

Analysis of Intermediate-Energy Nucleus-Nucleus Spallation, Fission, and Fragmentation Reactions with the LAQGSM code

S. G. Mashnik¹, K. K. Gudima², R. E. Prael¹, and A. J. Sierk¹

¹*Los Alamos National Laboratory, Los Alamos, NM 87545, USA*

²*Institute of Applied Physics, Academy of Science of Moldova, Kishinev, MD-2028, Moldova*

Abstract

The LAQGSM code has been recently developed at Los Alamos National Laboratory to simulate nuclear reactions for proton radiography applications. We have benchmarked our code against most available measured data both for proton-nucleus and nucleus-nucleus interactions at incident energies from 10 MeV to 800 GeV and have compared our results with predictions of other current models used by the nuclear community. Here, we present a brief description of our code and show illustrative results obtained with LAQGSM for neutron spectra measured recently by Nakamura's groups for reactions induced by light and medium nuclei on targets from ^{12}C to ^{208}Pb at several incident energies from 95 to 600 MeV/nucleon and with the recent GSI measurements of spallation, fission, and fragmentation yields from A+p and A+A reactions at incident energies near and below 1 GeV/nucleon. Further necessary work is outlined.

Introduction

During recent years, for a number of applications like Accelerator Transmutation of nuclear Waste (ATW), Accelerator Production of Tritium (APT), Rare Isotope Accelerator (RIA), Proton Radiography (Prad), astrophysical work for NASA, and other projects, we have developed at the Los Alamos National Laboratory an improved version of the Cascade-Exciton Model (CEM), contained in the code CEM2k, to describe nucleon-, pion-, and photo-induced reactions at incident energies up to about 5 GeV [1, 2] and the Los Alamos version of the Quark-Gluon String Model, realized in the high-energy code LAQGSM [3], to describe both particle- and nucleus-induced reactions at energies up to about 1 TeV/nucleon.

Both codes have been tested against most of the available data and compared with predictions of other modern codes [1]-[12]. Our comparisons show that these codes describe a large variety of spallation, fission, and fragmentation reactions quite reliably and often have a better predictive power than some other available Monte-Carlo codes.

In the present paper, we outline our models and show several typical results for nucleus-nucleus reactions demonstrating that LAQGSM is a reliable event generator that can be used both in applications and in fundamental nuclear research.

Since LAQGSM uses modules of CEM2k to describe the preequilibrium stages of nuclear reactions and evaporation/fission of excited compound nuclei, it is convenient for us to discuss both codes in this paper, although we show only results from LAQGSM.

CEM2k and LAQGSM Codes

A detailed description of the initial version of the CEM may be found in [13], therefore we outline here only its basic assumptions. The CEM assumes that reactions occur in three stages. The first stage is the IntraNuclear Cascade (INC) in which primary particles can be re-scattered and produce secondary particles several times prior to absorption by or escape from the nucleus. The excited residual nucleus remaining after the cascade determines the particle-hole configuration that is the starting point for the preequilibrium stage of the reaction. The subsequent relaxation of the nuclear excitation is treated in terms of an improved Modified Exciton Model (MEM) of preequilibrium decay followed by the equilibrium evaporative final stage of the reaction. Generally, all three stages contribute to experimentally measured outcomes.

The improved cascade-exciton model in the code CEM2k differs from the older CEM95 version [14] by incorporating new approximations for the elementary cross sections used in the cascade, using more precise values for nuclear masses and pairing energies, employing a corrected systematics for the

level-density parameters, adjusting the cross sections for pion absorption on quasi-deuteron pairs inside a nucleus, allowing for nuclear transparency of pions, including the Pauli principle in the preequilibrium calculation, and improving the calculation of the fission widths. Significant refinements and improvements in the algorithms used in many subroutines lead to a decrease of computing time by up to a factor of 6 for heavy nuclei, which is very important when performing simulations with transport codes. Essentially, CEM2k has a longer cascade stage, less preequilibrium emission, and a longer evaporation stage with a higher initial excitation energy, compared to its precursors CEM97 [15] and CEM95 [14]. Besides the changes to CEM97 and CEM95 mentioned above, we also made a number of other improvements and refinements, such as: (i) imposing momentum-energy conservation for each simulated event (the Monte-Carlo algorithm previously used in CEM provided momentum-energy conservation only statistically, but not exactly for the cascade stage of each event), (ii) using real binding energies for nucleons at the cascade stage instead of the approximation of a constant separation energy of 7 MeV used in previous versions of the CEM, (iii) using reduced masses of particles in the calculation of their emission widths instead of using the approximation of no recoil used previously, and (iv) a better approximation of the total reaction cross sections. On the whole, this set of improvements leads to a much better description of particle spectra and yields of residual nuclei and a better agreement with available data for a variety of reactions. Details, examples, and further references may be found in [1, 2, 4].

The Los Alamos version of the Quark-Gluon String Model (LAQGSM) [3] is a further development of the Quark-Gluon String Model (QGSM) by Amelin, Gudima, and Toneev (see [16] and references therein) and is intended to describe both particle- and nucleus-induced reactions at energies up to about 1 TeV/nucleon. The core of the QGSM is built on a time-dependent version of the intranuclear-cascade model developed at Dubna, often referred in the literature simply as the Dubna intranuclear Cascade Model (DCM) (see [17] and references therein). The DCM models interactions of fast cascade particles (“participants”) with nucleon spectators of both the target and projectile nuclei and includes interactions of two participants (cascade particles) as well. It uses experimental cross sections (or those calculated by the Quark-Gluon String Model for energies above 4.5 GeV/nucleon) for these elementary interactions to simulate angular and energy distributions of cascade particles, also considering the Pauli exclusion principle. When the cascade stage of a reaction is completed, QGSM uses the coalescence model described in [17] to “create” high-energy d, t, ^3He , and ^4He by final-state interactions among emitted cascade nucleons outside of the colliding nuclei. After calculating the coalescence stage of a reaction, QGSM moves to the description of the last slow stages of the interaction, namely to preequilibrium decay and evaporation, with a possible competition of fission using the standard version of the CEM [13]. If the residual nuclei have atomic numbers with $A \leq 13$, QGSM uses the Fermi break-up model to calculate their further disintegration instead of using the preequilibrium and evaporation models. LAQGSM differs from QGSM by replacing the preequilibrium and evaporation parts of QGSM described according to the standard CEM [13] with the new physics from CEM2k [1, 2] and has a number of improvements and refinements in the cascade and Fermi break-up models (in the current version of LAQGSM, we use the Fermi break-up model only for $A \leq 12$). A detailed description of LAQGSM and further references may be found in [3].

Originally, both CEM2k and LAQGSM were not able to describe fission reactions and production of light fragments heavier than ^4He , as they had neither a high-energy-fission nor a fragmentation model. Recently, we addressed these problems [6, 7] by further improving our codes and by merging them with the Generalized Evaporation Model code GEM2 developed by Furihata [18, 19].

Our current versions of CEM2k and LAQGSM were incorporated recently into the MARS [20] and LAHET [21] transport codes and are currently being incorporated into MCNPX [22]. This will allow others to use our codes as event-generators in these transport codes to simulate reactions with targets of practically arbitrary geometry and nuclide composition.

Illustrative Results

Recently, Nakamura’s group measured neutron double-differential cross sections from reactions induced by He, C, Al, and Ar nuclei on C, Al, Cu, and Pb targets at several incident energies from 95 to 600 MeV/nucleon (see [23] and references therein). We have calculated all these cross sections using LAQGSM. As an example, Figure 1 shows our results for 560 MeV/nucleon ^{40}Ar on C, Cu, and Pb

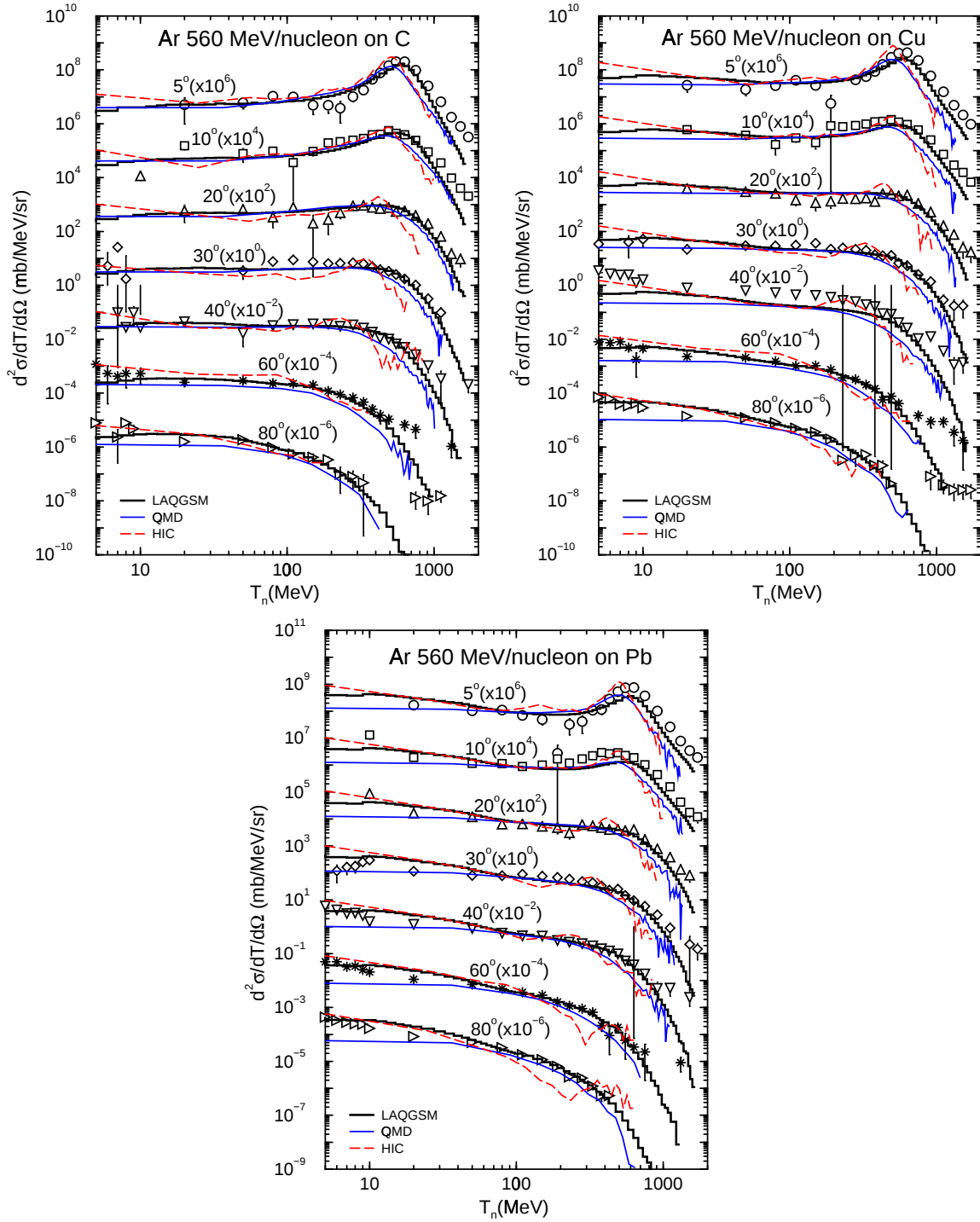


Figure 1. Comparison of measured [23] double differential cross sections of neutrons from 560 MeV/nucleon Ar beams on C, Cu and Pb with our LAQGSM results and calculations by QMD [24] and HIC [25] from Iwata *et al.* [23].

compared with experimental data and calculations with the QMD [24] and HIC [25] models kindly provided to us by Nakamura's group. We see that LAQGSM describes these data quite well and agrees with the measurements better than do QMD and HIC. Similar results are obtained for all the other reactions measured by this group.

Recently at GSI in Darmstadt, Germany, a large number of measurements have been performed using inverse kinematics for interactions of ^{56}Fe , ^{208}Pb and ^{238}U at 1 GeV/nucleon and ^{197}Au at 800 MeV/nucleon with liquid ^1H . These measurements provide a very rich set of cross sections for production of practically all possible isotopes from such reactions in a “pure” form, *i.e.*, individual cross sections from a specific given bombarding isotope (or target isotope, when considering reactions in the usual kinematics, $p + A$). Such cross sections are much easier to compare to models than the “camouflaged” data from γ -spectrometry measurements. These are often obtained only for a natural composition of isotopes in a target and are mainly for cumulative production, whereas measured cross sections contain contributions not only from the direct production of a given isotope, but also from all its decay-chain precursors. In addition, many reactions where a beam of light, medium, or heavy ions with energy near to or below 1 GeV/nucleon interact with different nuclei, from the lightest, d , to the heaviest, ^{208}Pb were measured recently at GSI. References on these measurements and many tabulated experimental cross sections may be found on the Web page of Prof. Schmidt [26]. We have analyzed with CEM2k and LAQGSM all measurements done at GSI of which we are aware, both for proton-nucleus and nucleus-nucleus interactions. Some examples of our CEM2k and LAQGSM results compared with the GSI data and calculations by other current models for proton-nucleus reactions may be found in [1,2,4,6,7,9-12]. This paper is devoted to nucleus-nucleus reactions, but for completeness sake, we show in Fig. 2 just one example of LAQGSM results for $p+A$ interactions; namely, spallation, fission, and fragmentation product yields from $p(1\text{ GeV}) + ^{238}\text{U}$ compared with the GSI data [27, 28]. Similar results are obtained for all other $p+A$ reactions measured at GSI for which we could find data.

We performed our calculation of this reaction in 2002, after the measured spallation product cross sections were published in [27], and published our results in the 2002 LANL Theoretical Division Report of Activity [29]. The experimental data on fission and fragmentation products were published only in 2003 [28]; therefore the LAQGSM results for fission and fragmentation products shown in the two upper panels of Fig. 2 are pure predictions; they agree amazingly well with the experimental data.

We note that all the results shown in the figures of this paper were calculated within a single approach, without fitting any parameters of LAQGSM.

Below we focus only on nucleus-nucleus reactions measured recently at GSI, and we start our analysis with the lightest target, d , namely with the reaction $^{238}\text{U}(1\text{ GeV}/A) + d$ shown in Fig. 3. One can see that LAQGSM merged with GEM2 (LAQGSM+GEM2) describes quite well both the spallation and fission product cross sections and agrees with most of the GSI data with an accuracy of a factor of two or better.

Fig. 4 shows an example of a reaction on a heavier target, ^9Be , namely the reaction 1 GeV/nucleon $^{86}\text{Kr} + ^9\text{Be}$ measured by Voss [31], compared with our LAQGSM+GEM2 results. No fission mechanism is involved in this reaction and all the measured products published in [31] and shown in this figure are described by our code only via spallation. Although LAQGSM+GEM2 underestimates significantly the yields of neutron-rich Rb isotopes, otherwise there is a good agreement between the calculations and data for all the other measured cross sections.

Fig. 5 shows an example of a reaction on a heavier target, ^{27}Al , namely the reaction 790 MeV/nucleon $^{129}\text{Xe} + ^{27}\text{Al}$ measured at GSI by Reinhold *et al.* [32] and compared with LAQGSM+GEM2 results. Although both the projectile and target are heavier than for the example shown in Fig. 4, LAQGSM+GEM2 describes all the products from the reaction shown in Fig. 5 as well using only spallation. A very good agreement between the data and calculations may be seen for all measured cross sections, except for the neutron-rich Cs isotopes, whose charge is bigger than that of initial Xe nuclei of the beam, being produced by picking up a proton from the Al target rather than by spallation processes. The situation observed in Fig. 4 for the production of neutron-rich Rb isotopes involves the same process.

Finally, Fig. 6 shows a heavy-ion-induced reaction measured at GSI [33, 34], namely the yields of measured spallation products from the interaction of a 950 MeV/nucleon ^{238}U beam with copper compared with our results. LAQGSM+GEM2 describes most of these data with an accuracy of a factor of two or better (the fission and fragmentation products are not yet published and we show here only the measured spallation yields, though we calculated all the products from this reaction).

Fig. 7 show an example of several exotic reactions, namely fragmentation of secondary beams of neutron-rich unstable $^{19,20,21}\text{O}$ and stable $^{17,18}\text{O}$ isotopes on ^{12}C targets at beam energies near

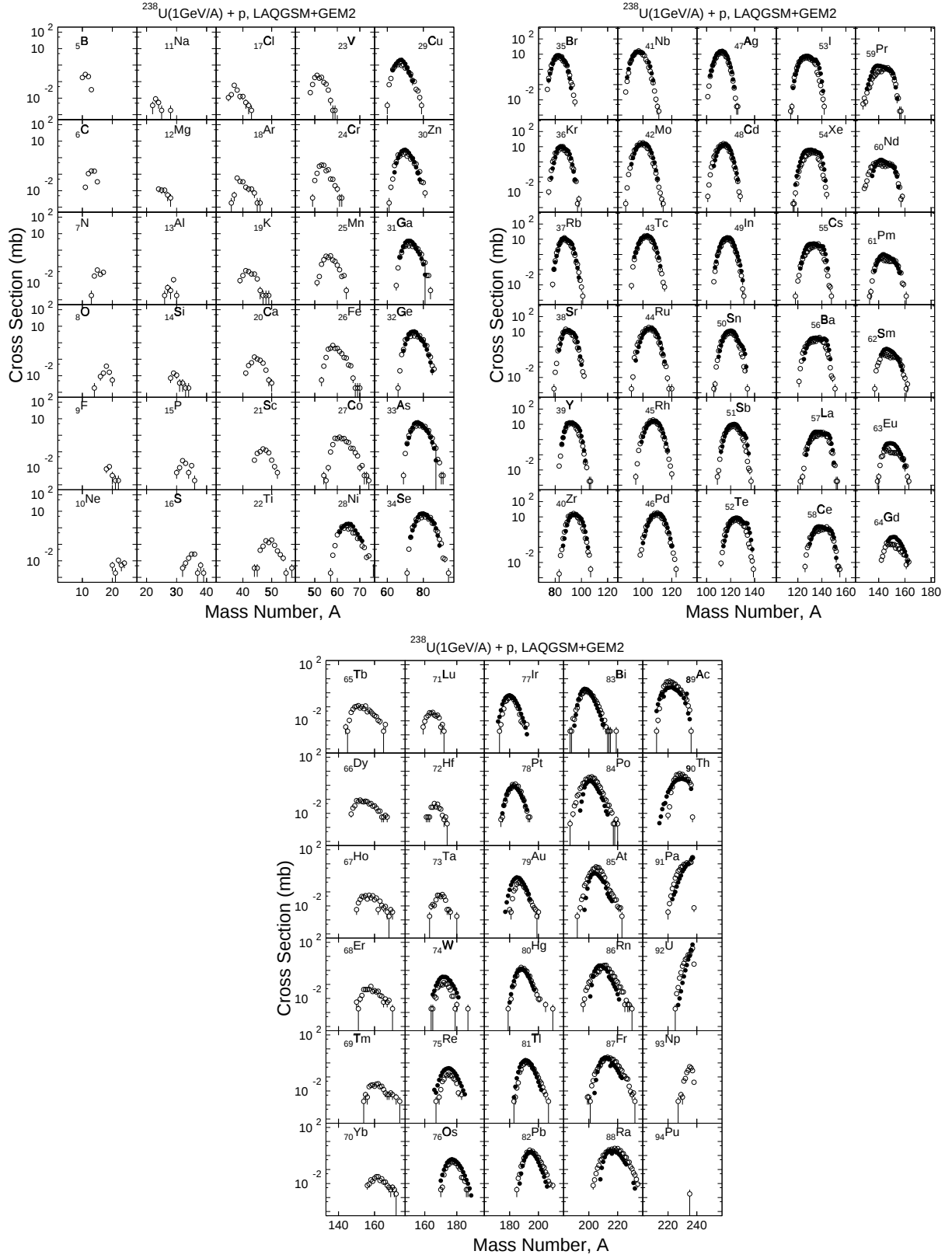


Figure 2. Comparison of measured [27, 28] spallation, fission, and fragmentation product cross sections of the reaction $^{238}\text{U}(1 \text{ GeV/A}) + p$ (filled circles) with our LAQGSM+GEM2 results (open circles). Experimental data for isotopes from B to Co and from Tb to Ta are not yet available so we present here only our predictions.

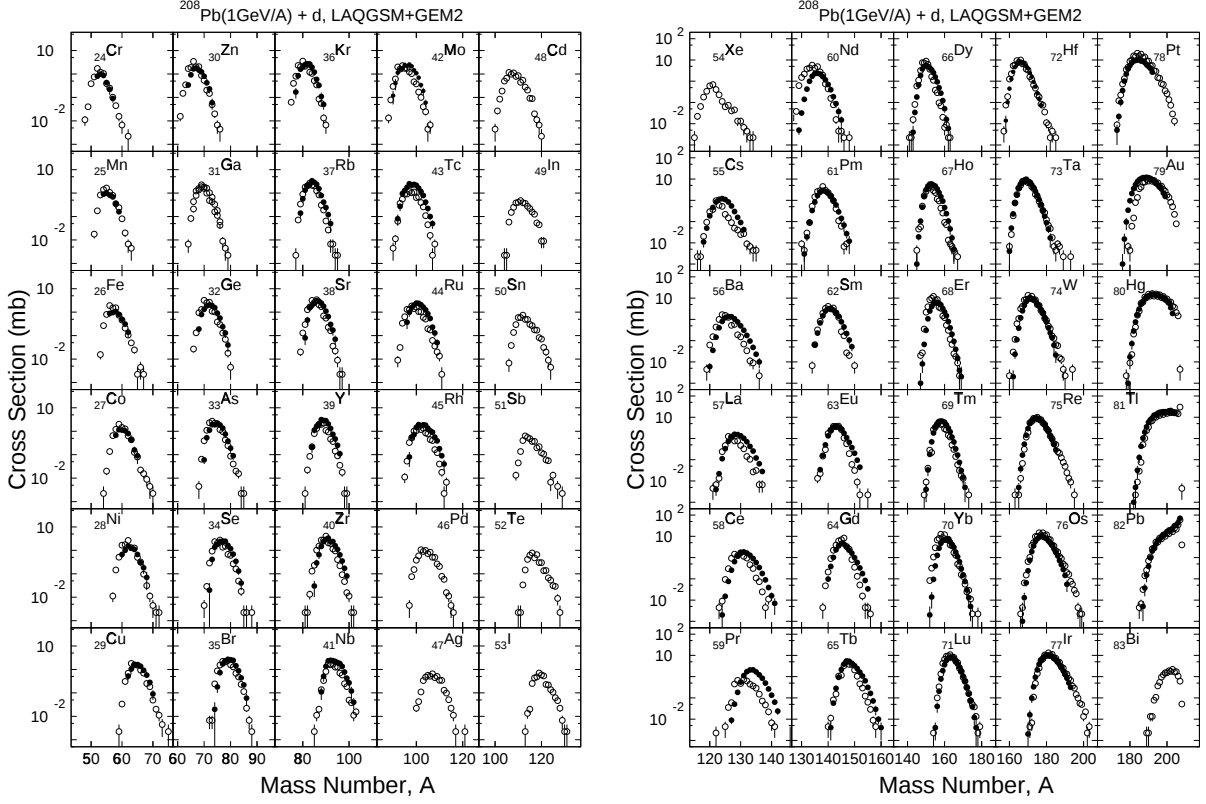


Figure 3. The same as in Fig. 2 but for the reaction $^{208}\text{U}(1\text{ GeV/A}) + d$. Experimental data (filled circles) are from [30]; open circles show our LAQGSM+GEM2 results.

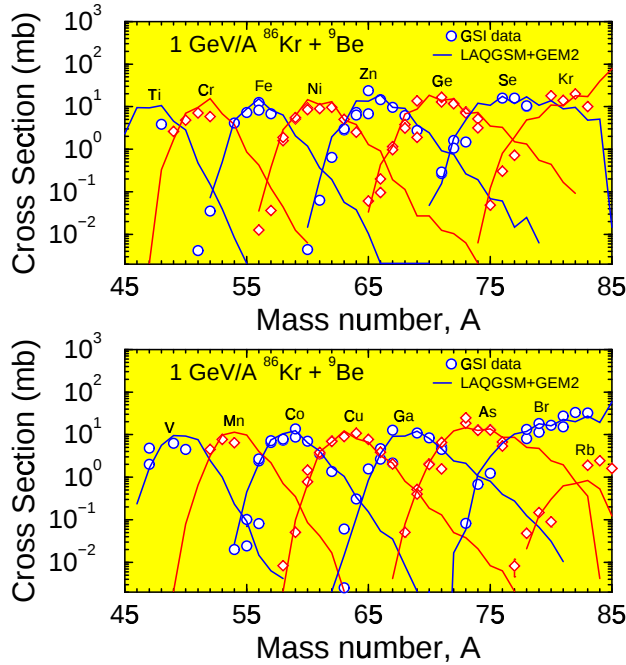


Figure 4. Comparison of all measured [31] cross sections of products from the reaction $^{86}\text{Kr} + ^9\text{Be}$ at 1 GeV/nucleon (symbols) with our LAQGSM+GEM2 results (lines).

600 MeV/nucleon measured recently at GSI [35], compared with our LAQGSM+GEM2 results. The secondary beams of $^{17-21}\text{O}$ ions were produced in the fragmentation of a primary ^{40}Ar beam at 720 MeV/nucleon on a beryllium target (see more details in [35]). The authors of this measurement reproduced reasonably well the general trend of their data with the empirical parameterization EPAX [36] and with two versions of the “abrasion-ablation” model [37, 38]. Nevertheless, the present version of the EPAX parameterization does not contain any physical description and does not reproduce the odd-odd effects in the production cross sections.

Both versions of the abrasion-ablation model [37, 38] do take into account even-even effects using experimental ground-state masses and pairing shifts of $12\sqrt{A}$ MeV, but apparently both calculations overestimate the effect [35]. We note that both EPAX [36] and the abrasion-ablation model [37] failed to reproduce well the recent GSI measurement of the 1 GeV/A $^{208}\text{Pb} + \text{Cu}$ reaction [39].

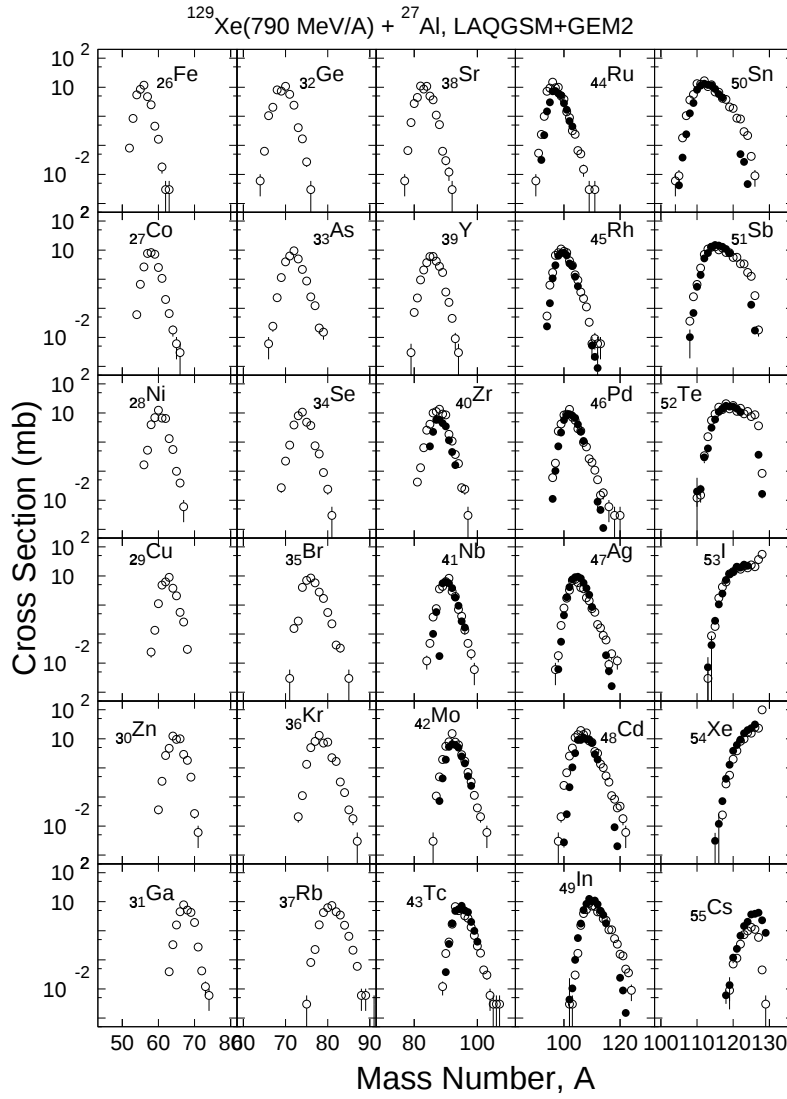


Figure 5. Comparison of all measured [32] cross sections of products from the reaction $^{129}\text{Xe} + ^{27}\text{Al}$ at 790 MeV/nucleon (filled circles) with our LAQGSM+GEM2 results (open circles). Isotopes from Fe to Y are not measured yet and we present here only our predictions.

This suggests we look first at the 1 GeV/A $^{208}\text{Pb} + ^{64}\text{Cu}$ reaction [39] that gave problems to EPAX [36] and the abrasion-ablation model [37] before trying to describe with LAQGSM+GEM2 the exotic measurements [35] shown in Fig. 7. Our LAQGSM+GEM2 results for all cross sections measured by de Jong *et al.* [39] are compared with experimental data in Fig. 8. One can see that LAQGSM+GEM2 describes reasonably well all the measured data and we do not see any shifts either to the neutron-rich or to the neutron-deficient regions observed in [39] for EPAX and the abrasion-ablation model. After addressing this reaction, we calculated with LAQGSM+GEM2 the reactions induced by neutron-rich $^{17-21}\text{O}$ beams on ^{12}C targets measured in [35] and shown in Fig. 7 as

filled circles. For completeness sake, we show in Fig. 7 calculated cross sections for the production of all O, N, and C isotopes, including the ones not measured in [35], as well as yields of B and Be isotopes not measured at all, just as predictions. One can see that LAQGSM+GEM2 describes reasonably well all the measured cross sections, and no worse than the abrasion-ablation model or phenomenological approximation EPAX do. LAQGSM+GEM2 also predicts significant yields for both neutron-rich and neutron-deficient products not yet measured in [35].

In recent years, we observed in the literature an increased interest in production and study of both neutron-rich and neutron-deficient nuclei from different A+A reactions. We analyzed some of these reactions with LAQGSM+GEM2. One illustrative example is shown in Fig. 9, where we compare the recent GSI measurement by Ozawa *et al.* [40] of the reaction ^{40}Ar (1.05 GeV/nucleon) + ^9Be with our results. LAQGSM+GEM2 describes most of the measured neutron-rich product yields quite well and reproduces correctly the change of the measured cross sections in an interval covering about six orders of magnitude. We believe that some of the overestimation by LAQGSM+GEM2 of the measured very neutron-rich product yields is related more to the limited statistics of our Monte-Carlo calculation (for the last measured neutron-rich nuclides with the lowest cross sections, we have only one or two simulated events) than to some serious physics problems of our code.

Further Work

From the results presented here and in the cited references, we conclude that LAQGSM describes well (and without any refitted parameters) a large variety of medium- and high-energy nuclear reactions induced both by nuclei and particles and is suitable for evaluations of nuclear data for applications and to study basic problems in nuclear reaction science. Merging our LAQGSM code with the Generalized

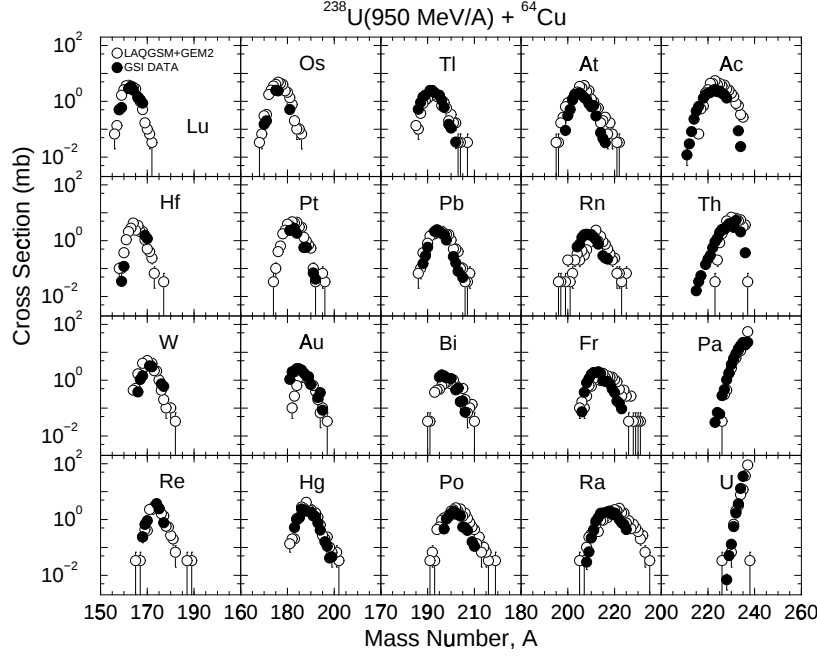


Figure 6. Comparison of all measured [33, 34] cross sections of products from the reaction $^{238}\text{U} + ^{64}\text{Cu}$ at 950 MeV/nucleon (filled circles) with our LAQGSM+GEM2 results (open circles).

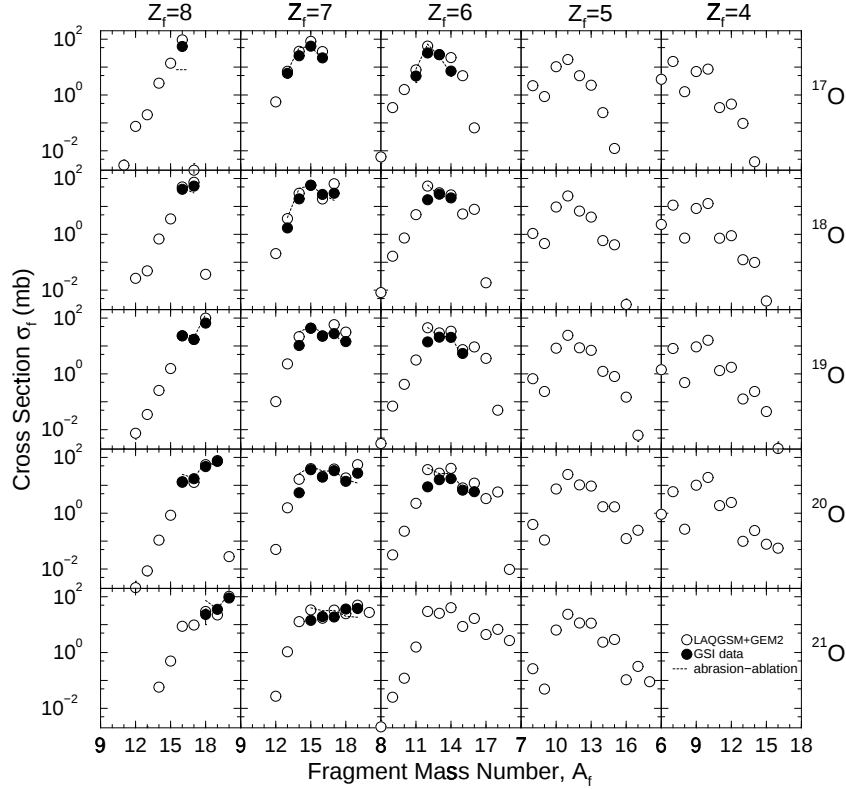


Figure 7. Cross sections of projectile fragments with nuclear charges Z_f (shown on the top) and masses A_f (shown on the bottom) produced from $^{17-21}\text{O}$ beams (shown on the right) in a ^{12}C target. Experimental data (filled circles) are from [35]. Open circles show our LAQGSM+GEM2 results for the measured cross sections and predictions for several unmeasured isotopes. Dashed lines show results by the abrasion-ablation model [37] from [35].

Evaporation Model code GEM2 by Furihata [18, 19] allows us to describe reasonably well many fission and fragmentation reactions in addition to the spallation reactions already described well by LAQGSM. This does not mean that LAQGSM+GEM2 is without

problems. For instance, it does not reproduce well the mass distributions for some fission-fragment elements from the reaction 1 GeV/A $^{238}\text{U} + ^{208}\text{Pb}$ measured recently at GSI [41], although it still reproduces very well the integral mass- and charge-distributions of all products. We think that the main reasons for this problem are the facts that the current version of LAQGSM does not take into account electromagnetic-induced fission [42], and because the GEM2 code by Furihata merged at present with our LAQGSM does not consider at all the angular momentum of emitted particles, and of the compound nuclei. Both these factors are especially important for reactions with heavy ions and less important for reactions with light ions or protons; this would explain why the code works well in the case of reactions induced by particles and light and medium nuclei but fails in the case of U+Pb. Besides the problem of angular momentum, the current version of GEM2 has several more drawbacks related to its lack of self-consistency (see details in [6]). We may choose to use a model similar to the GEM2 approach in

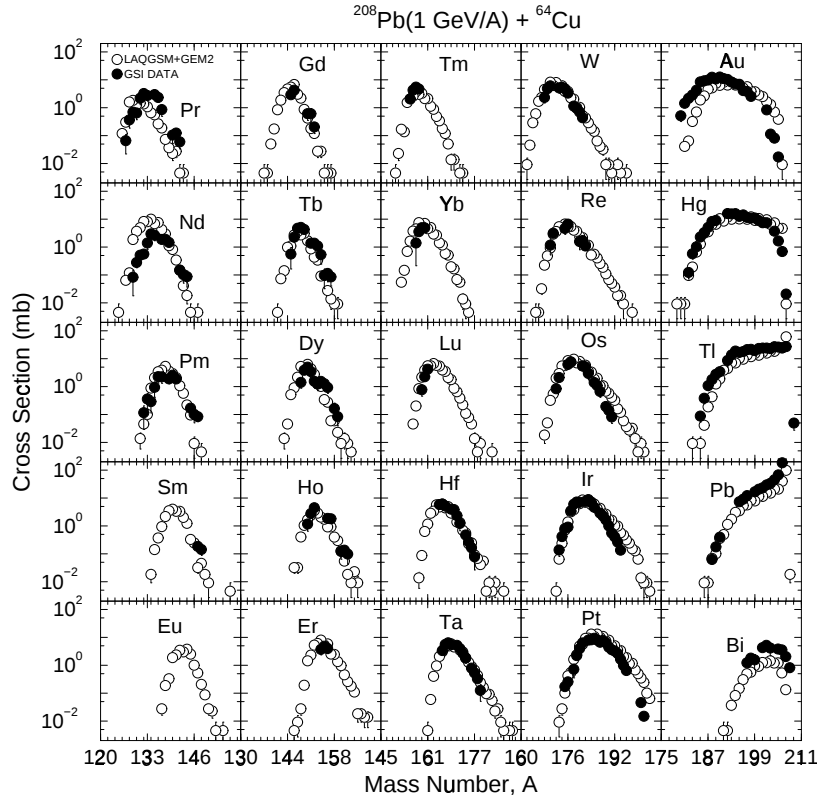


Figure 8. Comparison of all measured [39] cross sections of products from the reaction $^{208}\text{Pb} + ^{64}\text{Cu}$ at 1 GeV/nucleon (filled circles) with our LAQGSM+GEM2 results (open circles).

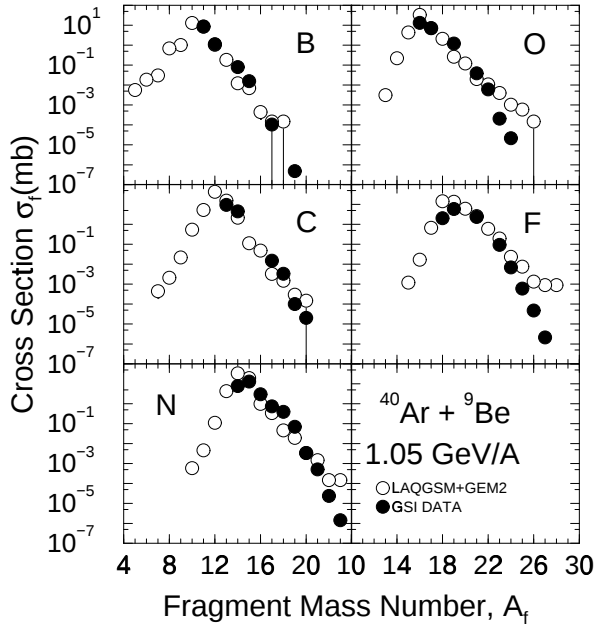


Figure 9. Experimental production cross sections [40] for B to F isotopes from a 1.05 GeV/nucleon ^{40}Ar beam on a ^9Be target (filled circles) compared with our LAQGSM+GEM2 results (open circles).

the future versions of our codes, but it must be significantly extended and further improved. Our work on LAQGSM and CEM2k is not completed; we continue their further development and improvement. Besides GEM2, we have investigated the well known code GEMINI by Charity [43] as an alternative way to describe production of various fragments by merging GEMINI with both LAQGSM and CEM2k, and we have also tested the thermodynamical fission model by Stepanov [44] with its own parameterizations for mass and charge widths, level-density parameters, fission barriers, *etc.*, merging it with both CEM2k and LAQGSM to describe fission. In addition, we have started to extend CEM2k and LAQGSM and to develop our own fission model, as briefly noted in [7].

The preliminary results we found for spallation, fission, and fragmentation products from several reactions we tested so far using these approaches are very promising and we will present our results from these studies in future papers.

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