawback of the MLP according to reference [22].

In the MLP, the collective effect term is strictly based on the ratio of Debye length to velocity. This modification leads to a readjustment of the contribution from the collective effect term, particularly near the Bragg peak ($x_{t/f} \approx 1$), where the revised theory exhibits higher stopping power. Moreover, near the Bragg peak, the particle velocity approaches the plasma thermal velocity, and the contribution of large-angle Coulomb scattering is significantly enhanced. Although the MLP is derived from the Fokker-Planck equation and attempts to incorporate both binary collisions and collective effects, its approximation of strong scattering may be inadequate to fully capture the complex dynamics near the Bragg peak, resulting in discrepancies in predictions. In other energy ranges, the results from all three models show good agreement. The cause of the increasing discrepancy between the results of this work and those of the reference LP literature as particle energy increases may be attributed to limitations in how the present model handles the relative velocity between the incident particles and the background particles when the incident particles are in a high-energy state.

According to reference [43], incident particles in plasma do not lose energy completely. Once their energy decreases to the minimum value E_m, the incident particles no longer exchange energy with the electrons or ions in the plasma. In this work, the definition of range refers to the definition given by He Bin et al. [44], that is, the distance traveled by the incident particles as their energy decreases from E_0 to E_m. The selection of E_m needs to ensure that the electron stopping power and the ion stopping power remain positive, and its value is close to the maximum of electron and ion temperature. Figure 8 [Figure 8: see original paper] shows the calculation results of the range. As shown in the figure, the particle range increases with ambient temperature.

The primary reason is that the increase in the thermal velocity of the background particles reduces the relative velocity difference between the incident particles and the background particles, thereby decreasing the efficiency of energy transfer, which means that the energy loss of the incident particles decreases. Although changes in the Coulomb logarithm or degree of ionization may have secondary effects, the dominant role of the thermal velocity leads to an overall downward trend, resulting in an increase in the range. As the particle energy decreases, the electron stopping power gradually declines, while the ion stopping power increases. However, once the energy drops to the minimum threshold, a sudden drop in the ion stopping power occurs. Range also decreases with the increase of electron number density as the number of effective collisions between particles in the plasma and the incident particles has increased.

IV. CALCULATION AND VALIDATION OF ENERGY LOSS FOR PARTICLES

Building on the previous section's calculation of energy loss and range for α particles, this section focuses on recoil tritons and deuterons. The physical modeling and physics list in Geant4 are shown in Figure 6 B. The recoil deuteron and triton energy spectrum are obtained using a nuclear database visualization program called JANIS 4.0 (Java-based nuclear information software) developed by the Nuclear Energy Agency (NEA) [45].

The recoil energy spectrum data from the ENDF evaluation database are exported in JANIS and processed according to the method given by Knoll to obtain the results [46]. As shown in Figure 9 [Figure 9: see original paper], the maximum energy of the recoil deuteron is 12.5 MeV with a peak cross-section of 123 mb, and the maximum energy of the recoil triton is 10.5 MeV with a peak cross-section of 78 mb. Therefore, in the subsequent energy loss calculations, the energy of the recoil deuteron ranges from 0 to 12.5 MeV, and the energy of the recoil triton ranges from 0 to 10.5 MeV.

The fraction of energy E_i transferred to the ions in the plasma and the fraction of energy E_e transferred to the electrons by the incident particles with initial kinetic energy E_0 can be expressed as Eq. (9)(10). This section focuses on the ratio of energy transferred to ions relative to the initial energy of incident particles, denoted as $\eta = E_i/E_0$.

Figure 10 [Figure 10: see original paper] illustrates η for both recoil deuterons and tritons, respectively. It can be observed that under the same temperature conditions, the electron number density is positively correlated with η. Here, the electron number density is the independent variable, while η is the dependent variable. However, when the electron number density increases to a certain extent, the transfer ratio tends to saturate.

In the low-energy region ($v_p \ll v_i$), the stopping power of ions plays a dominant role, and in contrast, in the high-energy region ($v_p \gg v_e$), the stopping power of electrons is dominant. For example, taking the deuteron energy as 2 MeV, when the environmental temperature is 3 keV, the thermal velocity of the background electrons is less than the velocity of the incident deuterons, and thus the ion stopping power does not dominate. The maximum value it can reach is only 0.16, as shown by the orange line in Figure 10(a) [Figure 10: see original paper]. When the environmental temperature is 30 keV, the thermal velocity of the background ions is greater than the velocity of the incident deuterons, and at this point, the ion stopping power dominates and increases with the material density, reaching a maximum of 0.62, as shown by the orange line in Figure 10(b) [Figure 10: see original paper].

A comparison between (a) and (b), or (c) and (d), reveals that the plasma temperature also influences η. A higher ambient temperature implies a higher thermal velocity of the background particles, allowing the stopping power of the ions to dominate at a lower energy range. A higher value of η is conducive to the generation of higher-energy ions in the environment, which is an important factor in maintaining self-sustained fusion. Observations in low-density regions reveal that η of low-energy recoil deuterons and tritons may also exceed η of high-energy recoil deuterons and tritons at specific densities and temperatures, as shown in the crossing area of the lines in the lower left corner of the graph in Figure 10(d) [Figure 10: see original paper], further illustrating that energy loss of charged particles in high-temperature and high-density plasma is a nonlinear process.

Figure 11 [Figure 11: see original paper] shows the calculation of mean collision path (λ) with recoil deuterons and recoil tritons as the incident particles. The mean collision path represents the average distance between two consecutive elastic or inelastic collisions of charged particles when considering electromagnetic energy loss. As seen from the figure, the improved Geant4 calculates a mean collision path 5 to 10 times that of the original Geant4. This is because the original Geant4 used G4BraggModel, G4BetheBlochModel, and G4ICRU49NuclearStoppingModel to calculate the energy loss of recoil deuteron and triton. These models cannot accurately handle electromagnetic energy loss in plasma under high-temperature and high-density conditions, overestimating stopping power contributions from electrons and ions, thus causing a decrease in mean collision path. After embedding the MLP, it can be anticipated that more deuteron and triton will remain in relatively high energy states, leading to more fusion reactions and more fusion neutrons. This difference is also reflected in neutron calculation in the following section.

For further clarification, the following test is performed. Figure 12 [Figure 12: see original paper] shows a comparison with calculation under ambient temperature and low density conditions. Although the mean collision paths for both cases increase with the energy of incident deuterium particles, the energy loss in plasma is significantly greater than in conventional materials. This is due to the more pronounced effects of electron and ion stopping power and collective effects in high-temperature and high-density plasma. This leads to a much higher recoil particle range in normal materials than in extreme environments. Figure 13 [Figure 13: see original paper] shows the calculated total stopping power for plasma density ranging from 10 to 1000 g/cm^3 and temperature from 3 keV to 30 keV. The MLP has higher computational accuracy at extremely low and high velocities and is applicable to a wide range of plasma conditions, from classical to quantum and from weakly coupled to strongly coupled. However, it still fails to address the issue of overestimation of stopping power near the Bragg peak.

V. CALCULATION AND VALIDATION OF FUSION NEUTRON

This section presents the calculations of neutron energy spectrum and emission angles in D-T fusion reactions. The physical modeling and particle source settings are referenced from Figure 6, whose density is 50 g/cm^3 and temperature is 30 keV. It should be noted that only the secondary neutrons produced by the D-T fusion reaction are considered in this study, as this is the most significant and highest-energy-yielding reaction in fusion. Neutrons from other reactions are currently excluded from the analysis. As mentioned in Section III A, UserSteppingAction is employed for tallying. Whenever secondary neutrons are produced, their information is retained or discarded based on their origin. It also records the number of D-T fusion events and the associated energy release. This section does not consider subsequent reactions of secondary particles, such as the recoil deuteron colliding with ambient particles and reacting again. However, this process is crucial, as it is an important mechanism for plasma self-heating and the production of ultra-high-energy neutrons.

The overall neutron energy spectrum is shown in Figure 14 [Figure 14: see original paper]. As the energy of deuterium increases, the spectrum gradually broadens, the percentages of neutrons in the medium-energy region decrease, and ultra-high-energy neutrons with energies higher than 15 MeV begin to appear. This has provided certain insights for the experimental production of such ultra-high-energy neutrons.

Figure 15 [Figure 15: see original paper] illustrates the spectrum with output angles θ for deuteron sources with energies of 200 keV, 400 keV, 600 keV, and 800 keV. The angle has been divided equally into twenty parts. For a deuteron with an energy of 200 keV, the energy spectrum broadens from 13.14 MeV to

15.13 MeV. For 400 keV, it broadens from 12.86 MeV to 15.64 MeV. For 600 keV, it broadens from 12.68 MeV to 16.04 MeV, and for 800 keV, it broadens from 12.50 MeV to 16.44 MeV. Overall, the secondary neutrons are emitted isotropically. It should be noted that the term "isotropically" here is used in the context of simulations with the same deuteron energy. That is to say, when $E = 200$ keV, the neutron flux at each angle tends to be consistent, as shown in Figure 15(a) [Figure 15: see original paper]; when $E = 400$ keV, the neutron flux at each angle tends to be consistent, as shown in Figure 15(b) [Figure 15: see original paper], and so on.

In 2022, Youssef et al. [47] compared experimental data of fusion reactions with simulation results from Geant4, MCUNED, ENEA-JSI, and DDT codes. The results showed that the Geant4 simulation data had poor agreement with the experimental data. To further verify this work, a Geant4 model was constructed for simulation calculations according to the experimental conditions of the reference. The model was set with a D-T plasma of density 50 g/cm^3 and temperature 3 keV within a sphere of radius 1.8 cm, and deuterons with an emission energy of 180 keV. Figure 16 [Figure 16: see original paper] shows the neutron spectrum of the reference, original Geant4, and this work. The comparison indicates that the neutrons in this work are mainly concentrated in the intermediate energy range, and the spectrum broadening is less pronounced than in the reference.

It is speculated that the reasons for this difference are as follows. First, the simulation conditions may not be completely consistent with the experimental conditions. Second, it also indicates that the improved Geant4 is not entirely accurate and still needs to be further refined in subsequent work. However, compared with the results from the original Geant4 simulations, the outcomes of this study demonstrate significant improvements.

VI. CONCLUSION

This study implemented a modified Li-Petrasso (LP) energy loss theory within the Geant4 framework to address the transport properties of charged particles in high-temperature, dense plasmas, a critical challenge in ICF research. By incorporating binary collision terms, collective plasma effects, and quantum degeneracy corrections, the enhanced model enables accurate calculations of stopping power, mean collision path, and energy transfer dynamics for particles such as α particles, recoil deuterons, and recoil tritons under extreme plasma conditions. The results show that the improved Geant4 is able to calculate the energy loss of charged particles in extreme environments. It is capable of calculating important parameters in the fusion process, such as neutron spectrum and energy transfer ratios, and it can also compute the production of ultra-high-energy neutrons. Additionally, this work has been compared with experimental data, and the results demonstrate a significant improvement in consistency with the experimental data, thereby validating the accuracy of the work. For the first time, this study completed a relatively complete simulation of charged particle energy loss and secondary neutron spectrum in D-T fusion using Geant4.

However, the results show that there is still a drawback around the Bragg peak. It can help researchers understand the characteristics of ICF and achieve more accurate fusion simulations. Future work should focus on continuously improving the computational model, investigating the secondary neutron spectrum in different fusion reactions, researching the production of ultra-high-energy neutrons, and exploring the energy deposition of secondary particles in plasmas.

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