ELEMENTARY PARTICLE PHYSICS AND FIELD THEORY

Simulation of nuclear relaxation in Geant4 hadronic physics

N. A. Chalyi · V. N. Ivanchenko

Received: 18 August 2025 / Revised: 2 October 2025 / Accepted: 20 October 2025

Abstract
This work presents the latest developments of the pre-compound model and nuclear relaxation module simulated in Geant4 toolkit in view of the future experiments with the high-energy large hadron collider and the nuclotron-based ion collider facility in the moderate energy region. These processes have a significant impact on spectra of low energy neutrons, protons, and ions in nuclear interactions, which affect various application domains. The paper presents the model modifications and validation. Updated hadronic models created in Geant4 are included in the public release of Geant4 11.4.

Keywords Simulation · Geant4 · Nuclear de-excitation · Neutrons · Protons · Pre-compound model

Introduction

Geant4 simulation toolkit [1–3] includes a wide range of physical models for simulating hadron- and ion-nucleus interactions. At high (above several gigaelectronvolts) interaction energies, it is necessary to simulate the formation and decay of quark-gluon strings. For such energies, Geant4 uses the FTF [4, 5] and QGSM [6] models. Cascade models are used at moderate energies below several gigaelectronvolts. In Geant4, the main cascade models are BIC [7], BERT [8] and INCL++ [9, 10]. After the string formation and nuclear cascade, the wounded nucleus de-excites. Any hadronic model requires a nuclear relaxation mechanism describing de-excitation through the emission of neutrons, protons, light ions, and gamma rays. Models used for simulation of de-excitation are almost entirely data-driven, with the data collected in international databases (e.g., EXFOR) based on the analysis of many experiments. In all cases, a residual nucleus after a high energy hadronic interaction, remains in the excited state, which requires modeling the transition process of the nucleus to the equilibrium state. Some models, for example BERT, have algorithms for modeling the relaxation of excited nuclei. However, most of high-energy models use centralized models from Geant4 toolkit, namely the pre-compound model [11, 12] and the nuclear relaxation module, which, in turn, consists of the evaporation model [13, 14], multi-fragmentation [15], Fermi break-up decays [15, 16], fission [17] and nuclear gamma transitions [18].

Low-energy processes of hadron physics have a significant impact on the shape of hadron showers in calorimeters used in high-energy physics. These models are actively employed in ATLAS, CMS, and other CERN LHC experiments, as well as in the upcoming MPD and SPD experiments at the nuclotron-based ion collider facility (NICA) in Dubna, Russia. In collider experiments, the primary collision usually produces a wide energy spectrum of hadrons and ions. These particles interact with the material of detectors, in particular calorimeters. Multiple secondary protons and neutrons produced in nuclear fragmentation, make a significant contribution to the total energy delivered in calorimeters. In addition, low-energy hadron physics in Geant4,

 https://doi.org/10.1007/s11182-025-03618-6

Published online: 10 November 2025

is especially important in medical Monte Carlo applications, namely proton and ion therapy, in which the modeling accuracy directly depends on how well the production of low energy secondary neutrons and light ions is simulated.

This work presents reorganization of Geant4-simulated models of the nuclear relaxation. The aim of this reorganization is to prepare a set of low-energy models, which corresponds to new challenges of the new-generation experiments conducted in high energy physics. Reorganization includes principal modifications of the pre-compound model, which provides a smooth transition from the kinetic reaction stage governed by high-energy inelastic interactions to the equilibrium phase, which is described by the nuclear relaxation module models, in which the evaporation model plays an important role. The paper also presents a new algorithm of integrating and sampling one-dimensional probability density functions of final states optimized for the described models instead of disparate algorithms previously used in Geant4. Validation results are presented for Geant4 11.4beta. This software will be publicly released with the Geant4 version 11.4 in December 2025.

Architecture of nuclear relaxation module simulated in Geant4

The low-energy hadron interaction simulated in Geant4, is based on a consistent description of the nuclear relaxation stages, which is critical for reproducing the processes of fragmentation, evaporation and generation of secondary particles. Within this approach, the key role belongs to complementary models covering different energy regimes and types of nuclear decays. The new flow chart proposed in this work, is shown in Fig. 1. The main modification of the long-standing structure [3] involves a reposition of the multi-fragmentation model [15] in front of the pre-compound model. So, highly-excited heavy nuclei ($A > 50$) with the high excitation energy first decay into several lighter fragments, which de-excite separately with pre-compound and de-excitation models. This change in the order of models, allows creating adequate initial conditions for the pre-compound model assumed in the original prescription [11].

Two processes are considered in the pre-compound model [11]: an exciton transition or emission of neutron, proton, or light ion up to alpha. The sampling is performed *via* the de-excitation loop. In the updated model, checks are performed after each iteration, and the loop is interrupted, if one of the following conditions is satisfied:

- Residual $Z<9$ and $A<17$
- The exciton number reaches equilibrium
- The excitation energy of the residual nucleus is below the *Pre-compound min excitation*
- The excitation energy of the residual nucleus is below the *Pre-compound max excitation*

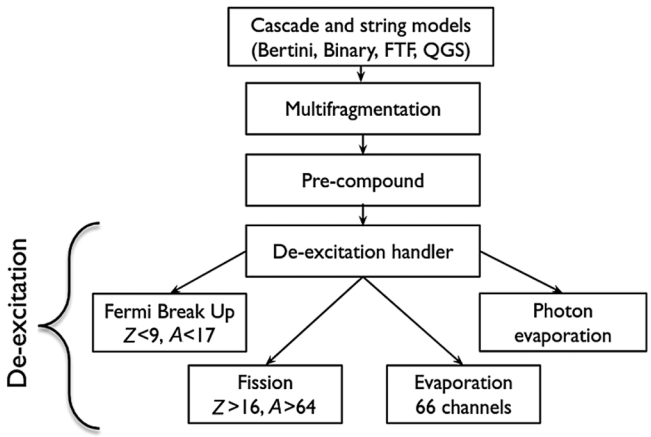

Fig. 1 Flow chart of hadronic physics simulated in Geant4 11.4

Table 1 Relaxation module parameters in Geant4 11.4.

Parameters	Default value, unit
Minimum energy per nucleon for the multi-fragmentation model	30, MeV/u
Pre-compound min excitation	100, keV/u
Pre-compound max excitation	30, MeV/u
Level density	0.075, 1/MeV
Tolerance	10, eV
Width of level	200, keV
Minimum lifetime	10 ns

Another modification shown in Fig. 1 is the Fermi break-up [16], which is now applied for any excitation energy of the light fragment at $Z<9$ and $A<17$. In previous Geant4 versions [3], there is a limited excitation energy, and the evaporation model is responsible for the light fragments decay with the high excitation energy. The choice of the energy limit is arbitrary and is not based on theoretical arguments. This reduces the possibility of improving the simulation accuracy. The new version allows using different models for the light fragment de-excitation, the only technical requirement is that such a model should follow the *G4VFermiBreakUp* interface and provide the final state sampling for any excitation energy of the primary fragment.

In the new version, after the pre-compound model, there is a choice (using Z and A) between the Fermi break-up and de-excitation models. De-excitation includes the possibility of fission, gamma transitions, and 66 evaporation channels. Computation of the emission probability of neutrons, protons, and light ions is based on the classical model [13].

After these modifications, the number of parameters used for sampling of relaxation was reduced. Table 1 summarizes the main parameters of the relaxation module. *Level density* of nucleons inside nuclei is a key parameter used in all models presented in Fig. 1. It defines probabilities of the emission of nucleons and nuclear fragments. De-excitation is performed as a chain of binary decays. After each decay, the residual nucleus may acquire the excited state. *Tolerance* is the numerical accuracy of the final nuclear level in the case with a quasi-stable residual isomer. *Width of level* is used for levels with very low lifetime. The de-excitation loop is stopped, if the residual fragment is in the ground or excited state with the lifetime longer than *Minimum lifetime*. In the new version, this time limit is closer to that in the Geant4 radioactive decay module. So, the excited isomer with the mentioned lifetime, can transport and further decay.

New method of integrating and sampling one-dimensional distributions

The proposed new method is intended for integrating and sampling one-dimensional distribution functions. In general, in Geant4 models, there are two types of the data used in the run time:

- The data initialized prior to the simulation of the first event, for example, cross section tables, which are kept in shared memory in the form of static *G4PhysicsTable* objects
- Dynamic distributions, which are different for each new sampling

The latter represents simulation of the nuclear relaxation. For any sampling of hadronic collision, the residual fragment is different, and its initial excitation energy is also different. The number of final opened channels and probability distribution functions are therefore also different. It is difficult to tabulate functions for each energy, because it requires a fine grid in energy and huge data structures. Thus, in the majority of relaxation models, the distribution function parameters are recomputed for each sampling. Let us introduce a new universal method implemented in the utility class *G4VSIntegration*, which provides functionality for the calculation of integrals

Table 2 Default *G4VSIntegration* parameter values for the nuclear relaxation

Parameters	Default values, unit
Accuracy	0.001
Reduction factor	0.25
Max factor	1.05
Energy bin	1, MeV
Min bin	0.1 MeV
Max bin	2 MeV

over the distribution function and sampling values of the random variable distribution for one-dimensional final state probability density functions. The key methods of this class include the following:

– *InitialiseIntegrator()*—initialization of integration parameters (see Table 2)
– *ComputeIntegral(Emin, Emax)*—calculation of the probability density function integral between *Emin* and *Emax*
– *SampleValue()*—the sample generation according to the given distribution between *Emin* and *Emax*
– *ProbabilityDensityFunction(E)*—returns the probability density value for a specific energy *E*

The integral over the probability density function $F(E)$ is computed to get the total probability of the given decay channel. This integration is performed numerically using the *Energy bin* defined in a user code (Table 2), depending on conversions of the integral, the bin size may be increased or decreased. *Min bin* and *Max bin* parameters limit the bin size value during this procedure. The integration procedure is limited by the value of the unitless parameter *Accuracy*. During this integration, the function is analyzed, and its maximum $F_{\max}$ is identified. For sampling, $F_{\max}$ value is multiplied by *Max factor* to preserve a correct estimation of the maximum. Two energies E_1 and E_2 are defined, which correspond to $F(E_1) = F_{\max} * q$, where q is the reduction factor, $F(E_2) = F(E_1) * q$. Additionally, the remaining energy interval splits into two parts at the energy $E_3 = (E_{\max} -$

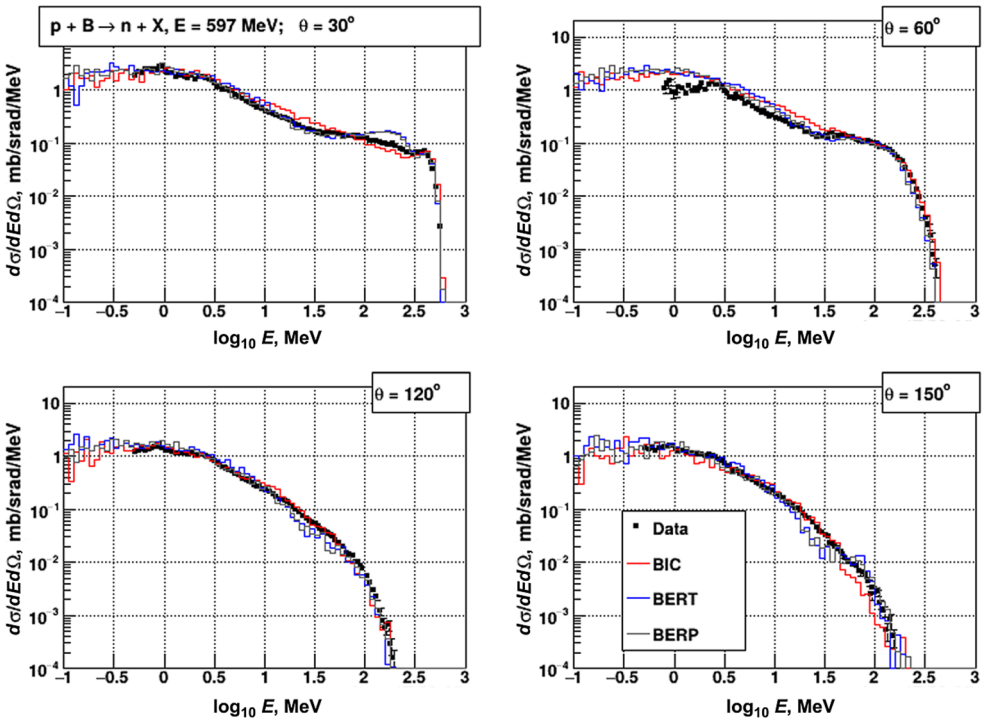

Fig. 2 Double-differential cross-section of neutron production by proton beam at 597 MeV at 4 different angles in boron as a function of the neutron kinetic energy. Points indicate the data from [19], histograms for Geant4 predictions: *BIC* Binary cascade [7], *BERT* Bertini cascade [8], *BERP* Bertini cascade with the Geant4 native pre-compound model

E_2)/2. As a result of integration, the function is prepared for the energy sampling using four energy intervals, the maximum of probability density function being checked in each interval. The default set of parameters for relaxation models (see Table 2) is obtained from the testing suite based on the EXFOR data for setups from different experiments with the beam energy ranging from 14 MeV to 3 GeV, and several targets from lithium to uranium. Using a significant number ($>10^7$) of events, no case is observed when $F(E)$ exceeds $F_{\max}$ value.

This method is effective for probability density functions of pre-compound and de-excitation models. The typical function is shown in Figs. 2 and 3. One can see double differential distributions of the neutron production from the boron and oxygen targets. This energy spectrum at any polar angle has one wide peak at the low neutron energy and a long tail up to the maximum neutron energy. The method is effective for this case, as it allows sampling the long tail with a sharp decrease in the probability density function for the high energy secondary emission, which exists in many cases of pre-compound or evaporation decays. The speed-up effect for usage of this method may not be visible in ordinary simulation, because the nuclear relaxation in the current Geant4 does not require a significant simulation time. In previous Geant4 versions, the relaxation was significantly optimized.

For high energy physics experiments, the total simulation time between previous versions 11.3 and 11.4 is not seen, because it has already been partially implemented in de-excitation models. The advantages of the new method include unification of the approach to integrating and sampling the random variable distribution for arbitrary one-dimensional functions of the probability density of final states, reducing the computational load and enhancing the possibility of adaptation to other physical models. For example, in low-energy applications like Geant4 DNA physics simulation, the effect from using the new utility may be a factor two or even more. An important advantage of the new utility is the possibility to customize parameters for a consumer.

Results and discussion

The pre-compound model [11, 12] describes the intermediate phase between the primary inelastic collision and thermodynamic equilibrium, considering the particle emission before a complete system thermalization. Its application is relevant for nuclei with the excitation energy ranging from tens to hundreds of megaelectronvolts, where the “memory” of the initial state of the system is yet preserved.

The evaporation model [13] describes the thermal-equilibrium stage, simulating the nucleon and light-cluster emission (e.g., α-particles) through a probabilistic account of the level density of the daughter nucleus, cross-section of back reactions and kinematic constraints. This approach dominates at low excitation energies and predicts secondary particle spectra, including angular distributions.

The Fermi break-up model [15, 16] is used for light nuclei ($A<17$) with the high excitation energy. The model assumes a fragmentation into several light nuclei without the intermediate thermalization stage. The decay probability is calculated through the phase space of available channels, 4-momentum conservation is built-in due to the two-body decay. In the default Fermi break-up model, the total number of decay channels is 991.

The change in the overall design of the de-excitation module allows more flexible combination of sub-models for sampling the nuclear relaxation and more simple usage of alternative models. The number of parameters used for the model steering, is reduced. These modifications are essential for a simulation of future experiments, in which more strong requirements are applied for the accurate simulation in Geant4. These are Phase-2 LHC experiments and experiments with NICA. In NICA, the energy of hadrons or ions produced in a collision, is below 10 GeV. Therefore, cascade models should be used for the description of such interaction. Testing setups with the data from EXFOR are adequate to this task. In our previous research [12], we present validation results for moderate heavy targets. In this work, we compare Geant4 predictions for the double-differential cross-section for light targets. As shown in Figs. 2 and 3, for 597 MeV beam, three cascade models (Binary cascade, Bertini cascade, and INCL++) describe the data well with almost similar accuracy. In these experiments, the

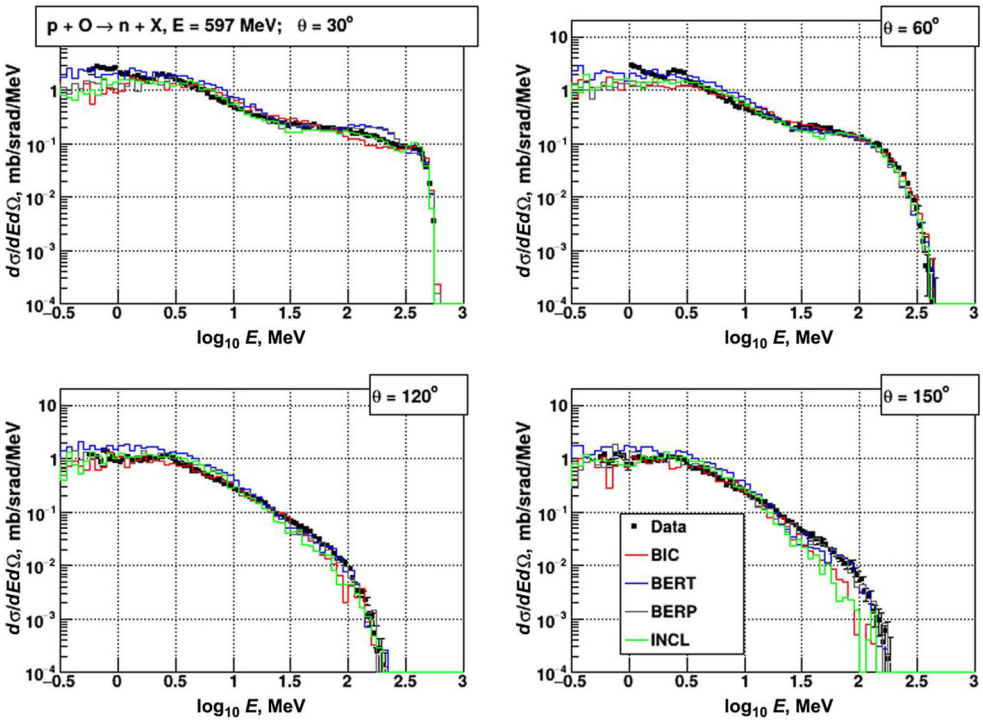

Fig. 3 Double-differential cross-section of neutron production by proton beam at 597 MeV at 4 different angles in oxygen as a function of the neutron kinetic energy. Points indicate the data from [19], histograms for Geant4 predictions: *BIC* Binary cascade [7], *BERT* Bertini cascade [8], *BERP* Bertini cascade with the Geant4 native pre-compound model, *INCL* INCL++ cascade [9, 10]

minimum polar angle for neutrons is 30 degrees. In the case of the forward scattering (Fig. 4), only the Binary cascade can reproduce the neutron flux.

Conclusions

This work presented a critical update to the Geant4 model configuration for nuclear relaxation simulations. These modifications were proposed in view of future HEP experiments, in particular, SPD experiment [21] at the NICA in Dubna, which is currently in progress. Modifications reported in this study, were supported by validation results showing a good simulation accuracy of the neutron production by the Binary cascade in light targets. In our previous research [12], we presented results for heavy targets. A new universal utility *G4VSIntegration* was introduced in Geant4, which is expected to be used not only by nuclear relaxation models

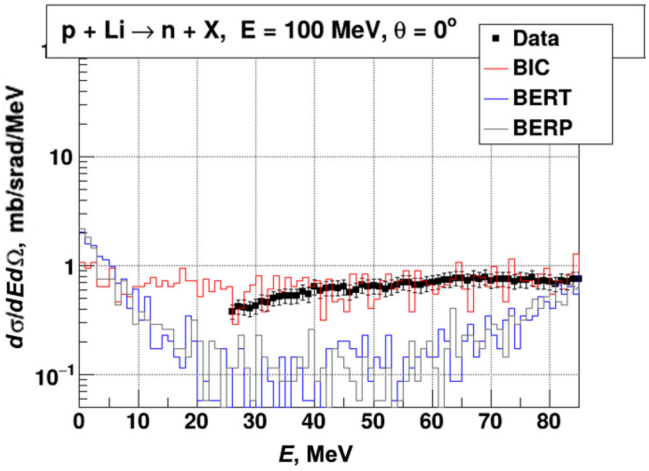

Fig. 4 Double-differential cross-section of neutron production by proton beam at 100 MeV in lithium as a function of the neutron kinetic energy. Points indicate the data from [20], histograms for Geant4 predictions: *BIC* Binary cascade [7], *BERT* Bertini cascade [8], *BERP* Bertini cascade with Geant4 the native pre-compound model, *INCL* INCL++ cascade [9, 10]

but also in other cases. All described modifications were included in the developed Geant4 version and will be publicly available in the new Geant4 release 11.4 in December 2025.

Funding This work was carried out under the government contract No. FSWM-2025-0023 of the Ministry of Science and Higher Education of the Russian Federation.

Author Contribution V.N.I. proposed and developed the model code and performed validation; N.A.C. developed test software, conducted tests and wrote the manuscript. Both authors have read and agreed to the published version of the manuscript.

Data availability The data are available on request.

Conflict of interest The authors have no competing interests to declare that are relevant to the content of this article.

References

1. Agostinelli, S., et al.: Geant4—a simulation toolkit. Nucl. Instrum. Meth. A **506**, 250–303 (2003). https://doi.org/10.1016/S0168-9002(03)01368-8
2. Allison, J., Amako, K., et al.: Geant4 developments and applications. IEEE Trans Nucl Sci **53**(1), 270–278 (2006). https://doi.org/10.1109/TNS.2006.869826
3. Allison, J., et al.: Recent developments in Geant4. Nucl Instrum Meth A **835**, 186–225 (2016). https://doi.org/10.1016/j.nima.2016.06.125
4. Andersson, B., Gustafson, G., Nilsson-Almqvist, B.: A model for low p_T hadronic reactions, with generalizations to hadron–nucleus and nucleus–nucleus collisions. Nucl. Phys. B. **281**, 289–309 (1987). https://doi.org/10.1016/0550-3213(87)90257-4
5. Nilsson-Almqvist, B., Stenlund, E.: Interactions between hadrons and nuclei: the lund monte Carlo—FRITIOF version 1.6. Comput Phys Commun **43**(3), 387–397 (1987). https://doi.org/10.1016/0010-4655(87)90056-7
6. Kaidalov, A.B., Ter-Martirosyan, K.A.: Pomeron as quark-gluon strings and multiple hadron production at SPS-Collider energies. Phys. Lett. B. **117**(3–4), 247–251 (1982). https://doi.org/10.1016/0370-2693(82)90556-1
7. Wright, D.H., Kelsey, M.H.: The geant4 bertini cascade. Nucl Instrum Meth A **804**, 175–188 (2015). https://doi.org/10.1016/j.nima.2015.09.058
8. Folger, G., Ivanchenko, V.N., Wellisch, J.P.: The binary cascade: nucleon nuclear reactions. Eur. Phys. J. A **21**, 407–417 (2004). https://doi.org/10.1140/epja/i2003-10219-7
9. Mancusi, D., Boudard, A., et al.: Extension of the Lìège intranuclear-cascade model to reactions induced by light nuclei. Phys Rev C **90**, 54602 (2014). https://doi.org/10.1103/PhysRevC.90.054602
10. Kaitaniemi, P., et al.: INCL intra-nuclear cascade and ABLA de-excitation models in Geant4. Prog Nucl Sci Technol **2**, 788–793 (2011). https://doi.org/10.15669/pnst.2.788
11. Gudima, K.K., Mashnik, S.G., Toneev, V.D.: Cascade-exciton model of nuclear reactions. Nucl Phys A **401**, 329–361 (1983). https://doi.org/10.1016/0375-9474(83)90532-8
12. Chalyi, N.A., Ivanchenko, V.N.: Geant4 pre-compound model upgrade. Russ. Phys. J. **1**, 1962–1968 (2025). https://doi.org/10.1007/s11182-024-03333-8
13. Dostrovsky, I., Fraenkel, Z., Friedlander, G.: Monte Carlo calculations of nuclear evaporation processes. III. Applications to low-energy reactions. Phys Rev **116**(3), 683–702 (1959). https://doi.org/10.1103/PhysRev.116.683
14. Kalbach, C.: Exciton number dependence of the griffin model two-body matrix element. Z. Phys. A **287**, 319–322 (1987). https://doi.org/10.1007/BF01481712
15. Bondorf, J.P., Botvina, A.S., et al.: Statistical multifragmentation of nuclei. Phys Rep **257**(3), 133–221 (1995). https://doi.org/10.1016/0370-1573(94)00097-M
16. Fermi, E.: High energy nuclear events. Prog. Theor. Phys. **5**(4), 570–583 (1950). https://doi.org/10.1143/ptp/5.4.570
17. Viola, V.E., Kwiatkowski, K., Walker, M.: Phys. Rev. C **31**, 1550 (1985). https://doi.org/10.1103/PhysRevC.31.1550
18. Iljinov, A.S., et al.: Phenomenological statistical analysis of level densities, decay widths and lifetimes of excited nuclei. Nucl. Phys. A. **543**(3), 517–557 (1992). https://doi.org/10.1016/0375-9474(92)90278-r
19. Amian, W.B., Byrd, R.C., et al.: Differential neutron production cross sections for 597-MeV protons. Nucl Sci Eng **115**(1), 1–12 (1993). https://doi.org/10.13182/NSE93-A35517
20. Nakao, N., et al.: Development of a quasi-monoenergetic neutron field using the 7Li(p,n)7Be reaction in the 70–210 MeV energy range at RIKEN. Nucl. Instrum. Meth. A **420**, 218–231 (1999). https://doi.org/10.1016/S0168–9002(98)01146-2
21. The SPD Collaboration, et al.: Technical design report of the spin physics detector at NICA (2024)

Authors and Affiliations

N. A. Chalyi[1] · V. N. Ivanchenko[1]

✉ N. A. Chalyi
nchalyi@mail.tsu.ru

[1] National Research Tomsk State University, Tomsk, Russian Federation