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Title: Validation and Verification of MCNP6 Against High-Energy Experimental Data and Calculations by Other Codes. II. The LAQGSM Testing Primer

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Intended for: The MCNP6 Code Package

Validation and Verification of MCNP6 Against High-Energy Experimental Data and Calculations by Other Codes. II. The LAQGSM Testing Primer

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Abstract

MCNP6 has been Validated and Verified (V&V) against various recent intermediate- and high-energy measurements as well as against calculations by later versions of MCNPX using different event generators and against results by LAQGSM03.03/01, CEM03.03, INCL+ABLA, INCL4.5+ABLA07, ISABEL+ABLA07, TALYS, ALICE-IPPE, EPAX, ABRABLA, HIPSE, and AMD, used as stand alone codes. New, **/VALIDATION_LAQGSM/** and **/VALIDATION_CEM/** subdirectories in the **/MCNP6/Testing/** directory were created where 18 MCNP6 test-problems that exercise physics of LAQGSM and 18 problems to test MCNP6 with CEM are presented so far together with template files of MCNP6 results, experimental data, and results by other codes. README files that contain short descriptions of every input file, the experiment, the quantity of interest that the experiment measures and its description in the MCNP6 output files, and the publication reference of that experiment are presented for every test-problem. Templates for plotting the corresponding results with **xmgrace** as well as pdf files with figures representing the final results of our V&V efforts are presented. More than a dozen problems or technical "bugs" in MCNP6 and/or in MCNPX discovered during our current V&V of MCNP6 are either fixed already, or are in working process and will be fixed before the next release of MCNP6. Our results show that MCNP6 using our LAQGSM and CEM event generators describes, as a rule, reasonably well different intermediate- and high-energy measured data and agrees very well with similar results obtained with MCNPX and other codes. Here, we describe the V&V of MCNP6 using the LAQGSM event-generator. The test-suite for V&V of MCNP6 using CEM was presented in a separate, first primer of this series. This primer isn't meant to be read from cover to cover. Readers may skip some sections and go directly to a test-problem they are interested in.

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1. Introduction

Following an increased interest in intermediate- and high-energy nuclear reactions in relation to such projects as Accelerator Production of Tritium (APT), Accelerator Transmutation of nuclear Wastes (ATW), Spallation Neutron Source (SNS), Rare Isotope Accelerator (RIA), Proton Radiography (PRAD) as a radiographic probe for the Advanced Hydro-test Facility, NASA needs, and others, the US Department of Energy has supported during the last decade our work on the development of improved versions of the Cascade-Exciton Model (CEM) and of the Los Alamos version of the Quark Gluon String Model (LAQGSM). The latest versions of our codes, CEM03.03 and LAQGSM03.03, have been incorporated recently as event generators in MCNP6 [1, 2], the latest and most advanced LANL Monte Carlo transport code and the principal code product produced by the XCP-3 and D-5 LANL Groups representing a merger of MCNP5 [3] and MCNPX [4]. As multilateral Validation and Verification (V&V) of all our codes is very important and necessary, we decided to V&V specific capabilities of LAQGSM and CEM as event generators in MCNP6.

New, **/VALIDATION_LAQGSM/** and **/VALIDATION_CEM/** subdirectories in the **/MCNP6/Testing/** directory were created where 18 MCNP6 test-problems that exercise physics in LAQGSM and 18 problems to test MCNP6 with CEM are presented so far together with template files of MCNP6 results, experimental data, and results by other codes. README files that contain short descriptions of every input file, the experiment, the quantity of interest that the experiment measures and its description in the MCNP6 output files, and the publication reference of that experiment are presented for every test-problem. Templates for plotting the corresponding results with **xmgrace** as well as pdf files with figures representing the final results of our V&V efforts are presented.

In this primer, we describe the V&V of MCNP6 using the LAQGSM event-generator. The test-suite for V&V of MCNP6 using CEM was presented to a separate, first primer [5] of this series.

To help novice users of MCNP6 and MCNPX, as well as advanced users of MCNP but without sufficient experience in working with our high-energy event generators LAQGSM and CEM, we present here the whole text of all our V&V input files together with a brief description of the corresponding parts of the output files, and provide also extensive comparisons of our MCNP6 results with available experimental data and predictions by other codes.

2. A Brief Survey of LAQGSM and CEM Physics

A detailed description of LAQGSM and CEM may be found in our recent lectures [6] and references therein. Therefore, we present here only a very brief survey of the LAQGSM and CEM physics to help the MCNP6 users chose the proper event generators in their problems as well as a minimum information about the evaporation model used by our codes, needed to better understand several of our current MCNP6 test-problems.

The basic versions of both our LAQGSM and CEM event generators are the so-called "03.01" versions, namely LAQGSM03.01 [7] and CEM03.01 [8]. **While the CEM code calculates nuclear reactions induced only by nucleons, pions, and photons, and only at incident energies below $\sim$ 5 GeV, the LAQGSM code calculates nuclear reactions induced by almost all types of elementary particles as well as by heavy-ions in a very broad**

range of incident energies, up to ∼ 1 TeV/nucleon. LAQGSM assumes that nuclear reactions occur generally in three stages, just like CEM does. 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. When the cascade stage of a reaction is completed, LAQGSM uses the coalescence model to "create" high-energy d, t, ^{3}He, and ^{4}He by final-state interactions among emitted cascade nucleons, already outside of the target (see Fig. 1 below).

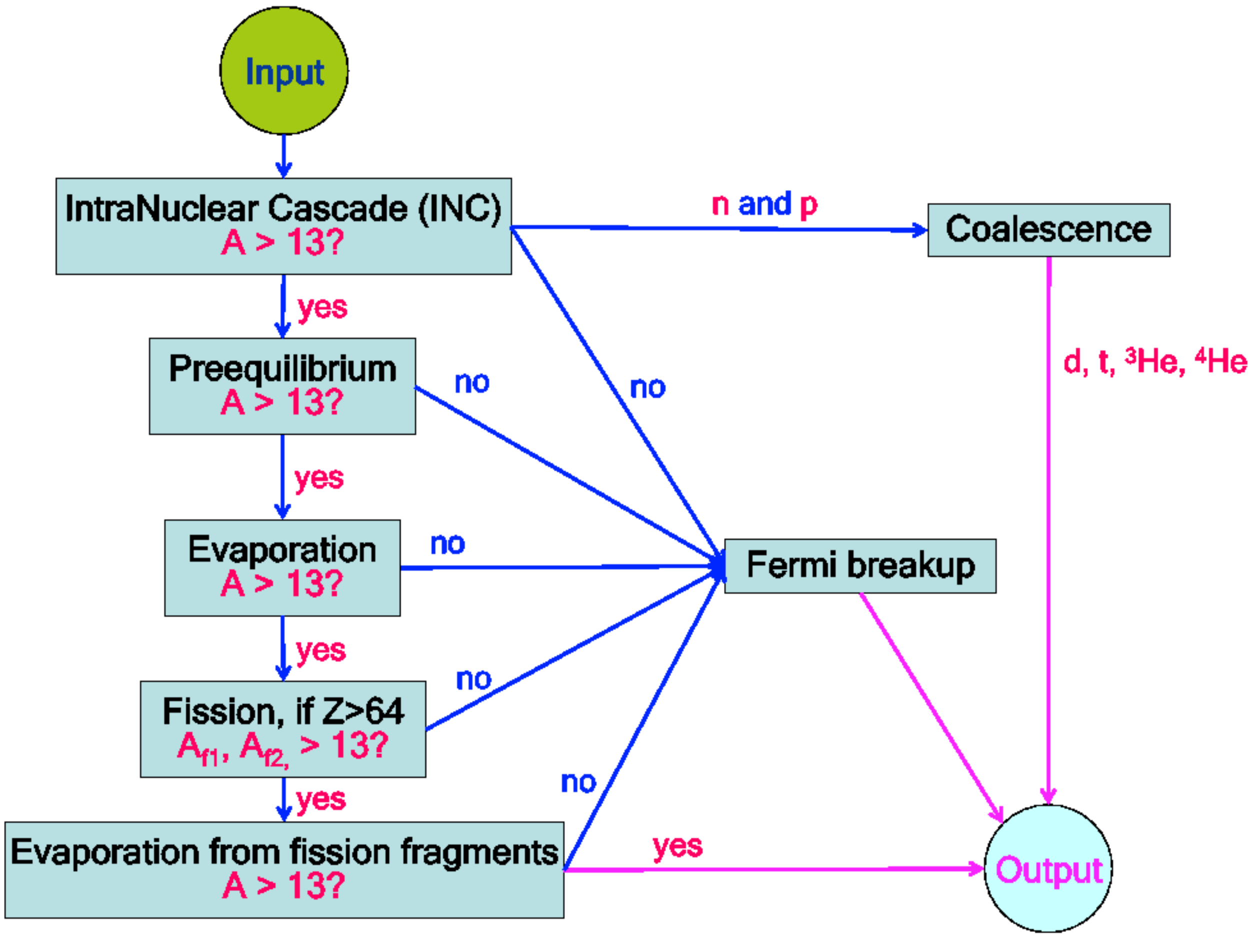

Figure 1: Flow chart of nuclear-reaction calculations by LAQGSM03.03 and CEM03.03

The emission of the cascade particles determines the particle-hole configuration, Z, A, and the excitation energy that is the starting point for the second, preequilibrium stage of the reaction. The subsequent relaxation of the nuclear excitation is treated in terms of an improved version of the modified exciton model of preequilibrium decay followed by the equilibrium evaporation/fission stage of the reaction. Generally, all four components may contribute to experimentally measured particle spectra and other distributions. But if the residual nuclei after the INC have atomic numbers with $A \leq 12$, LAQGSM uses the Fermi breakup model to calculate their further disintegration instead of using the preequilibrium and evaporation models. Fermi breakup is much faster to calculate and gives results very similar to the continuation of the more detailed models to much lighter nuclei. Note that the INC of LAQGSM is completely different from the one in CEM.

The main difference of the following, so-called "03.02" versions of LAQGSM and CEM from the basic "03.01" versions is that the latter use the Fermi breakup model to calculate the disintegration of light nuclei instead of using the preequilibrium and evaporation models only after the INC, when the excited nuclei after the INC have a mass number $A \leq 12$, but do not use the Fermi breakup model at the preequilibrium, evaporation, and fission stages, when, due to emission of preequilibrium particles or due to evaporation or to a very asymmetric fission, we get an excited nucleus or a fission fragment with $A \leq 12$. This problem was solved in the 03.02 versions of LAQGSM and CEM [9], where the Fermi breakup model is used at any stage of a reaction, when we get an excited nucleus with $A \leq 12$.

In addition, the routines that describe the Fermi breakup model in the basic 03.01 version of our codes were written several decades ago in the group of Prof. Barashenkov at JINR, Dubna, Russia, and are far from being perfect, though they are quite reliable and are still used currently without any changes in some transport codes. First, these routines allow in rare cases production of some light unstable fragments like ^{5}He, ^{5}Li, ^{8}Be, ^{9}B, etc., as a result of a breakup of some light excited nuclei. Second, these routines allowed in some very rare cases even production of "neutron stars" (or "proton stars"), i.e., residual "nuclei" produced via Fermi breakup that consist of only neutrons (or only protons). Lastly, in some very rare cases, these routines could even crash the code, due to cases of divide by zero. All these problems of the Fermi breakup model routines are addressed and solved in the 03.02 version of our codes [9]. Several bugs are also fixed in 03.02 in comparison with its predecessor. On the whole, the 03.02 versions describe nuclear reactions on intermediate and light nuclei, and production of fragments heavier than ^{4}He from heavy targets much better than their predecessors, almost do not produce any unstable unphysical final products, and are free of the known bugs.

However, even after solving these problems and after implementing the improved Fermi breakup model into LAQGSM03.02 and CEM03.02 [9], in some very rare cases, our event generators still could produce some unstable products via very asymmetric fission, when the excitation energy of such fragments was below 3 MeV and they were not checked and not disintegrated with the Fermi breakup model (see details in [10]). This problem was addressed in the 03.03 versions of our codes, where we force such unstable products to disintegrate via Fermi breakup independently of their excitation energy. Several more bugs were fixed in the 03.03 version as well. A schematic outline of a nuclear reaction calculation by LAQGSM03.03 or CEM03.03 is shown in Fig. 1. We emphasize that the occurrence of these problems even in the 03.01 versions is quite rare, allowing stand-alone calculations of many nuclear reactions to proceed without problems, but are unacceptable when the event generators are used inside transport codes doing large-scale simulations. Let us note here that the "03.03" version of CEM produced as described above (see more details in [10]) is used at present only in MARS15 [11]. In the latest versions of MCNPX, 2.7.A [12], 2.7.B [13], 2.7.C [14], 2.7.D [15], 2.7.E [16], and 2.7.0 [17] and in MCNP6 [2] (as well as in the Monte Carlo Radiative Energy Deposition (MRED) code developed at Vanderbilt University for single event effect studies [18]) we use now a new modification of CEM03.02 which does not produce any fission fragments with $A < 13$. Therefore, there is no need to use the "standard 03.03" version.

Let us mention that until very recently, we have called the latest version of CEM in MCNP6/X "CEM03.02" (to not confuse it with the version used at FNAL in MARS15) though its physics corresponds to CEM03.03. We have participated with it in the recent Benchmark of Spallation Models organized at the International Atomic Energy Agency during 2008-2009 [19], and it is referred there as "CEM03.02". As one can see from the numerous and various results presented at the Web-site of that Benchmark [19], the results by "CEM03.02" are practically the same as those by "CEM03.03", just as we expected. The situation with different names of the latest version of CEM in MCNP6/X as "CEM03.02" and as "CEM03.03" in MARS15 was confusing for people outside our Group, as kindly pointed out to us by one of the referees of our recent paper on Validation and Verification of MCNP6 [20]. To address this, we decided to call in Ref. [20] and in all our following publications the latest version of CEM we use at LANL (and in MRED at Vanderbilt University) also as "CEM03.03". This is why we refer here to it as to "CEM03.03".

As several our test-problems address a specific question of the evaporation model used by our LAQGSM and CEM, let us recall here the main assumptions of the evaporation model, without discussing at all the INC, the preequilibrium, the fission, and the coalescence models used by LAQGSM and CEM (we direct readers interested in details of these models to our lectures [6] and references therein).

LAQGSM03.01 and CEM03.01 and their later versions use an extension of the Generalized Evaporation Model (GEM) code GEM2 by Furihata [21]–[23] after the preequilibrium stage of reactions to describe evaporation of nucleons, complex particles, and light fragments heavier than ^{4}He (up to ^{28}Mg) from excited compound nuclei and to describe their fission, if the compound nuclei are heavy enough to fission ($Z \geq 65$). The GEM is an extension by Furihata of the Dostrovsky evaporation model [24] as implemented in LAHET [25] to include up to 66 types of particles and fragments that can be evaporated from an excited compound nucleus plus a modification of the version of Atchison's fission model [26]–[28] used in LAHET. Many of the parameters were adjusted by Furihata for a better description of fission reactions when using it in conjunction with the extended evaporation model.

A very detailed description of the GEM, together with a large amount of results obtained for many reactions using the GEM coupled either with the Bertini or ISABEL INC models in LAHET may be found in [21, 22]. Therefore, we present here only the main features of the GEM, following mainly [22] and using as well useful information obtained in private communications with Dr. Furihata.

Furihata did not change in GEM the general algorithms used in LAHET to simulate evaporation and fission. The decay widths of evaporated particles and fragments are estimated using the classical Weisskopf-Ewing statistical model [29]. In this approach, the decay probability P_j for the emission of a particle j from a parent compound nucleus i with the total kinetic energy in the center-of-mass system between ϵ and $\epsilon + d\epsilon$ is

$$P_j(\epsilon)d\epsilon = g_j \sigma_{inv}(\epsilon) \frac{\rho_d(E - Q - \epsilon)}{\rho_i(E)} \epsilon d\epsilon, \tag{1}$$

where E [MeV] is the excitation energy of the parent nucleus i with mass A_i and charge Z_i, and d denotes a daughter nucleus with mass A_d and charge Z_d produced after the emission of ejectile j with mass A_j and charge Z_j in its ground state. σ_{inv} is the cross section for the inverse reaction, ρ_i and ρ_d are the level densities [MeV]$^{-1}$ of the parent and the daughter nucleus, respectively. $g_j = (2S_j + 1)m_j/\pi^2\hbar^2$, where S_j is the spin and m_j is the reduced mass of the emitted particle j. The Q-value is calculated using the excess mass $M(A, Z)$ as $Q = M(A_j, Z_j) + M(A_d, Z_d) - M(A_i, Z_i)$. In GEM2, four mass tables are used to calculate Q values, according to the following priorities, where a lower priority table is only used outside the range of validity of the higher priority one: (1) the Audi-Wapstra mass table [30], (2) theoretical masses calculated by Möller *et al.* [31], (3) theoretical masses calculated by Comay *et al.* [32], (4) the mass excess calculated using the old Cameron formula [33]. As does LAHET, GEM2 uses Dostrovsky's formula [24] to calculate the inverse cross section σ_{inv} for all emitted particles and fragments

$$\sigma_{inv}(\epsilon) = \sigma_g \alpha \left(1 + \frac{\beta}{\epsilon}\right) \ , \tag{2}$$

which is often written as

$$\sigma_{inv}(\epsilon) = \begin{cases} \sigma_g c_n (1 + b/\epsilon) & \text{for neutrons} \\ \sigma_g c_j (1 - V/\epsilon) & \text{for charged particles} \ , \end{cases}$$

where $\sigma_g = \pi R_b^2$ [fm^2] is the geometrical cross section, and

$$V = k_j Z_j Z_d e^2 / R_c \tag{3}$$

is the Coulomb barrier in MeV.

One important new ingredient in GEM2 in comparison with LAHET, which considers evaporation of only 6 particles (n, p, d, t, ^{3}He, and ^{4}He), is that Furihata includes the possibility of evaporation of up to 66 types of particles and fragments and incorporates into GEM2 several alternative sets of parameters b, c_j, k_j, R_b, and R_c for each particle type.

The 66 ejectiles considered by GEM2 for evaporation are selected to satisfy the following criteria: (1) isotopes with $Z_j \leq 12$; (2) naturally existing isotopes or isotopes near the stability line; (3) isotopes with half-lives longer than 1 ms. All the 66 ejectiles considered by GEM2 are shown in Table 1.

Table 1. The evaporated particles considered by GEM2

Z_j	Ejectiles						
0	n						
1	p	d	t				
2	^{3}He	^{4}He	^{6}He	^{8}He			
3	^{6}Li	^{7}Li	^{8}Li	^{9}Li			
4	^{7}Be	^{9}Be	^{10}Be	^{11}Be	^{12}Be		
5	^{8}B	^{10}B	^{11}B	^{12}B	^{13}B		
6	^{10}C	^{11}C	^{12}C	^{13}C	^{14}C	^{15}C	^{16}C
7	^{12}N	^{13}N	^{14}N	^{15}N	^{16}N	^{17}N	
8	^{14}O	^{15}O	^{16}O	^{17}O	^{18}O	^{19}O	^{20}O
9	^{17}F	^{18}F	^{19}F	^{20}F	^{21}F		
10	^{18}Ne	^{19}Ne	^{20}Ne	^{21}Ne	^{22}Ne	^{23}Ne	^{24}Ne
11	^{21}Na	^{22}Na	^{23}Na	^{24}Na	^{25}Na		
12	^{22}Mg	^{23}Mg	^{24}Mg	^{25}Mg	^{26}Mg	^{27}Mg	^{28}Mg

Note that when including evaporation of up to 66 particles in GEM2, its running time increases significantly compared to the case when evaporating only 6 particles, up to ^{4}He. The major particles emitted from an excited nucleus are n, p, d, t, ^{3}He, and ^{4}He. For most cases, the total emission probability of particles heavier than α is negligible compared to those for the emission of these light ejectiles. Our detailed study of different reactions (see, *e.g.*, [34] and references therein) shows that if we study only nucleon and complex-particle spectra or only spallation and fission products and are not interested in light fragments, we can consider evaporation of only 6 types of particles in GEM2 and save much computing time, getting results very close to the ones calculated with the more time consuming "66" option. In LAQGSM03.01 and

CEM03.01, we have introduced an input parameter called **nevtype** that defines the number of types of particles to be considered at the evaporation stage. The index of each type of particle that can be evaporated corresponds to the particle arrangement in Table 1, with values, *e.g.*, of 1, 2, 3, 4, 5, and 6 for n, p, d, t, ^{3}He, and ^{4}He, with succeeding values up to 66 for ^{28}Mg. All 66 particles that can possibly evaporate are listed in LAQGSM03.01 and CEM03.01 together with their mass number, charge, and spin values in the **block data bdejc**. For all ten examples of inputs and outputs of CEM03.01 included in Appendices 1 and 2 of the CEM03.01 User Manual [8], whose results are plotted in the figures in Appendix 3 of [8], we have performed calculations taking into account only 6 types of evaporated particles (**nevtype = 6**) as well as with the "66" option (**nevtype = 66**) and we provide the corresponding computing time for these examples in the captions to the appropriate figures shown in Appendix 3 of Ref. [8]. The "6" option can be up to several times faster than the "66" option, providing meanwhile almost the same results. Therefore we recommend that users of LAQGSM and CEM use 66 for the value of the input parameter **nevtype** only when they are interested in all fragments heavier than ^{4}He; otherwise, we recommend the value of 6 for **nevtype**. Alternatively, users may choose intermediate values of **nevtype**, for example 9 if one wants to calculate the production of ^{6}Li, or 14 for modeling the production of ^{9}Be and lighter fragments and nucleons only, while still saving computing time compared to running the code with the maximum value of 66.

3. V&V of MCNP6 using LAQGSM03.03

To help the users of MCNP6, in all the following subsections, we describe the test problems (input and output files and comparisons with experimental data and results by other models) exactly as they are presented in the **VALIDATION_LAQGSM** subdirectory in the basic **MCNP6/Testing** directory.

Before presenting our results, let us mention that the easiest way to calculate (in MCNP6) spectra of secondary particles and cross section of products from a thin target is to use either the **noact=-2** option on the **LCA** card of the MCNP6 input file, or the special **GENXS** option of MCNP6. The first option (**noact=-2**) was developed for the MCNPX code and is described in detail in Section 5.4.6.1 of the MCNPX Manual [35]; it migrated later to MCNP6 exactly as implemented in MCNPX [35]. The second option (**GENXS**) was developed by Dr. Richard Prael especially for MCNP6 and is described in detail in Ref. [36]. Both these documents [35, 36] are included in the package to be distributed to the MCNP6 users. Below, in cases of test-problems with thin targets, we show examples of using either the first or the second option (note that in Sections 3.6, 3.7, and 3.8 of the CEM Testing Primer [5], we show examples of using both these options of MCNP6).

3.1. Test-Problem #1: Si600CuREP

This MCNP6 problem is to test the applicability of MCNP6 using the LAQGSM03.03 event generator for different NASA (shielding for missions in space), medical (cancer treatment with heavy-ions), and FRIB (the U.S. DOE Facility for Rare Isotope Beams, a continuation and modification of the former Rare Isotope Production (RIA) project) applications.

This test problem calculates with MCNP6 the neutron spectra at 5, 10, 20, 30, 40, 60, and 80 degrees from interaction of a 600 MeV/nucleon ^{28}Si beam with a thin ^{64}Cu target and compares the results with experimental data and with results by other models.

Let us mention that one of the major reasons for this test problem was to investigate and fix a "bug" observed by Dr. Igor Remec of ORNL when he calculated this reaction with MCNPX 2.7.B (see Ref. [20] for more details). Dr. Remec called our attention to a problem he observed in the MCNPX 2.7.B for neutron spectra at forward angles. For unknown reasons, MCNPX 2.7.B using LAQGSM03.01 strongly overestimates the neutron spectra at forward angles (see the cyan lines in Fig. 8 of Ref. [20] and in Fig. 2 below), while LAQGSM03.01 used as a stand alone code describes such spectra very well (see the black lines on Fig. 8 of Ref. [20] and the green lines in Fig. 2 below). A special investigation by Dr. Mike James of the LANL D-5 Group has identified a previously unobserved error in the MCNPX implementation of LAQGSM03.01, which caused that problem. This implementation error was fixed by Mike James in the 2.7.0 version of MCNPX [17] by replacing completely the relatively old LAQGSM03.01 with the latest version LAQGSM03.03. Such a replacement was also done in MCNP6 by Dick Prael. As we can see from Fig. 8 of Ref. [20] and in Fig. 2 below, the current version of MCNP6 describes these measured neutron spectra very well, just as LAQGSM03.03 and LAQGSM03.01 do as stand alone codes.

We calculate this test-problem using the **NOACT=-2** option for the 8th parameter of the **LCA** card of the MCNP6 input file. As we have presented a detailed description of the use of **NOACT=-2** option to calculate particle spectra from thin targets in the test-problem #6 of the CEM Testing Primer [5], and have provided additional examples of its use in test problems #7 and #8 of Ref. [5], we do not need to discuss the input and output files for this case. Therefore, we limit ourselves to only providing the text of the input file as well as describing where to find the results in the MCNP6 output files. The input file for this test problem is **Si600CuREP**. It is presented in the subdirectory **/VALIDATION_LAQGSM/Inputs/** and is also shown below.

Si600CuREP:

```
MCNP6 test with LAQGSM03.03: 600 MeV/A Si28 + Cu64 -> n spectra
C to test Dick Prael fix of the bug observed by Igor Remec
c as test-problem for NASA application
1   1  -8.96  -501        imp:n=1
2   0         501  -502  imp:n=1
99  0         502        imp:n=0

501   so 0.01
502   so 1
c
c  tally surfaces
c
250    kz    0    0.001906278     1  $  2.5 deg
750    kz    0    0.017332380     1  $  7.5 deg
125    kz    0    0.049148523     1  $ 12.5 deg
175    kz    0    0.099413326     1  $ 17.5 deg
225    kz    0    0.171572875     1  $ 22.5 deg
275    kz    0    0.270990054     1  $ 27.5 deg
325    kz    0    0.405858517     1  $ 32.5 deg
375    kz    0    0.588790706     1  $ 37.5 deg
425    kz    0    0.839662820     1  $ 42.5 deg
```

```
575    kz    0    2.463912811     1  $ 57.5 deg
625    kz    0    3.690172332     1  $ 62.5 deg
775    kz    0    20.34649121     1  $ 77.5 deg
825    kz    0    57.69548054     1  $ 82.5 deg

m1     29064   1.0  $ Cu64 target, density 8.96 g/cc
lca 7j -2 j 1    $ LAQGSM
c nps 1000
nps 1e7
prdmp 2j -1
sdef par=14028 erg=16800 vec=0 0 1 dir 1
phys:# 16800
phys:h 3000
phys:n 3000
phys:a 3000
phys:d 3000
phys:t 3000
phys:s 3000
phys:/ 3000
phys:z 3000
mode n h # a d t s / z *
c
f1:n  502
fs1   -250 -750 -125 -175 -225 -275 -325 -375 -425 -575 -625 -775 -825 T
c The following Segment Divisor card is needed to get 1/sr for n-spectra
sd1   0.00598020  $ 2pi(cos0 -cos2.5)
      0.04777332  $ 2pi(cos2.5 - cos7.5)
      0.09518306  $ 2pi(cos7.5 - cos12.5)
      0.14186840  $ 2pi(cos12.5 - cos17.5)
      0.18747403  $ 2pi(cos17.5 - cos22.5)
      0.23165287  $ 2pi(cos22.5 - cos27.5)
      0.27406869  $ 2pi(cos27.5 - cos32.5)
      9.31439869  $ 2pi(cos32.5 - cos37.5)
      0.35233592  $ 2pi(cos37.5 - cos42.5)
      1.25649713  $ 2pi(cos42.5 - cos57.5)
      0.47470090  $ 2pi(cos57.5 - cos62.5)
      1.54132190  $ 2pi(cos62.5 - cos77.5)
      0.53980995  $ 2pi(cos77.5 - cos82.5)
      7.10330556  $ 2pi(cos82.5 - cos180)
      12.5663706  $ 4pi
c     Boundaries of the neutron energy bins: 0-1 MeV; 1-3 MeV, ...
e1    1     3     5     7     9     11    13    15    17    19
      22.5  27.5  32.5  37.5  42.5  47.5  52.5  57.5  62.5  67.5
      72.5  77.5  82.5  87.5  92.5  97.5  105   115   125   135
      145   155   165   175   185   195   205   215   225   235
      245   255   265   275   285   295   305   315   325   335
      345   355   365   375   385   395   405   415   425   435
```

```
      445   455   465   475   485   495   505   515   525   535
      545   555   565   575   585   595   605   615   625   635
      645   655   665   675   685   695   705   715   725   735
      745   755   765   775   785   795   805   815   825   835
      845   855   865   875   885   895   905   915   925   935
      945   955   965   975   985   995  1025  1075  1125  1175
     1225  1275  1325  1375  1425  1475  1525  1575  1625  1675
     1725  1775  1825  1875  1925  1975
em1 2279.85 135r $ multiply to sig_inelastic = 2279.85 mb, as predicted
c                 by LAQGSM03.03, file Si600Cu0303.out, Nov 9, 2009; needed
c                 to get the spectra in [mb/sr/MeV], after dividig the flux
c                 to the energy bins with divisor136.exe to get [1/MeV]
c
c
e0   2000
f11:n   502
f21:h   502
f31:d   502
f41:t   502
f51:s   502
f61:a   502
f71:/   502
f81:z   502
f91:*   502
dbcn  20j  0  7j  1  2j  0  1
```

Spectra by MCNP6 at 5, 10, 20, 30, 40, 60, and 80 (±2.5) degrees are tabulated in units of [mb/sr/proton] in the output file Si600CuREP_c.o (calculated with the "continue" option using the auxiliary input file inp_Si600CuREP; the first MCNP6 output calculated with the main input file Si600CuREP is Si600CuREP.o; both of these output files are presented in subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**) as tally 1, respectively, in the "segments":
1) segment: 250 -750
2) segment: 250 750 -125
3) segment: 250 750 125 175 -225
4) segment: 250 750 125 175 225 275 -325
5) segment: 250 750 125 175 225 275 325 375 -425
6) segment: 250 750 125 175 225 275 325 375 425 575 -625
7) segment: 250 750 125 175 225 275 325 375 425 575 625 775 -825

Note that to get the units of [mb] needed for the normalization of the calculated spectra to the total reaction cross section, we use the Energy Multiplier card **EM1** in our input file Si600CuREP with the value 2279.85 on it for all the 136 energy bins of our tally **F1**: 2279.85 is the value of the total inelastic (reaction) cross section in [mb] as calculated by LAQGSM03.03 used as a stand alone code.

In a similar manner, to get the units of [1/sr] for the MCNP6 calculated spectra, we use in our input file the Segment Divisor card **SD1** with values of the solid angles for each "segment" identifying the needed angles of 5, 10, 20, 30, 40, 60, and 80 ($\pm$2.5) degrees.

Last, to get the units of [1/MeV] in the final spectra, we need to divide the MCNP6 tables for the "segments" listed above by the value of the corresponding energy bins. We could do this with the Energy Multiplier card **EM1** or with the Segment Divisor card **SD1** mentioned above. In order to keep this MCNP6 input as simple as possible, we chose to not do so with the **EM1** or **SD1** cards in the current test-problem; instead, after all MCNP6 calculations are completed, we divide the corresponding MCNP6 results using a little auxiliary routine we wrote to make this division.

To help plot these spectra with **xmgrace** (see file Si600Cu_REP.pdf), the final MCNP6 results are copied to separate files REP5.dat, REP10.dat, REP20.dat, REP30.dat, REP40.dat, REP60.dat, and REP80.dat, respectively. The file Si600Cu_REP.fig is a template for plotting the figure with **xmgrace**.

Besides the MCNP6 results, for comparison, we present here also results by LAQGSM03.01 used as a stand alone code (files 5_01.dat, 10_01.dat, 20_01.dat, 30_01.dat, 40_01.dat, 60_01.dat, and 80_01.dat, for 5, 10, 20, 30, 40, 60, and 80 degrees, respectively), by the latest version of LAQGSM used as a stand alone code, LAQGSM03.03 (files 5_03.dat, 10_03.dat, 20_03.dat, 30_03.dat, 40_03.dat, 60_03.dat, and 80_03.dat, respectively), as well as results obtained by Igor Remec with MCNPX 2.7.B using LAQGSM03.01 in a standard calculation mode (files I_5.dat, I_10.dat, I_20.dat, I_30.dat, I_40.dat, I_60.dat, and I_80.dat, respectively). The results by MCNPX 2.7.B were kindly provided us by Dr. Igor Remec.

The experimental data for this test problem are published in Ref. [37]. Numerical values of experimental data were obtained from the authors of the measurement (performed at the Heavy Ion Medical Accelerator in Chiba (HIMAC) facility of the National Institute of Radiological Science (NIRS), Japan via Dr. Igor Remec of the Oak Ridge National Laboratory. Experimental neutron spectra in units of [mb/MeV/sr] for angles of 5, 10, 20, 30, 40, 60, and 80 degrees are presented in files 5exp.dat, 10exp.dat, 20exp.dat, 30exp.dat, 40exp.dat, 60exp.dat, and 80exp.dat, respectively, in the subdirectory:
/VALIDATION_LAQGSM/Experimental_data/Si600Cu_l/.

For convenience of plotting with **xmgrace** spectra at all angles on a single figure and to compare spectra at different angles with each other, the experimental data (and the results by LAQGSM03.01 used as a stand alone code) at 5 degrees were multiplied by 10^6, at 10 degrees by 10^5, at 20 degrees by 10^4, etc., as is shown in the legend of the figure (see file Si600Cu_REP.pdf). (Note that results by MCNP6, by LAQGSM03.03 used as a stand alone code, and by MCNPX 2.7.B, as described below, are not multiplied in the separate files provided here; instead, they were multiplied only in the figure, while plotting the figure with **xmgrace**.)

The final results for this problem are shown below in Fig. 2. We see a very good agreement between our current MCNP6 results using the LAQGSM03.03 event generator and the calculations with LAQGSM03.03 and LAQGSM03.01 used as stand alone codes. We observe also a pretty good agreement of our results with the experimental data. For comparison, we show in Figure 2 also the results calculated by Dr. Remec at ORNL using MCNPX 2.7.B (with the wrong implementation of LAQGSM03.01 as mentioned above); we see that those old results strongly overestimate the neutron spectra at forward angles. Fortunately, that implementation "bug" was fixed in both MCNPX 2.7.0 and MCNP6 and now both our transport codes describe well particle spectra emitted in the laboratory system in the forward direction from this and other similar nuclear reactions.

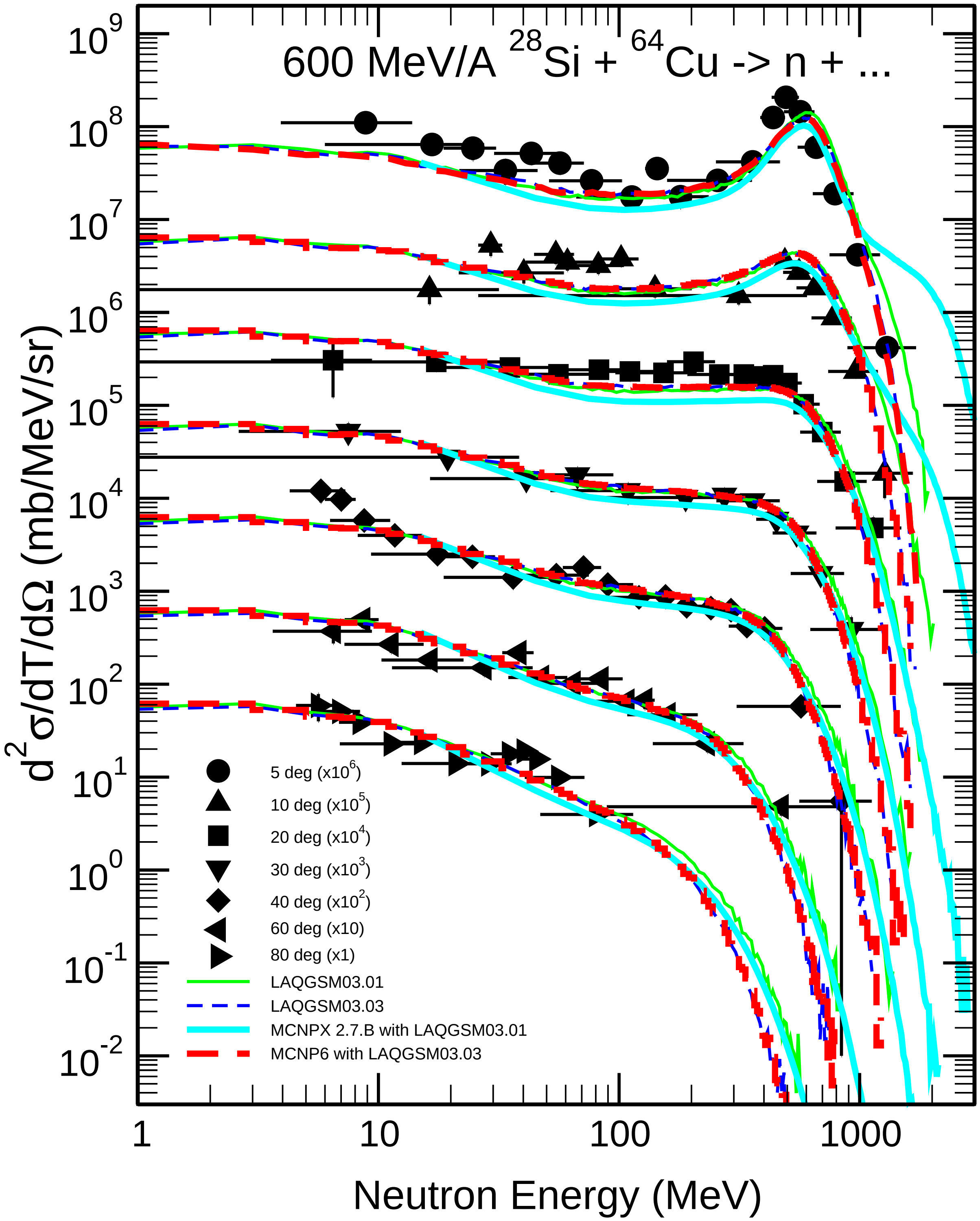

Figure 2: Experimental neutron spectra [37] at 5°, 10°, 20°, 30°, 40°, 60°, and 80° from a relatively thin Cu target bombarded with a 600 MeV/nucleon ^{28}Si beam compared with results by LAQGSM03.01 [7] and LAQGSM03.03 [6] used as stand alone codes, with our MCNP6 results using LAQGSM03.03 with the **noact=-2** option for the 8th parameter of the LCA card, as well as with results by MCNPX 2.7.B [13] obtained by Dr. Igor Remec at ORNL using LAQGSM03.01, as indicated.

3.2. Test-Problem #2: inp71corREP

This MCNP6 problem is to test the applicability of MCNP6 using the LAQGSM03.03 event generator for several NASA (shielding for missions in space) and FRIB (the initial U.S. DOE project known as Rare Isotope Production (RIA), updated in 2008 as “Facility for Rare Isotope Beams” (FRIB), under construction at present at MSU) applications. It was also used to check and correct an error observed in the input file **inp71** of the MCNPX test-problem adopted later also as a test-problem for the MCNP6 Suite: **/Testing/MCNPX_EXTENDED/heavyions/**. In addition, we used this test problem to study, understand, and fix the “implementation bug” mentioned in the previous Section 3.1.

We calculate this test-problem using the **NOACT=-2** option for the 8th parameter of the **LCA** card of the MCNP6 input file. As we have presented a detailed description of the use of **NOACT=-2** option to calculate particle spectra from thin targets in the test-problem #6 of the CEM Testing Primer [5], and have provided additional examples of its use in test problems #7 and #8 of Ref. [5], we do not need to discuss in detail the input and output files for this case. Therefore, we limit ourselves to only providing the text of the input file as well as describing where to find the results in the MCNP6 output files. We discuss below only some points of the input file needed to understand the observed (and corrected here) error in the input file **inp71** of the MCNPX test-problem adopted later also as a test-problem for the MCNP6 Suite: **/Testing/MCNPX_EXTENDED/heavyions/**.

The input file for this test problem is **inp71corREP**. It is presented in the subdirectory **/VALIDATION_LAQGSM/Inputs/** and is also shown below.

inp71corREP:

```
MCNP6 test with LAQGSM03.03: 135 MeV/A He4+Cu64 -> n spectra
c a correct version of the inp71 test-problem from */MCNPX_E*/heavyions/
c use of the latest, August 2010, version (REP) of MCNP6 with LAQGSM03.03
1   1  -10   -501      imp:n=1
2   0         501  -502  imp:n=1
99  0         502      imp:n=0

501   so 0.01
502   so 1
c
c  tally surfaces
c
5      kz    0    0.007654253     1
10     kz    0    0.031091151     1
15     kz    0    0.071796643     1
20     kz    0    0.132474088     1
25     kz    0    0.217442414     1
30     kz    0    0.333332652     1
35     kz    0    0.49028952      1
40     kz    0    0.704086505     1
45     kz    0    0.999997346     1
50     kz    0    1.420272373     1
```

```
55     kz    0    2.03959969      1
60     kz    0    2.999987744     1
65     kz    0    4.598886921     1
70     kz    0    7.548583695     1
75     kz    0    13.92808003     1
80     kz    0    32.16299385     1
85     kz    0    130.6423246     1
90     pz    0
95     kz    0    130.6503105    -1
100    kz    0    32.16399202    -1
105    kz    0    13.92837571    -1
110    kz    0    7.548708346    -1
115    kz    0    4.598950644    -1
120    kz    0    3.000024513    -1
125    kz    0    2.039622728    -1
130    kz    0    1.420287681    -1
135    kz    0    1.000007961    -1
140    kz    0    0.704094093    -1
145    kz    0    0.490295058    -1
150    kz    0    0.333336738    -1
155    kz    0    0.217445427    -1
160    kz    0    0.132476276    -1
165    kz    0    0.071798167    -1
170    kz    0    0.031092115    -1
175    kz    0    0.007654721    -1

m1  29064 1
lca 7j -2 j 1    $ LAQGSM
c nps 1000
nps 1e6
prdmp 2j -1
sdef par=a erg=540 vec=0 0 1 dir 1
phys:# 600
phys:h 600
phys:n 600
phys:a 600
phys:d 600
phys:t 600
phys:s 600
phys:/ 600
phys:z 600
mode n h # a d t s / z
c
f1:n  502
fs1   -5 -10 -20 -25 -35 -45 -55 -75 -85 105 115 125 135
      145 155 T
c sd1   0.17453  0.17453  0.34907  0.17453  0.34907  0.34907
```

```
c       0.34907 0.69814 0.34907
c       0.69814  0.34907  0.34907 0.34907  0.34907 0.34907
c       0.87266 12.56636
c The initial sd card (above) was wrong
c
c The following Segment Divisor card is needed to get 1/sr for n-spectra
sd1   0.02391  $ 2pi(cos0 -cos5)
      0.07155  $ 2pi(cos5 - cos10)
      0.28347  $ 2pi(cos10 - cos20)
      0.20976  $ 2pi(cos20 - cos25)
      0.54762  $ 2pi(cos25 - cos35)
      0.70500  $ 2pi(cos35 - cos45)
      0.83900  $ 2pi(cos45 - cos55)
      1.97768  $ 2pi(cos55 - cos75)
      1.07859  $ 2pi(cos75 - cos85)
      2.17382  $ 2pi(cos85 - cos105)
      1.02918  $ 2pi(cos105 - cos115)
      0.94850  $ 2pi(cos115 - cos125)
      0.83900  $ 2pi(cos125 - cos135)
      0.70400  $ 2pi(cos135 - cos145)
      0.54726  $ 2pi(cos145 - cos155)
      0.58869  $ 2pi(cos155 - cos180)
      12.56637 $ 4pi
c     Boundaries of the neutron energy bins: 0-1 MeV; 1-3 MeV, ...
e1    1     3     5     7     9     11    13    15    17    19
      22.5  27.5  32.5  37.5  42.5  47.5  52.5  57.5  62.5  67.5
      72.5  77.5  82.5  87.5  92.5  97.5  105   115   125   135
      145   155   165   175   185   195   205   215   225   235
      245   255   265   275   285   295   305   315   325   335
      345   355   365   375   385   395   405   415   425   435
      445   455   465   475   485   495   505   515   525   535
      545   555   565   575
em1 1258.34 73r $ multiply to sig_inelastic = 1258.34 mb, as predicted
c                by LAQGSM03.01, calculation of 6/10/2002. This is needed
c                to get the spectra in [mb/sr/MeV], after dividig the flux
c                to the energy bins, to get [1/MeV]
c
c
e0   600
f11:n   502
f21:h   502
f31:d   502
f41:t   502
f51:s   502
f61:a   502
f71:/   502
f81:z   502
```

```
dbcn  20j  0  7j  1  2j  0  1
```

We calculate the neutron spectra using the **F1** tally on the surface of a sphere (surface # 502) with a radius equal to 1 cm, using a source of 540 MeV monoenergetic alpha particles in its center (i.e., a source of ^{4}He with the bombarding energy of $540/4 = 140$ MeV/nucleon), with the beam in the Z-axis direction. To get the double-differential spectra of secondary neutrons at needed angles, it is very convenient to divide the surface of the sphere (surface # 502) in "segments", corresponding to our angles, and to tally the neutron separately in all these "segments". For this, we use "tally surfaces" of cones on the Z-axis defined as:

```
5       kz    0    0.007654253     1
10      kz    0    0.031091151     1
15      kz    0    0.071796643     1
20      kz    0    0.132474088     1
25      kz    0    0.217442414     1
30      kz    0    0.333332652     1
35      kz    0    0.49028952      1
40      kz    0    0.704086505     1
45      kz    0    0.999997346     1
50      kz    0    1.420272373     1
55      kz    0    2.03959969      1
60      kz    0    2.999987744     1
65      kz    0    4.598886921     1
70      kz    0    7.548583695     1
75      kz    0    13.92808003     1
80      kz    0    32.16299385     1
85      kz    0    130.6423246     1
90      pz    0
95      kz    0    130.6503105    -1
100     kz    0    32.16399202    -1
105     kz    0    13.92837571    -1
110     kz    0    7.548708346    -1
115     kz    0    4.598950644    -1
120     kz    0    3.000024513    -1
125     kz    0    2.039622728    -1
130     kz    0    1.420287681    -1
135     kz    0    1.000007961    -1
140     kz    0    0.704094093    -1
145     kz    0    0.490295058    -1
150     kz    0    0.333336738    -1
155     kz    0    0.217445427    -1
160     kz    0    0.132476276    -1
165     kz    0    0.071798167    -1
170     kz    0    0.031092115    -1
175     kz    0    0.007654721    -1
```

Let us provide here a useful hint: we have chosen the numbers for the surfaces for these cones not arbitrarily, but so that they help us know at once the angle a given cone provides:

So, surface #5 is a cone on the Z-axis starting at the origin, Z=0; it provides us an angle of 5 degrees relative to the Z-axis. Similarly, surface #10 provides us an angle of 10 degrees, etc. From here, we have that the "segment" of the sphere (surface # 502) cut by the cones #10 and #20 corresponds to an angle of 15 ± 5 degrees, the second angle for which we need to calculate the neutron spectra. In a similar way, other cones have the surface numbers and provide just the angles to get the remaining 30 ± 5, 50 ± 5, 80 ± 5, and 110 ± 5 degrees in order to calculate our spectra. It is clear that the first spectrum, at 0 ± 5 degrees, is tallied on the surface of the sphere (surface # 502) cut by the cone #5.

Let us recall here that the **F1** tally of MCNP6 provides us current of particles (neutrons, in our case) over a surface in units of [particles/projectile], while we need our final neutron spectra in units of [mb/MeV/sr] (per projectile), as they were measured in the experiment. To get the units of mb, we multiply our MCNP6 spectra with the total inelastic cross section, $\sigma_{in} = 1258.34$ mb, as calculated by LAQGSM03.01 used as a stand alone code; for this, we use the Energy Multiplier Card **EM1**

```
em1 1258.34 73r $ multiply to sig_inelastic = 1258.34 mb, as predicted
c                 by LAQGSM03.01, calculation of 6/10/2002. This is needed
c                 to get the spectra in [mb/sr/MeV], after dividig the flux
c                 to the energy bins, to get [1/MeV]
```

with this value for all of the 74 energy bins defined by the **E1** card:

```
c     Boundaries of the neutron energy bins: 0-1 MeV; 1-3 MeV, ...
e1    1     3     5     7     9     11    13    15    17    19
      22.5  27.5  32.5  37.5  42.5  47.5  52.5  57.5  62.5  67.5
      72.5  77.5  82.5  87.5  92.5  97.5  105   115   125   135
      145   155   165   175   185   195   205   215   225   235
      245   255   265   275   285   295   305   315   325   335
      345   355   365   375   385   395   405   415   425   435
      445   455   465   475   485   495   505   515   525   535
      545   555   565   575
```

To get the needed units of [1/MeV] for our spectra, we need to divide the MCNP6 results by the corresponding energy bin widths (in MeV). Note that we could do this with the **EM1** card, using on it σ_{in} divided by different values for the corresponding energy bins, as was done in the test-problem presented in Section 3.8 of Ref. [5]. However, in order to keep this MCNP6 input as simple as possible, we chose to not do so with the **EM1** in the current test-problem; instead, after all MCNP6 calculations are completed, we divide the corresponding MCNP6 results using a little auxiliary routine we wrote to make this division.

Finally, to get the units of [1/sr] in our spectra, we need to divide the **F1** MCNP6 tally results by the values of the solid angles for the "segments" where we count the neutrons. It is convenient to do this with the Segment Divisor Card **SD1**, where we provide the solid angle for each "segment" (we calculate them separately with a calculator before starting our MCNP6 run).

```
c sd1   0.17453  0.17453  0.34907  0.17453  0.34907  0.34907
c       0.34907 0.69814 0.34907
c       0.69814  0.34907  0.34907 0.34907  0.34907 0.34907
```

```
c       0.87266 12.56636
c The initial sd card (above) was wrong
c
c The following Segment Divisor card is needed to get 1/sr for n-spectra
sd1   0.02391  $ 2pi(cos0 -cos5)
      0.07155  $ 2pi(cos5 - cos10)
      0.28347  $ 2pi(cos10 - cos20)
      0.20976  $ 2pi(cos20 - cos25)
      0.54762  $ 2pi(cos25 - cos35)
      0.70500  $ 2pi(cos35 - cos45)
      0.83900  $ 2pi(cos45 - cos55)
      1.97768  $ 2pi(cos55 - cos75)
      1.07859  $ 2pi(cos75 - cos85)
      2.17382  $ 2pi(cos85 - cos105)
      1.02918  $ 2pi(cos105 - cos115)
      0.94850  $ 2pi(cos115 - cos125)
      0.83900  $ 2pi(cos125 - cos135)
      0.70400  $ 2pi(cos135 - cos145)
      0.54726  $ 2pi(cos145 - cos155)
      0.58869  $ 2pi(cos155 - cos180)
      12.56637 $ 4pi
```

For comparison, in the first four commented lines above, we show the values used on the **SD1** card in the input file **inp71** of the MCNPX test-problem adopted later also as a test-problem for the MCNP6 Suite: **/Testing/MCNPX_EXTENDED/heavyions/**. We can see that the values of the solid angles shown on the commented lines from **inp71** were not correct; therefore, we use here our correct values, as shown above.

All other details of the input file are either described in the CEM Testing Primer [5] or are self-explanatory; therefore, we do not discuss them here.

Spectra calculated by MCNP6 with LAQGSM03.03 using the correct input, **inp71corREP**, for angles of 0, 15, 30, 50, 80, and 110 (±5) degrees are tabulated in units of [mb/sr] in the output file **/VALIDATION_LAQGSM/Templates/LINUX/inp71corREP.o** as tally 1 for "segments":
1) segment: -5
2) segment: 5 10 -20
3) segment: 5 10 20 25 -35
4) segment: 5 10 20 25 35 45 -55
5) segment: 5 10 20 25 35 45 55 75 -85
6) segment: 5 10 20 25 35 45 55 75 85 -105 115

respectively, as well as in the MCTAL file inp71corREP.m. The same results but already divided by the energy bins (after the MCNP6 calculations are completed, using a little auxiliary routine we wrote to make this division, as mentioned above), to get the [1/MeV] units for our spectra, providing the final units of [mb/MeV/sr], as measured and tabulated in the published data, are presented in the files 0_m6REP.dat, 15_m6REP.dat, 30_m6REP.dat, 50_m6REP.dat, 80_m6REP.dat, and 110_m6REP.dat, respectively. These files are used by **xmgrace** to plot the figure shown in the file He135Cu_xf4.pdf, presented below in Figure 3. The file He135Cu_xf4.fig

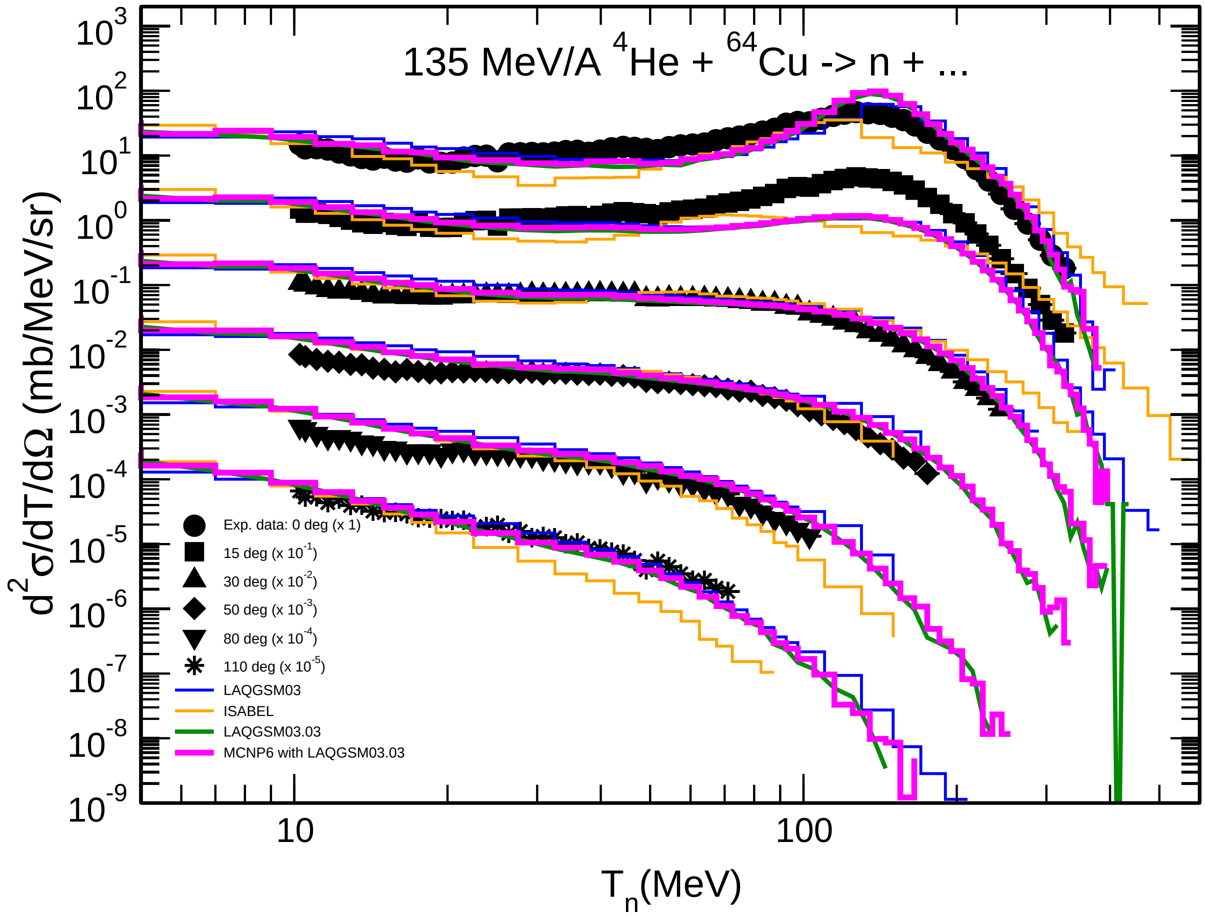

Figure 3: Experimental neutron spectra [39, 40] at 0, 15, 30, 50, 80, and 110 degrees (symbols) from a thin Cu target bombarded with a 135 MeV/nucleon ^{4}He beam compared with results by LAQGSM03 [41] and ISABEL [42] + MPM preequilibrium [50] + Dresner evaporation [51] model used as stand alone codes as published in Ref. [38], and with our current MCNP6 results using the LAQGSM03.03 event generator and calculations by LAQGSM03.03 [10] used as a stand alone code, as indicated.

is a template for plotting this figure with **xmgrace**.

Besides the MCNP6 results, for comparison, we present here also results by LAQGSM03.03 used as a stand alone code (files 0_L0303.dat, 15_L0303.dat, 30_L0303.dat, 50_L0303.dat, 80_L0303.dat, and 110_L0303.dat, for angles of 0, 15, 30, 50, 80, and 110 degrees, respectively).

For comparison, we also present our earlier results by LAQGSM03 [41] used as a stand alone code (files: 0_laqgsm03.dat, 15_laqgsm03.dat, 30_laqgsm03.dat, 50_laqgsm03.dat, 80_laqgsm03.dat, and 110_laqgsm03.dat, respectively) and by ISABEL INC [42] followed by the MPM [50] preequilibrium and Dresner evaporation model [51] used as a stand alone code (files: 0_isabel.dat, 15_isabel.dat, 30_isabel.dat, 50_isabel.dat, 80_isabel.dat, and 110_isabel.dat, respectively). These earlier results are published in the paper [38].

The experimental data for this problem are published in figures of Ref. [39]. Tabulated values of these data are taken from the CD distributed with the Handbook [40]. Experimental neutron spectra in units of [mb/MeV/sr] for angles of 0, 15, 30, 50, 80, and 110 degrees are presented in files 0_135He4Cu64exp.dat, 15_135He4Cu64exp.dat, 30_135He4Cu64exp.dat, 50_135He4Cu64exp.dat, 80_135He4Cu64exp.dat, and 110135He4Cu64exp.dat, respectively, in the subdirectory **/VALIDATION_LAQGSM/Experimental_data/inp71cor/**, together with files with all calculation result and figures.

From Figure 3, we see very good agreement between the MCNP6 results calculated using the **NOACT=-2** option for the 8th parameter of the **LCA** card with the LAQGSM03.03 event generator and the calculations by LAQGSM03.03 used as a stand alone code. Both these results agree well with the experimental data and with older calculations by LAQGSM03 [41] and by ISABEL [42] + MPM preequilibrium [50] + Dresner [51] evaporation model used as a stand alone codes. The test-results obtained with the old input file **inp71** of the MCNPX test-problem adopted later also as a test-problem for the MCNP6 Suite: **/Testing/MCNPX_EXTENDED/heavyions/** do not agree well with the measured data. An even worse agreement with the measured spectra at forward angles was obtained using the initial version of MCNP6 and older versions of MCNPX, which both contained the implementation error mentioned in Section 3.1. As both these problems were solved, we do not present here the wrong results. Now, both the MCNP6 and MCNPX 2.7.0 transport codes describe well such neutron spectra from this and other similar nucleus-nucleus reactions.

3.3. Test-Problems #3: inp75cor_bREP

This MCNP6 exercise is to test the applicability of MCNP6 using the LAQGSM03.03 event generator for FRIB, the initial U.S. DOE project known as "Rare Isotope Production" (RIA), updated in 2008 as "Facility for Rare Isotope Beams" (FRIB), presently under construction at Michigan State University.

It is the last example we present in the current Primer which was used by us to study, understand, and fix the "implementation bug" mentioned in Section 3.1.

Finally, this exercise is also to test a new capability of MCNP6, namely, to tally separately particles and antiparticles (π^+ and π^-, in this example).

This problem calculates with MCNP6 the neutron, proton, deuteron, triton, ^{3}He, ^{4}He, as well as charged and neutral pion angle-integrated energy spectra from interaction of a 400 MeV/A ^{238}U beam with a thick ^{6}Li target. There are no measured data for this test-problem, but extensive simulations with MCNPX for such interactions were performed several year ago by Dr. Itacil Gomes [43, 44] to support the RIA project.

One of the main initial reasons to address this test-problem was to check some suspicious MCNPX results for this reaction, presented at the ICRS11/RPSD2008 conference and published in the LANL Report LA-UR-08-2218 [45], we detected only after the ICRS11/RPSD2008 conference and publication of Ref. [45]. What made the situation even more difficult, is that those suspicious MCNPX results were obtained with an MCNPX input similar to the one adopted later in the MCNP6 Suite **/Testing/MCNPX_EXTENDED/heavyions/**, as the file **inp75**. Our main concern about those MCNPX results calculated using the LAQGSM03.01 event generator was related with the neutron and proton spectra from a thick ^{6}Li target bombarded with a 400 MeV/nucleon ^{238}U beam shown on page 18 of Ref. [45]. In spite of the fact that the incident energy of the beam was of only 400 MeV/nucleon, the nucleon spectra emitted from the bombarded thick ^{6}Li target were not vanishing and far from approaching a zero value up to 2000 MeV, the maximum energy shown in the figure on page 18 of Ref. [45]. As the Fermi energy of the intranuclear nucleons is only of the order of several tens of MeV and LAQGSM does not consider any collective or other "exotic" mechanisms which could provide such energetic secondary nucleons from the thick ^{6}Li target, that figure clearly indicates us that something was wrong with those MCNPX results.

This is why we decided to investigate in detail this reaction with MCNP6, looking at spectra not only of nucleons, but of all secondary particles produced from such interactions, up to their maximum possible energy, as calculated by MCNP6. Our initial results calculated with a "historical" version of MCNP6 which used the same LAQGSM03.01 [7] event generator as employed in the MCNPX calculations published in Ref. [45] shocked us: With a 400 MeV/nucleon beam, we got spectra of nucleons emitted from our thick target with energies up to 5.4 GeV, and pion spectra up to 2.5 GeV, which was undoubtably an error. Our investigation has shown that this was related with the same unobserved error in the implementation of LAQGSM03.01 in MCNPX and the initial version of MCNP6 discussed above in Section 3.1. After that error was fixed, we get correct results for such (and other similar) reactions, as is proved below by the results of the current test-problem.

The input file for this test problem is **inp75cor_bREP**. It is presented in the subdirectory **/VALIDATION_LAQGSM/Inputs/** and is also shown below.

inp75cor_bREP:

```
RIA target test
1 1 5e-2  -3  -99
2 0  3  -99
99 0  99

1  pz 0.0
2  pz 1.0
3  cx 1.5
99 so 100.0

mode # n a t d s h / * z
m1  3006  1
phys:# 100000
phys:n 10000
phys:h 10000
phys:a 10000
phys:t 10000
phys:d 10000
phys:s 10000
phys:/ 10000
phys:* 10000
phys:z 10000
lca  9j 1
imp:# 1 1 0
imp:n 1 1 0
sdef par=92238 erg=95200 pos 0 0 -2 rad=d1 axs 0 0 1 vec 0 0 1 dir 1
si1   0 0.2
sp1   -21 1
c nps 500
```

```
nps 1e6
prdmp 2J -1
e0 0.0 99i 104000.0
f4:# 2
sd4  1
f1:n 3
e1 1 99i 10000
f11:h 3
e11 1 99i 10000
f21:a 3
e21 1 99i 10000
f31:d 3
e31 1 99i 10000
f41:t 3
e41 1 99i 10000
f51:s 3
e51 1 99i 10000
f71:/ 3
e71 1 99i 10000
f81:* 3
e81 1 99i 10000
c f91:z 3
c e91 1 99i 10000
f94:z 1
e94 1 99i 10000
f61:# 3
e61 1 99i 100000
print
c dbcn  20j  0  7j  1  2j  0  1
dbcn  20j  0  5j  -1  j  1  2j  0  1  $ dbcn(27)=-1 provides pi+ separately of pi-
```

Let us mention that particle spectra from thick targets are usually calculated or measured in units of [particles/MeV/projectile] and such spectra, generally, can not be compared directly with spectra from thin targets which usually are presented in units of [mb/MeV(/projectile)]. In other words, we can not compare quantitatively the spectra calculated with MCNP6 from a thick target with spectra calculated by LAQGSM used as a stand alone code from a thin target. Besides, we do not have experimental data for the current problem. However, if we normalize the spectra calculated with MCNP6 from our thick ^{6}Li target to the value of the total reaction cross section (2880.24 mb) as calculated by LAQGSM03.03 used as a stand alone code for this reaction on a thin ^{6}Li target we could compare qualitatively the present spectra calculated with MCNP6 with results by LAQGSM03.03 used as a stand alone code. Buy doing so, we can at least judge if the shape and the absolute value of the spectra calculated by MCNP6 from the thick ^{6}Li target do not contradict the results obtained with LAQGSM03.03 used as a stand alone code for a thin ^{6}Li target. As any thick material causes particles to slows down and may absorb all charged particles and ions transported through it, spectra of such particles and ions from any thick target must be lower than the corresponding spectra from thin targets. Also, they should have similar shapes, and must always encompass lower energies in comparison with spectra from thin targets.

Before presenting our results, let us mention here an important point about using the **Mode Card** and **Phys Card** in MCNP6: Initially, MCNP6 adopted the MCNPX concept to transport both particles and antiparticles, if particles are listed on the **mode** and **phys** cards. This is why in the initial version of the input file for this test-problem we have listed on these cards only the π^+, with its designator **/**, but do not list its antiparticle, the π^-, with its designator *****. This was valid in the version of MCNP6 we had and used when we run this test-problem, in April 2010. This approach really makes physics sense only for the electron/positron instance, and is contrary to the usual practice among other high-energy codes, where particles and their antiparticles are generally separate and separately-treated particle types (because their physics is usually quite different). In other words, the initial MCNP6 approach adopted from MCNPX would tally both π^+ and π^- together and would not allow us to calculate separately π^+ and π^- spectra, as discussed in some other of our test-problems with MCNP6 using CEM [5]. In the initial version of MCNP6, the compromise has been to assume that the presence of a particle on the **Mode Card**, and on appropriate tallies, implies the presence of the corresponding antiparticle when MCNPX emulation is in force (specified by **DBCN(29)=1**; see the last card of our current input file), but to keep particles and antiparticles separate when MCNP emulation is effective (specified by **DBCN(29)=0**). This compromise was reasonable, but we understand that the MCNP6 users need the capability to select this behavior independently of the **DBCN(29)** setting. This deficiency was solved in MCNP6 by Grady Hughes, when on May 11, 2010 he produced a new and more universal version of MCNP6 implementing an extra (backward compatibility) DBCN control, namely the **DBCN(27)** flag. Specifically, the logic implemented by Grady Hughes in the new version of MCNP6 is now as follows:

1) There will be no promotion of antiparticles in KCODE problems;
2) There will be no promotion of antiparticles for at most N, P, E problems;
3) Otherwise, **DBCN(27) = 1** turns **on** promotion regardless of DBCN(29);
4) Or, **DBCN(27) = -1** turns **off** promotion regardless of DBCN(29);
5) Otherwise, promotion is turned **on** when **DBCN(29) = 1**;
6) Or, **off** when **DBCN(29) = 0**.

To summarize, if users have an old version of MCNP6, they should uncomment the second from the end (**dbcn**) card in the input file provided above, comment the last (**dbcn**) card, comment the card **phys:* 10000**, and remove the π^- designator ***** from the **mode** card. But with a newer version of MCNP6, in order to transport π^-, the user should have the designator of π^- (which is ***** in MCNP6) on the **mode** card and have it on a **phys** card as well, as is shown in the current input file **inp75cor_bREP**. In addition, the last (**dbcn**) card of the current input file should be activate, while the second from the end card should be commented, as is shown in our example.

More details on the use of the DBCN options in MCNP6 calculations can be found in the recent report by Grady Hughes [46]. Let us note here that we are working at present to simplify the use of the DBCN option for MCNP6 users; many details described in Ref. [46] will be of interest only for MCNP6 developers, while the users will not need to know and/or (explicitly) use them in their applications.

Energy spectra of n, p, ^{4}He, d, t, ^{3}He, π^+, π^-, and π^0 calculated with MCNP6 using the LAQGSM03.03 event generator with the input file **inp75cor_bREP** are tabulated as tallies 1, 11, 21, 31, 41, 51, 71, 81, and 91, respectively, in units of [particles/projectile] in the output file **inp75cor_bREP.o** presented together with the MCTAL file **inp75cor_bREP.m** in the subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**.

To plot these spectra with **xmgrace**, the same results, already divided by the energy bins to get the calculated spectra in unites of [particles/MeV/projectile], are presented in the separate files n_6REP.dat, p_6REP.dat, he4_6REP.dat, d_6REP.dat, t_6REP.dat, he3_6REP.dat, pip_6REP.dat, and pim_6REP.dat, respectively. Finally, in order to compare qualitatively the current MCNP6 results with spectra by LAQGSM03.03 [10] and LAQGSM03.01 [7] used as a stand alone codes calculated from a thin ^{6}Li target in units of [mb/GeV], (and, also, [per projectile]), while plotting the MCNP6 spectra with **xmgrace**, we multiply them by 2880.23, the value of the total inelastic cross section in [mb] as calculated by LAQGSM03.03 used as a stand alone code. We also must convert the MCNP6 units for particle energies of [MeV] to [GeV], as used by LAQGSM03.03 and plotted here.

Results by LAQGSM03.01 [7] used as a stand alone code from a thin ^{6}Li target for energy spectra of n, p, d, t, ^{3}He, ^{4}He, π^{+}, and π^{-} in units of [mb/GeV] are presented in the files n_0301.dat, p_0301.dat, d_0301.dat, t_0301.dat, he3_0301.dat, he4_0301.dat, pi+_0301.dat, and pi-_0301.dat, respectively. Similar results in the same units by the latest version of LAQGSM, LAQGSM03.03 [10], are presented in the files n_0303.dat, p_0303.dat, d_0303.dat, t_0303.dat, he3_0303.dat, he4_0303.dat, pi+_0303.dat, and pi-_0303.dat, respectively.

All the mentioned results are plotted with **xmgrace** and are presented in the subdirectory **/VALIDATION_LAQGSM/Experimental_data/inp75cor/** in the pdf files n_6REP.pdf, p_6REP.pdf, d_6REP.pdf, t_6REP.pdf, He3_6REP.pdf, He4_6REP.pdf, pip_6REP.pdf, pim_6REP.pdf, as well as in the summary file with all eight plots U238_Li6_6REP.pdf. Templates for **xmgrace** are presented in the files n_6REP.fig, p_6REP.fig, d_6REP.fig, t_6REP.fig, He3_6REP.fig, He4_6REP.fig, pip_6REP.fig, pim_6REP.fig, respectively.

The final results for this test problem are shown below in Figure 4. We see that after the correction the problem of implementation of LAQGSM in MCNP6/X, as described in Section 3.1, the shape of all spectra calculated with MCNP6 from our thick ^{6}Li target are very similar to the ones provided by LAQGSM03.01 [7] and LAQGSM03.03 [10] used as stand alone codes from a thin ^{6}Li target. All spectra calculated with MCNP6 from the thick target are lower than the corresponding spectra from thin targets calculated with LAQGSM03.01 and LAQGSM03.03 used as stand alone codes, and all encompass lower energies in comparison with spectra from thin targets, just as we expected. These results prove to us that the mentioned problem observed in the neutron and proton spectra shown on page 18 of Ref. [45] was solved, and we do not need to show here the wrong results caused by that implementation problem. In both MCNP6 and MCNPX 2.7.0, that problem was solved.

3.4. Test-Problem #4: Pb1000LbREP

This MCNP6 problem is to test the applicability of MCNP6 using the LAQGSM03.03 event generator to describe backward emission of particles from thick targets bombarded by intermediate-energy (200–1000 MeV) protons. To be specific, the main aim of this problem is to study neutron emission at 175 degrees from a 1.0 GeV proton beam hitting a face plane of a cylindrical lead target that is 20 cm in diameter and 25 cm thick.

First, we need such information for shielding consideration, to be able to prevent cases when personnel may receive radiation from backward fluxes.

Second, it is much more difficult for all models to describe particle production at very backward angles than at intermediate or forward angles; that is, this problem is a good test to see how the LAQGSM03.03 event generator works in such a “difficult” kinematics region.

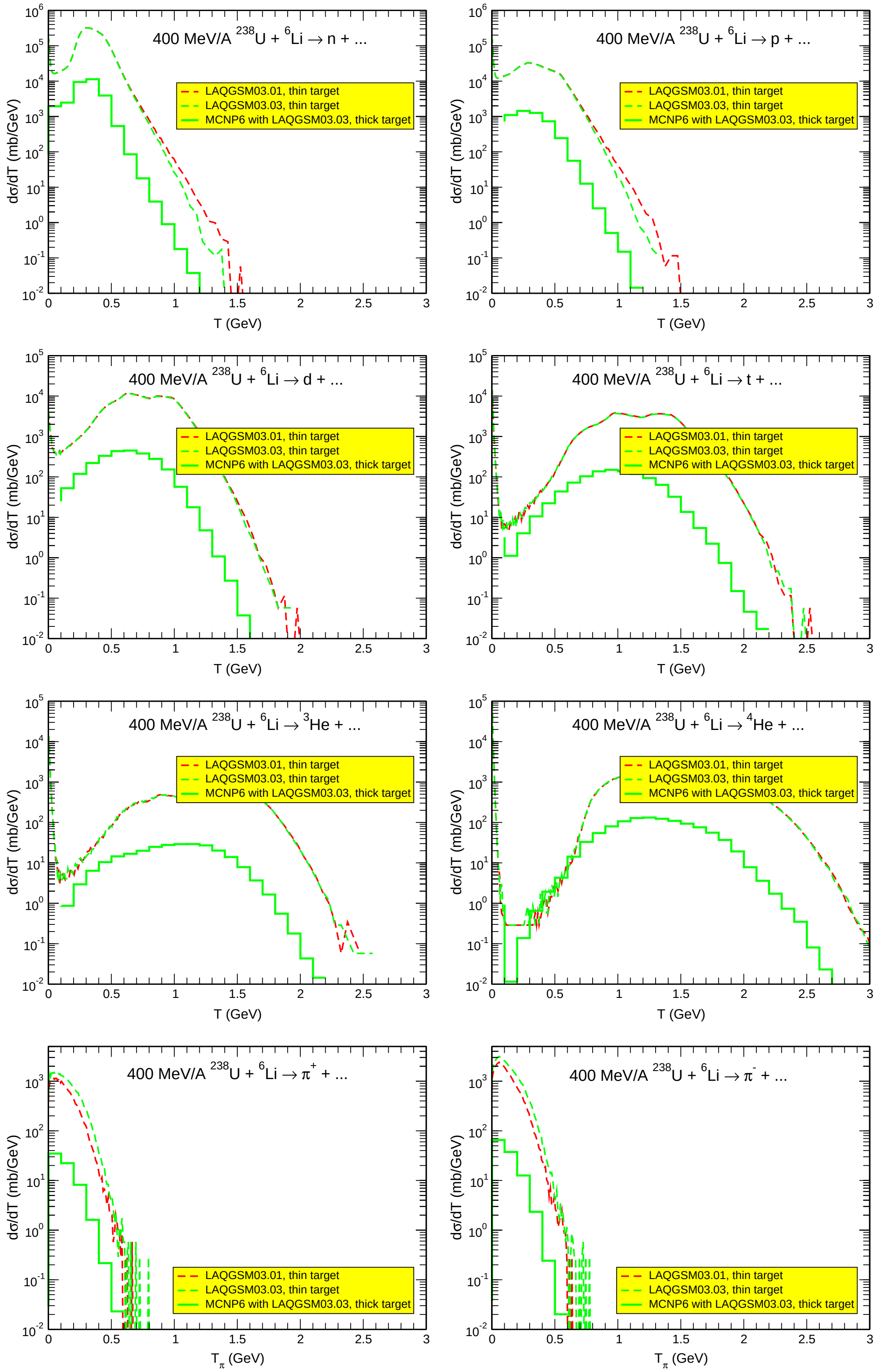

Figure 4: Energy spectra of n, p, d, t, ^{3}He, ^{4}He, π^+, and π^- from a ^{6}Li target bombarded with a 400 MeV/nucleon ^{238}U beam calculated with LAQGSM03.01 [7] and LAQGSM03.03 [10] codes used as stand alone codes (from a thin ^{6}Li target) and with MCNP6 using LAQGSM03.03 (from a thick ^{6}Li target; see details in the text), as indicated.

Third, spectra of secondary particles at very backward angles are of great academic interest, to understand the mechanisms of cumulative particle production, under investigation for four decades already, but still with many open questions (see, e.g., Ref. [47]).

The experimental data for this problem were measured at the Institute of High Energy Physics in Protvino, Russia using the calorimetric-time-of-flight (CTOF) technique and are published in Ref. [48].

Though the current problem is to model only interaction of 1000 MeV protons with a cylindrical lead target of 20 cm in diameter and 25 cm thick, the measurements were performed also at 200, 400, 600, and 800, MeV; therefore, we performed calculations with MCNP6 using the LAQGSM03.03 [10] event-generator at all these energies. In addition, for comparison, we performed similar calculations with MCNP6, but using the CEM03.03 [6], Bertini INC [49] followed by the Multistage Preequilibrium Model (MPM) [50] and the evaporation model described with the Dresner code EVAP [51], and using the INCL+ABLA [52, 53] event-generators. For a broader comparison, we use here also the results obtained at ORNL and kindly supplied us by Wei Lu and Franz Gallmeier with the 2.6.0 version of MCNPX [35] using CEM03.01 [8] (see more details in Ref. [48]). All these results are shown in Figure 5 together with the experimental data from Ref. [48].

Below, we present only the MCNP6 input for the case of 1000 MeV bombarding protons; it is called **Pb1000LbREP**. This input is more complicated than we had for the previous test-problems, therefore we provide also all the necessary information to help MCNP6 users understand all its details.

Pb1000LbREP:

```
MCNP6 test: 175 deg. n-spec. by LAQGSM03.03 to compare with exp. data
c
c     **cellcards **
c
    1  1 -11.35  -1 2 -3    $ m1 is Lead
    2  2 -0.001168  #1 -5
    3  0        5  -6
    6  0        6
  999  0       -999

c
c  *****surface card
c
    1  cz    10      $ diameter = 20 cm
    2  pz    0.0
    3  pz    25.0    $ 25 cm thick
    5  so    600
    6  so    800
    7  pz    -597.8168189
    8  pz    -597.6168189
  999  cz    10.000001

c  *
```

```
c  * Data Cards
c  *
c
c         Material cards
c
m1       82204.70h  1.400
         82206.70h 24.100
         82207.70h 22.100
         82208.70h 52.400
m2       7014.70h 1.555901784
         7015.60c 0.005778216
         8016.70h 0.448606754
         8017.60c 0.001079246
         1001.70h 0.06
         18000.35c 0.00934
         6000.60c 0.000383
c
c  importances
imp:n 1 1 1 0 0
imp:h 1 1 1 0 0
imp:p 1 1 1 0 0
imp:d 1 1 1 0 0
imp:t 1 1 1 0 0
imp:s 1 1 1 0 0
imp:a 1 1 1 0 0
imp:/ 1 1 1 0 0
imp:z 1 1 1 0 0
c *
c * source definition
c *
sdef erg=1000 par=h dir=1 vec= 0 0 1 x=d1 y=d2 z=0 ccc=999
sp1  -41 2.4 0
sp2  -41 2.4 0
 nps   1e7
c nps   1000
print   10 110   40
prdmp 2.e7 1.e6 1 10 1e6
LCA  9j 1
LCB 0 0 0 0 0 3500
c
c  tally
c
F11:n   5
SD11    1 753.9822369 1
FS11    -7 -8
FQ11    e u
TF11    6j 21
```

```
E11   1.059254E-03 1.188502E-03 1.333521E-03 1.496236E-03 1.678804E-03
      1.883649E-03 2.113489E-03 2.371374E-03 2.660725E-03 2.985383E-03
      3.349654E-03 3.758374E-03 4.216965E-03 4.731513E-03 5.308844E-03
      5.956621E-03 6.683439E-03 7.498942E-03 8.413951E-03 9.440609E-03
      1.059254E-02 1.188502E-02 1.333521E-02 1.496236E-02 1.678804E-02
      1.883649E-02 2.113489E-02 2.371374E-02 2.660725E-02 2.985383E-02
      3.349654E-02 3.758374E-02 4.216965E-02 4.731513E-02 5.308844E-02
      5.956621E-02 6.683439E-02 7.498942E-02 8.413951E-02 9.440609E-02
      1.059254E-01 1.188502E-01 1.333521E-01 1.496236E-01 1.678804E-01
      1.883649E-01 2.113489E-01 2.371374E-01 2.660725E-01 2.985383E-01
      3.349654E-01 3.758374E-01 4.216965E-01 4.731513E-01 5.308844E-01
      5.956621E-01 6.683439E-01 7.498942E-01 8.413951E-01 9.440609E-01
      1.059254E+00 1.188502E+00 1.333521E+00 1.496236E+00 1.678804E+00
      1.883649E+00 2.113489E+00 2.371374E+00 2.660725E+00 2.985383E+00
      3.349654E+00 3.758374E+00 4.216965E+00 4.731513E+00 5.308844E+00
      5.956621E+00 6.683439E+00 7.498942E+00 8.413951E+00 9.440609E+00
      1.059254E+01 1.188502E+01 1.333521E+01 1.496236E+01 1.678804E+01
      1.883649E+01 2.113489E+01 2.371374E+01 2.660725E+01 2.985383E+01
      3.349654E+01 3.758374E+01 4.216965E+01 4.731513E+01 5.308844E+01
      5.956621E+01 6.683439E+01 7.498942E+01 8.413951E+01 9.440609E+01
      1.059254E+02 1.188502E+02 1.333521E+02 1.496236E+02 1.678804E+02
      1.883649E+02 2.113489E+02 2.371374E+02 2.660725E+02 2.985383E+02
      3.349654E+02 3.758374E+02 4.216965E+02 4.731513E+02 5.308844E+02
      5.956621E+02 6.683439E+02 7.498942E+02 8.413951E+02 9.440609E+02
      1000
EM11  360000 120r  $ unit: n/sr/p
c
mode n h p d t s a / z
phys:h   1500.
phys:n   1500.
phys:p   1500
phys:/   1500
phys:z   1500
DBCN 28j 1
```

First, in the the input file **Pb1000LbREP**, we see that the lead cylinder, 20 cm in diameter and lying in the Z-axis from $Z = 0$ cm to $Z = 25$ cm, serves as the target for this problem and fills **cell #1**:

```
1  1 -11.35  -1 2 -3    $ m1 is Lead
```

defined by the **surface cards**:

```
1  cz    10      $ diameter = 20 cm
2  pz    0.0
3  pz    25.0    $ 25 cm thick .
```

Its **material** is defined also as #1, **m1**, as indicated by the useful comment on the cell card. The density of Pb is defined on the cell card as equal to 11.35 g/cm^3, and its composition is defined by the **material cards**:

```
m1        82204.70h  1.400
          82206.70h 24.100
          82207.70h 22.100
          82208.70h 52.400
```

As in the real experiment [48], the target was in a room filled with air. In our MCNP6 test-problem we surround the Pb-cylinder also with air, composed in our example of N, O, H, Ar, and C. The air is defined as material #2:

```
m2        7014.70h 1.555901784
          7015.60c 0.005778216
          8016.70h 0.448606754
          8017.60c 0.001079246
          1001.70h 0.06
          18000.35c 0.00934
          6000.60c 0.000383 .
```

In our problem, the air fills cell #2 and has a density of 0.001168 g/cm^3:

```
    2  2 -0.001168  #1 -5 .
```

The surface #5 is a sphere centered at origin with a radius $R = 600$ cm. Later, we tally our neutrons with the **tally card F11** just on the surface of this sphere

```
 F11:n   5 .
```

This means, we are not interested in what happens outside this sphere and can define all the "outside world", beyond this sphere, as "void"; the outside cells #3, #6, and #999 are of zero-density:

```
    3  0        5  -6
    6  0        6
  999  0       -999 .
```

This also means that we do not need to track particles in cells #6 and #999, and can set "importances" of all particles to 0 in these cells:

```
imp:n 1 1 1 0 0
imp:h 1 1 1 0 0
imp:p 1 1 1 0 0
imp:d 1 1 1 0 0
imp:t 1 1 1 0 0
imp:s 1 1 1 0 0
imp:a 1 1 1 0 0
imp:/ 1 1 1 0 0
imp:z 1 1 1 0 0 .
```

The beam of 1.0 GeV bombarding protons is defined on the **sdef** card:

```
sdef erg=1000 par=h dir=1 vec= 0 0 1 x=d1 y=d2 z=0 ccc=999 .
```

It is a mono-directional beam (**dir=1**) of protons (**par=h**) in the Z-direction (**vec= 0 0 1**) starting at $Z = 0$ (**z=0**) but, to account for the profile of the real experimental beam [48], it has a Gaussian distribution in both X- and Y-directions, as defined by the **Source Probability** cards:

```
sp1  -41 2.4 0
sp2  -41 2.4 0 .
```

The built-in function number **41**, used as a negative number on both **sp1** and **sp2** cards with the same parameters (**2.4 0**) identifies Gaussian distributions in both X- and Y-directions with the widths at half maximum (FWHM) of 2.4 cm and the mean of 0, i.e., with their maximum at $X = 0$ and $Y = 0$.

Note that on the **sdef** card, we use also the "Cookie-cutter rejection" (**ccc=999**), which accepts the simulated distribution of protons if it is within the cell #999, i.e., inside the cylinder of radius $R_{999} = 10.000001$ cm in the Z-direction, as defined by the surface #999

```
  999  cz    10.000001
```

and reject and resample it (truncate, so that all protons are inside this cylinder), if is not (see pages 3-52 to 3-68 in [3] for more details).

As our problem is symmetric about the Z-axis, we can tally the neutrons on a "ring" we cut from the sphere with a radius $R = 600$ cm defined by surface #5. If we cut this "ring" from the sphere with planes perpendicular to the Z-axis, $Z_7 = -597.8168189$ and $Z_8 = -597.6168189$, as defined by the surface cards

```
    7  pz    -597.8168189
    8  pz    -597.6168189 ,
```

then the middle of the ring $Z_m = -597.7168189$ determines an angle of 175 degree about the beam direction (600 cm$\times \cos 5^\circ = 597.7168189$ cm), i.e., exactly the angle where we want the neutrons tallied. Then, we can use the **Tally Segment Card**:

```
FS11    -7 -8
```

allowing us to subdivide the surface of the whole sphere into three sections, below $Z_7 = -597.8168189$, above $Z_8 = -597.6168189$, and between $Z_7 = -597.8168189$ and $Z_8 = -597.6168189$ and to calculate the neutron current with the card

```
F11:n   5
```

integrated over each of them, separately. The middle segment will provide us the current of neutrons emitted from the cylinder-target exactly at 175° — what we need in this problem.

Let us remind users that MCNP6 provides the results in units of **neutrons per incident proton**, while the experimental spectra were measured in units of **neutrons/sr/MeV per incident proton**. It is very easy to get the units of [1/MeV] for the MCNP6 spectra: For this, we need to divide the final MCNP6 results of the middle segment (**7 -8**) by the values of the corresponding energy bins, whose 121 boundaries are defined by the **Tally Energy Card**:

```
E11   1.059254E-03 1.188502E-03 1.333521E-03 1.496236E-03 1.678804E-03
      - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
      5.956621E+02 6.683439E+02 7.498942E+02 8.413951E+02 9.440609E+02
      1000 .
```

MCNP6 could do this division for us providing [1/MeV] in the calculated spectra, if we would instruct MCNP6 to do so with a corresponding **Energy Multiplier Card** in our input file. We do so, *e.g.*, in test-problems #6, #7, and #8 of the CEM Testing Primer [5] which have simpler input files. In the current test-problem, to keep the input file as simple as possible, we chose to not use this capability, but to divide instead the spectra from the final MCNP6 output files by the corresponding energy bins using a little post processing routine after the calculations are completed, just to get the needed units for plotting the final MCNP6 spectra.

It is a little more complicated to get the units of [1/sr] in the final spectra in this test-problem. For this, we divide the neutron spectrum tallied in the middle segment by the value of the solid angle of this segment. The solid angle Ω (in [sr]) of the "ring" where we tally neutrons is equal to the area of this ring, $S_{ring} = 2\pi Rh$ (where h is the "height" of the ring, i.e., $h = (Z_8 - Z_7) = 0.2$ cm, and R is the radius of the sphere, $R = 600$ cm), divided by the area of the whole sphere, $S_{sphere} = 4\pi R^2$, and multiplied by 4π: $\Omega = (2\pi Rh/4\pi R^2) \times 4\pi$. This is the same as multiplying the tallied spectra by the inverse of this quantity, $\Omega^{-1} = R^2/2\pi Rh$. To get [1/sr] in our final spectrum, we need to divide the tallied spectrum by $2\pi Rh = 753.9822369$ ([cm^2]) and to multiply it by $R^2 = 360000$ ([cm^2]). Here, we do the division for our middle segment with the **Segment Divisor Card (SD11)**

```
SD11    1 753.9822369 1
```

and multiply our spectra, at all 121 energy bins with the **Energy Multiplier Card (EM11)**:

```
EM11  360000 120r  $ unit: n/sr/p .
```

The energy of the bombarding proton beam is quite high, 1.0 GeV, and will produce numerous neutrons; we need to detect all of these emitted neutrons from our thick target. Some of the emitted neutrons are produced not directly by the bombarding protons, but via subsequent interactions inside the target of all types of secondary particles produced in an initial proton-iron collision. LAQGSM03.03, CEM03.03, and other event generators tested here can produce n, p, d, t, ^{3}He, ^{4}He, π^+, π^0, and π^- from an p+Pb interaction; therefore, we need to transport all these particles through our target. This is guaranteed using the **Mode Card**:

```
mode n h p d t s a / z
```

together with the **Phys Cards**:

```
phys:h   1500.
phys:n   1500.
phys:p   1500
phys:/   1500
phys:z   1500 .
```

Note that we do not need to specify additional **phys** cards to obtain the maximum energies of d, t, ^{3}He, and ^{4}He: They will be set to 1500 MeV for all particles. We can check this with **Print Table 101**, which provides us detailed information about all tracked particles, by adding **101** on the **print card**, like:

```
print   10 110 40 101 .
```

Finally, let us note here that the **Print Hierarchy Card (FQ)**

```
FQ11    e u
```

and the **Tally Fluctuation Card (TF)**

```
TF11    6j 21
```

are very useful for ordering printed output, by changing the default bin for a given tally specifying for which tally bin the chart and all the statistical analysis output will be printed. Both these cards are highly recommended for some problems in the MCNP5 and MCNPX manuals [3, 35]. However, in this particular test-problem, these cards are included more like examples and do not actually affect the neutron spectra we calculate here; in principle, we could omit both these cards in our MCNP6 input file and would get the same results.

As this problem requires quite a long computing time, we calculate it in several steps, using the **Continue-Run** option. Initially, we have run MCNP6 for several hours using the initial input file shown above with the command: **mcnp6 i=Pb1000LbREP n=Pb1000LbREP.**. The initial run provides us the output file **Pb1000LbREP.o**, the RUNTPE file **Pb1000LbREP.r**, and the MCTAL file **Pb1000LbREP.m**. In a second run, we would use only the RUNTPE file **Pb1000LbREP.r** from the first run and an auxiliary simple input file **inp-con** of only two cards

```
nps   1e7
continue
```

using the command: **mcnp6 c i=inp-con o=Pb1000LbREPc.o m=Pb1000LbREPc.m r=Pb1000LbREP.r**. Thereafter, if needed, we can make a third run, and so on (changing every time only the names of the corresponding output and MCTAL files) until we get the needed statistics.

The initial output file of this test-problem, **Pb1000LbREP.o**, together with the final output **Pb1000LbREP_7c.o** and MCTAL **Pb1000LbREP_7c.m** files are presented in the subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**. As mentioned above, the MCNP6 output file **Pb1000LbREP_7c.o** provides for the middle segment, between surfaces **7 -8**, the neutron spectrum at 175° in units of [neutrons/sr/proton], looking like:

```
- - - - - - - - - - - - - - - - - - - -
surface  5
 segment:           7       -8
      energy
    1.0593E-03   0.00000E+00 0.0000
    1.1885E-03   4.77316E-05 1.0000
    1.3335E-03   9.53951E-05 0.7071
- - - - - - - - - - - - - - - - - - - -
    1.0000E+03   0.00000E+00 0.0000
      total      1.37965E+00 0.0059
- - - - - - - - - - - - - - - - - - - -
```

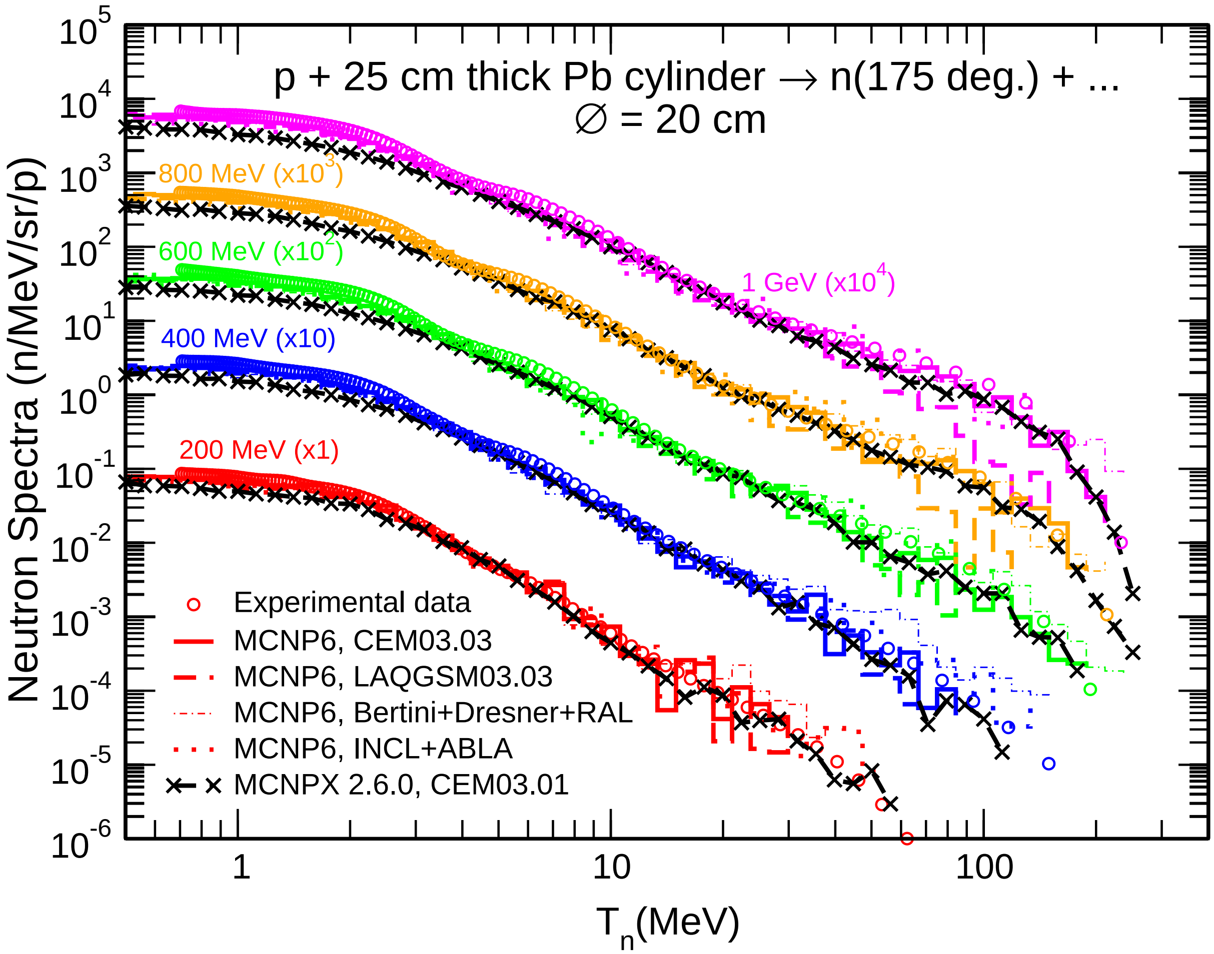

Figure 5: Experimental neutron spectra [48] at 175 degrees (symbols) from a thick Pb cylinder bombarded with 200, 400, 600, 800, and 1000 MeV protons compared with results by MCNP6 using the CEM03.03 [6], LAQGSM03.03 [10], Bertini INC [49] + Multistage Preequilibrium Model [50] + Dresner evaporation [51] + RAL fission model [26], and with INCL [52] + ABLA [53] event-generators, as well as with results by the 2.6.0 version of MCNPX [35] obtained by Wei Lu and Franz Gallmeier at ORNL using CEM03.01 [8], as indicated.

To plot this spectrum and compare it with the experimental data and results by other codes (see Figure 5), we convert it so that we have results in units of [1/MeV]. We do this separately with a little post processing routine written especially for this.

As the measurements [48] and calculations by other codes were done not only for incident protons of 1000 MeV, but also at 800 MeV, 600 MeV, 400 MeV, and 200 MeV, we performed calculations with MCNP6 at all these energies as well. For this, we had to change in the input file shown above only the incident energy of protons on the **sdef** card.

Our final MCNP6 results using LAQGSM03.03 for the incident proton energies of 1000, 800, 600, 400, and 200 MeV are presented in the files pb1000rep.dat, pb800rep.dat, pb600rep.dat, pb400rep.dat, and pb200rep.dat, of the subdirectory
/VALIDATION_LAQGSM/Experimental_data/Pb1000Lb/ and are plotted with **xmgrace**, as shown in Figure 5 and in the pdf file pPb_n_MCNP6_REP.pdf of the same subdirectory. A template to plot this figure with **xmgrace** is presented there as well in the file

pPb_n_MCNP6_REP.fig.

Experimental spectra in units of [neutron/MeV/sr/projectile] as functions of the neutron energy at incident proton energies of 1000, 800, 600, 400, and 200 MeV are presented in the same subdirectory in the files Pb1000_exp.dat, Pb800_exp.dat, Pb600_exp.dat, Pb400_exp.dat, and Pb200_exp.dat, respectively (the experimental errors are of the order of 8.5-9%, depending on the neutron energy).

For comparison, MCNP6 neutron spectra calculated with the CEM03.03 [6], Bertini [49] + MPM [50] + Dresner [51] + RAL [26], and INCL [52] + ABLA [53] event-generators at proton energies of 200, 400, 600, 800, and 1000 MeV are presented in the files Pb200C.dat, Pb400C.dat, Pb600C.dat, Pb800C.dat, and Pb1000C.dat for CEM03.03, in the files Pb200B.dat, Pb400B.dat, Pb600B.dat, Pb800B.dat, and Pb1000B.dat for Bertini+MPM+Dresner+RAL, and in the files Pb200I.dat, Pb400I.dat, Pb600I.dat, Pb800I.dat, and Pb1000I.dat for INCL+ABLA, respectively.

Finally, results by MCNPX2.6.0 [35] using the CEM03.01 [8] event-generator obtained at ORNL and kindly supplied us by Wei Lu and Franz Gallmeier as published in Ref. [48] for the incident proton energies of 200, 400, 600, 800, and 1000 MeV are presented in the files Pb200C_X.dat, Pb400C_X.dat, Pb600C_X.dat, Pb800C_X.dat, and Pb1000C_X.dat, respectively.

All these results are shown in Figure 5. We see that MCNP6 using LAQGSM03.03 describes well the experimental spectra [48] and agrees very well with results obtained with MCNP6 using CEM03.03, Bertini+MPM+Dresner+RAL, and INCL+ABLA event-generators, and with results by MCNPX using CEM03.01.

3.5. Test-Problems #5: inpl05REP with inp_inpl05

This MCNP6 problem is to test the applicability of MCNP6 using the LAQGSM03.03 event generator to calculate production of protons from intermediate energy heavy-ion induced reactions for different NASA (shielding for missions in space), medical (cancer treatment with heavy-ions), FRIB (Facility for Rare Isotope Beams), and for several U.S. DOE applications.

This test calculates with MCNP6 the proton double-differential spectra at 30, 70, 90, 110, and 150 degrees from interaction of a 1042 MeV/nucleon ^{40}Ar beam with a thin ^{40}Ca target and compares the results with experimental data and with calculations by the LAQGSM03.03 event generator used as a stand alone code.

We calculate this test-problem using the **NOACT=-2** option for the 8th parameter of the **LCA** card of the MCNP6 input file. As we have presented a detailed description of the use of **NOACT=-2** option to calculate particle spectra from thin targets in the test-problem #6 of the CEM Testing Primer [5], and have provided additional examples of its use in test problems #7 and #8 of Ref. [5], we do not need to discuss in detail the input and output files for this case. Therefore, we limit ourselves to only providing the text of the input file as well as describing where to find the results in the MCNP6 output files.

The input file for this test problem is **inpl05REP**. It is presented in the subdirectory **/VALIDATION_LAQGSM/Inputs/** and is also shown below.

inpl05REP:

```
MCNP6 test with LAQGSM03.03: 1042 MeV/A Ar40+Ca40 -> p spectra
c at 30, 70, 90, 110, and 150 deg to compare with Sandoval's et al.
```

```
C measurements and results by LAQGSM03.03 as a stand alone code
1   1  -10   -501      imp:h=1
2   0         501  -502  imp:h=1
99  0         502      imp:h=0

501   so 0.01
502   so 1
c
c  tally surfaces
c
5      kz    0    0.007654253     1
10     kz    0    0.031091151     1
15     kz    0    0.071796643     1
20     kz    0    0.132474088     1
25     kz    0    0.217442414     1
30     kz    0    0.333332652     1
35     kz    0    0.49028952      1
40     kz    0    0.704086505     1
45     kz    0    0.999997346     1
50     kz    0    1.420272373     1
55     kz    0    2.03959969      1
60     kz    0    2.999987744     1
65     kz    0    4.598886921     1
70     kz    0    7.548583695     1
75     kz    0    13.92808003     1
80     kz    0    32.16299385     1
85     kz    0    130.6423246     1
90     pz    0
95     kz    0    130.6503105    -1
100    kz    0    32.16399202    -1
105    kz    0    13.92837571    -1
110    kz    0    7.548708346    -1
115    kz    0    4.598950644    -1
120    kz    0    3.000024513    -1
125    kz    0    2.039622728    -1
130    kz    0    1.420287681    -1
135    kz    0    1.000007961    -1
140    kz    0    0.704094093    -1
145    kz    0    0.490295058    -1
150    kz    0    0.333336738    -1
155    kz    0    0.217445427    -1
160    kz    0    0.132476276    -1
165    kz    0    0.071798167    -1
170    kz    0    0.031092115    -1
175    kz    0    0.007654721    -1

mode n h d t s a # / * z
```

```
m1  20040 1
lca 7j -2 j 1    $ LAQGSM, no transport, only the 1st inelstic interaction
c nps 1000
nps 1e6
prdmp 2j -1
sdef par=18040 erg=41680 vec=0 0 1 dir 1
phys:# 45000
phys:h 3100
phys:n 3100
phys:a 6000
phys:d 5000
phys:t 5200
phys:s 5200
phys:/ 2200
phys:* 2200
phys:z 2200
c
f1:h  502
c defining our "segments" for angles of 30, 70, 90, 110, and 150 deg
fs1 -25 -35 -65 -75 -85 95 105 115 145 155 T
c
c The following Segment Divisor card is needed to get 1/sr for p-spectra
sd1   0.58869  $ 2pi(cos0 -cos25)
      0.54762  $ 2pi(cos25 - cos35)
      2.49150  $ 2pi(cos35 - cos65)
      1.02918  $ 2pi(cos65 - cos75)
      1.07859  $ 2pi(cos75 - cos85)
      1.09523  $ 2pi(cos85 - cos95)
      1.07859  $ 2pi(cos95 - cos105)
      1.02918  $ 2pi(cos105 - cos115)
      2.49150  $ 2pi(cos115 - cos145)
      0.54762  $ 2pi(cos145 - cos155)
      0.58869  $ 2pi(cos155 - cos180)
      12.56637 $ 4pi
c
c     Boundaries of the proton energy bins: 0-1 MeV; 1-3 MeV, ...
c     tabulated exactly as used by LAQGSM03.03 as stand alone code
e1    1     3     5     7     9     11    13    15    17    19
      22    27    32    37    42    47    52    57    62    67
      72    77    82    87    92    97    105   115   125   135
      145   155   165   175   185   195   205   215   225   235
      245   255   265   275   285   295   305   315   325   335
      345   355   365   375   385   395   405   415   425   435
      445   455   465   475   485   495   505   515   525   535
      545   555   565   575   585   595   605   615   625   635
      645   655   665   675   685   695   705   715   725   735
      745   755   765   775   785   795   805   815   825   835
```

```
        845   855   865   875   885   895   905   915   925   935
        945   955   965   975   985   995   1025  1075  1125  1175
        1225  1275  1325  1375  1425  1475  1525  1575  1625  1675
        1725  1775  1825  1875  1925  1975  2025  2075  2125  2175
        2225  2275  2325  2375  2425  2475  2525  2575  2625  2675
        2725  2775  2825  2875  2925  2975  3025  3075  3125  3175
        3225  3275  3325  3375  3425  3475  3525  3575  3625  3675
        3725  3775  3825  3875  3925  3975  4025  4075  4125  4175
        4225  4275  4325  4375  4425  4475  4525  4575  4625  4675
        4725  4775  4825  4875  4925  4975  5025  5075  5125  5175
c
em1 2200.92 199r $ multiply to sig_inelastic = 2200.92 mb, as predicted by
c                  LAQGSM03.03 in Ar1042Ca_a.out of 05/21/2010. This is needed
c                  to get the spectra in [mb/sr/MeV], after dividig the flux
c                  to the energy bins, to get [1/MeV]; we do this for every E-bin
c
c
e0   6000
f11:n   502
f21:h   502
f31:d   502
f41:t   502
f51:s   502
f61:a   502
f71:/   502
f81:z   502
f91:*   502
c dbcn  20j  0  7j  1  2j  0  1
dbcn  20j  0  5j  -1  j  1  2j  0  1  $ dbcn(27)=-1 provides pi+ separately of pi-
```

The experimental data for this problem were measured at the Berkeley Bevalac by an international team and were presented and discussed in the paper [54]. The complete set of experimental data is tabulated in the 118 page AIP document No. PAPS PRVCA 21-1321-118 available upon request from the Physics Auxiliary Publication Service of the American Institute of Physics.

Experimental proton spectra $d^2\sigma/dT/d\Omega$ in units of [mb/sr/MeV] as functions of proton kinetic energy in [MeV] at 30, 70, 90, 110, and 1530 degrees are presented in the files Ar1042Ca_30_p.dat, Ar1042Ca_70_p.dat, Ar1042Ca_90_p.dat, Ar1042Ca_110_p.dat, and Ar1042Ca_150_p.dat, respectively. For convenience of plotting all angles on a single figure and to compare spectra at different angles with each other, the experimental data at 70 degrees were multiplied by 10^{-1}, at 90 degrees by 10^{-2}, at 110 degrees by 10^{-3}, and at 150 degrees by 10^{-4}, as is shown on the plot (see file Ar1042Ca_p_6REP.pdf).

Proton spectra by MCNP6 at 30, 75, 90, 110, and 150 (± 5) degrees are tabulated in units of [mb/sr/projectile] in the final MCNP6 output file **inpl05REP_c.o** shown in the subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/** (calculated with the "continue" option using the auxiliary input file **inp_inpl05**; the first MCNP6 output calculated with the main input file, **inpl05REP**, is **inpl05REP.o**; it is shown in the same subdirectory) as tally 1,

respectively in the "segments":
1) segment: 25 -35
2) segment: 25 35 65 -75
3) segment: 25 35 65 75 85 95
4) segment: 25 35 65 75 85 -95 -105 115
5) segment: 25 35 65 75 85 -95 -105 -115 -145 155

and in the final MCTAL file **inpl05REP_c.m**.

Note that to get the units of [mb] needed for normalization of the calculated spectra to the total reaction cross section, we used the Energy Multiplier card **EM1** in our input file **inpl05REP** with the value 2200.92 on it for all the 200 energy bins of our tally **F1**: 2200.92 is the value of the total inelastic (reaction) cross section in [mb] as predicted by LAQGSM03.03 used for this reaction as a stand alone code. In a similar manner, to get the units of [1/sr] for the calculated spectra, we used in our input file the Segment Divisor card **SD1** with values of the solid angles for each "segment" corresponding to the angles of 30, 75, 90, 110, and 150 (±5) degrees. To get the calculated double differential spectra $d^2\sigma/dT/d\Omega$ at these angles in conventional units of [mb/sr/MeV], we still divide the tables from the MCNP6 output file at the "segments" described above to the values of the energy bins. We do this separately with a little post processing routine written especially for this, as mentioned in the previous section.

To plot our proton spectra with **xmgrace** (see file Ar1042Ca_p_6REP.pdf), the final MCNP6 results obtained as described above are copied to separate files 30_p_6REP.dat, 70_p_6REP.dat, 90_p_6REP.dat, 110_p_6REP.dat, and 150_p_6REP.dat, respectively. Besides the MCNP6 results, for comparison, we present here also results by LAQGSM03.03 as a stand alone code (files: 30_p_l.dat, 70_p_l.dat, 90_p_l.dat, 110_p_l.dat, and 150_p_l.dat, respectively).

The file Ar1042Ca_p_6REP.fig is a template for plotting the figure with **xmgrace**. The pdf file for the figure with final results for this problem is Ar1042Ca_p_6REP.pdf. All these files are presented in the subdirectory **/VALIDATION_LAQGSM/Experimental_data/inpl05/**.

Our results are shown below in Figure 6. We see that MCNP6 using LAQGSM03.03 describes well the measured proton spectra [54] and agrees very well with results obtained with LAQGSM03.03 event generator used as a stand alone code.

3.6. Test-Problems #6: Ne800Cu_REP with inp_6.7e6

This MCNP6 problem is to test the applicability of MCNP6 using the LAQGSM03.03 event generator to calculate production of deuterons from intermediate energy heavy-ion induced reactions for different NASA (shielding for missions in space), medical (cancer treatment with heavy-ions), FRIB (Facility for Rare Isotope Beams), and for some U.S. DOE applications.

This test calculates with MCNP6 the deuteron invariant spectra at 30, 45, 60, 90, and 130 degrees from interaction of a 800 MeV/A ^{20}Ne beam with a thin ^{64}Cu target and compares the results with experimental data and with results by the LAQGSM03.03 event generator used as a stand alone code.

We calculate this test-problem using the **NOACT=-2** option for the 8th parameter of the **LCA** card of the MCNP6 input file. As we have presented a detailed description of the use of **NOACT=-2** option to calculate particle spectra from thin targets in the test-problem #6 of the CEM Testing Primer [5], and have provided additional examples of its use in test problems #7 and #8 of Ref. [5], we do not need to discuss in detail the input and output files for this case.

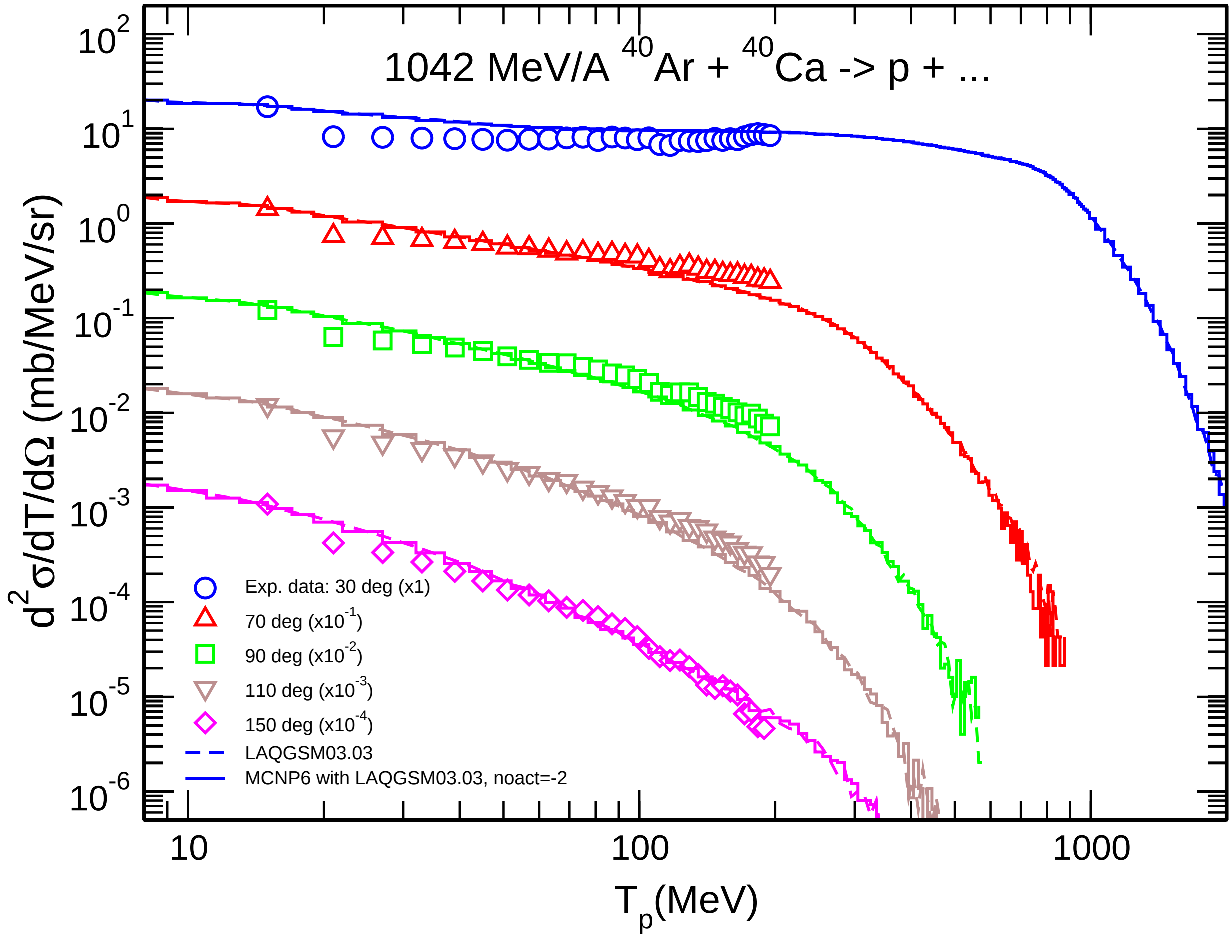

Figure 6: Experimental proton spectra [54] at 30, 70, 90, 110, and 150 degrees (symbols) from a thin ^{40}Ca target bombarded with a 1042 MeV/nucleon ^{40}Ar beam compared with results by LAQGSM03.03 [10] used as a stand alone code and by MCNP6 using the LAQGSM03.03 event-generator, as indicated.

Therefore, we limit ourselves to only providing the text of the input file as well as describing where to find the results in the MCNP6 output files.

The input file for this test problem is **Ne800Cu_REP**. It is presented in the subdirectory **/VALIDATION_LAQGSM/Inputs/** and is also shown below.

Ne800Cu_REP:

```
MCNP6 test with LAQGSM03.03: 800 MeV/A Ne20+Cu64 -> d invariant spectra
c Ed^3sigma/d^3p [mb/GeV^2/c^-3/sr] at 30, 70, 90, 110, and 150 deg
c to compare with Nagamiya's et al. measurements (LBL-8463)
c and results by LAQGSM03.03 as a stand alone code
1   1  -10   -501      imp:h=1
2   0          501  -502  imp:h=1
99  0          502      imp:h=0

501   so 0.01
```

```
502   so 1
c
c  tally surfaces
c
5      kz    0    0.007654253     1
10     kz    0    0.031091151     1
15     kz    0    0.071796643     1
20     kz    0    0.132474088     1
25     kz    0    0.217442414     1
30     kz    0    0.333332652     1
35     kz    0    0.49028952      1
40     kz    0    0.704086505     1
45     kz    0    0.999997346     1
50     kz    0    1.420272373     1
55     kz    0    2.03959969      1
60     kz    0    2.999987744     1
65     kz    0    4.598886921     1
70     kz    0    7.548583695     1
75     kz    0    13.92808003     1
80     kz    0    32.16299385     1
85     kz    0    130.6423246     1
90     pz    0
95     kz    0    130.6503105    -1
100    kz    0    32.16399202    -1
105    kz    0    13.92837571    -1
110    kz    0    7.548708346    -1
115    kz    0    4.598950644    -1
120    kz    0    3.000024513    -1
125    kz    0    2.039622728    -1
130    kz    0    1.420287681    -1
135    kz    0    1.000007961    -1
140    kz    0    0.704094093    -1
145    kz    0    0.490295058    -1
150    kz    0    0.333336738    -1
155    kz    0    0.217445427    -1
160    kz    0    0.132476276    -1
165    kz    0    0.071798167    -1
170    kz    0    0.031092115    -1
175    kz    0    0.007654721    -1

mode n h d t s a # / * z
m1  29064 1
lca 7j -2 j 1    $ LAQGSM, no transport, only the 1st inelstic interaction
c nps 50000
nps 1e7
c prdmp 2j -1
sdef par=10020 erg=16000 vec=0 0 1 dir 1
```

```
phys:# 16000
phys:h 3100
phys:n 3100
phys:a 6000
phys:d 5000
phys:t 5200
phys:s 5200
phys:/ 2200
phys:* 2200
phys:z 2200
c
f1:d  502
c defining our ``segments" for angles of 30, 45, 60, 90, and 130 deg
fs1 -25 -35 -40 -50 -55 -65 -85 95 105 115 125 135 T
c
c The following Segment Divisor card is needed to get 1/sr for d-spectra
sd1   0.58869  $ 2pi(cos0 -cos25)
      0.54762  $ 2pi(cos25 - cos35)
      0.33368  $ 2pi(cos35 - cos40)
      0.77445  $ 2pi(cos40 - cos50)
      0.43487  $ 2pi(cos50 - cos55)
      0.94850  $ 2pi(cos55 - cos65)
      2.10777  $ 2pi(cos65 - cos85)
      1.09523  $ 2pi(cos85 - cos95)
      1.07859  $ 2pi(cos95 - cos105)
      1.02918  $ 2pi(cos105 - cos115)
      0.94850  $ 2pi(cos115 - cos125)
      0.83900  $ 2pi(cos125 - cos135)
      1.84030  $ 2pi(cos135 - cos180)
      12.56637 $ 4pi
c
c     Boundaries of the proton energy bins: 0-1 MeV; 1-3 MeV, ...
c     tabulated exactly as used by LAQGSM03.03 as stand alone code
e1    1     3     5     7     9     11    13    15    17    19
      22    27    32    37    42    47    52    57    62    67
      72    77    82    87    92    97    105   115   125   135
      145   155   165   175   185   195   205   215   225   235
      245   255   265   275   285   295   305   315   325   335
      345   355   365   375   385   395   405   415   425   435
      445   455   465   475   485   495   505   515   525   535
      545   555   565   575   585   595   605   615   625   635
      645   655   665   675   685   695   705   715   725   735
      745   755   765   775   785   795   805   815   825   835
      845   855   865   875   885   895   905   915   925   935
      945   955   965   975   985   995   1025  1075  1125  1175
      1225  1275  1325  1375  1425  1475  1525  1575  1625  1675
      1725  1775  1825  1875  1925  1975  2025  2075  2125  2175
```

```
      2225  2275  2325  2375  2425  2475  2525  2575  2625  2675
      2725  2775  2825  2875  2925  2975  3025  3075  3125  3175
      3225  3275  3325  3375  3425  3475  3525  3575  3625  3675
      3725  3775  3825  3875  3925  3975  4025  4075  4125  4175
      4225  4275  4325  4375  4425  4475  4525  4575  4625  4675
      4725  4775  4825  4875  4925  4975  5025  5075  5125  5175
c
em1 2085.63 199r $ multiply to sig_inelastic = 2085.63 mb, as predicted by
c                  LAQGSM03.03 in Ne800Cu.out of 06/14/2010. This is needed
c                  to get the spectra in [mb/sr/MeV], after dividig the flux
c                  to the energy bins, to get [1/MeV]; we do this for every E-bin;
c   Then, we will multiply these double-differential spectra, d^2sigma/dT/dOmega,
c   by 1/p, to get the final invariant spectra Ed^3sigma/d^3p [mb/GeV^2/c^-3/sr],
c   coverting later also MeV^(-2) to GeV^(-2)
c
e0   6000
dbcn  20j  0  5j  -1  j  1  2j  0  1  $ needed to tally pi+ separately of pi-
```

The experimental data for this problem were measured at the Berkeley Bevalac by Prof. Shoji Nagamiya's Group [55] and are tabulated in the 181 page Lawrence Berkeley National Laboratory. Report No. LBL-8463 [56].

Experimental invariant deuteron spectra $Ed^3\sigma/d^3p$ in units of [mb/sr/GeV^2/c^{-3}] as functions of deuteron momentum in [MeV/c] at 30, 45, 60, 90, and 130 degrees are presented in the files 30_d_e.dat, 45_d_e.dat, 60_d_e.dat, 90_d_e.dat, and 130_d_e.dat, respectively. For convenience of plotting all angles on a single figure and to compare spectra at different angles with each other, the experimental data at 45 degrees were multiplied by 10^{-1}, at 60 degrees by 10^{-2}, at 90 degrees by 10^{-3} and at 130 degrees by 10^{-4}, as is shown on the plot (see file Ne800Cu_d_6REP.pdf).

The final MCNP6 output file **Ne800Cu_REP11_8c.o** is presented in the subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**. It is calculated with the "continue" option using the auxiliary input file **inp_6.7e6**; the first MCNP6 output calculated with the main input file, **Ne800Cu_REP**, is: **Ne800Cu_REP11.o**. Deuteron spectra as calculated by MCNP6 at 30, 45, 60, 90, and 130 (±5) degrees are tabulated in units of [mb/sr/projectile] as segments for tally 1, where the segments corresponding to our angles are, respectively:
1) segment: 25 -35
2) segment: 25 35 40 -50
3) segment: 25 35 40 50 55 -65
4) segment: 25 35 40 50 55 65 85 95
5) segment: 25 35 40 50 55 65 85 -95 -105 -115 -125 135 .

Note that to get the units of [mb] needed for normalization of the calculated spectra to the total reaction cross section, we used the Energy Multiplier card **EM1** in our input file **Ne800Cu_REP** with the value 2085.63 on it for all the 200 energy bins of our tally F1: 2085.63 is the value of the total inelastic (reaction) cross section in [mb] as predicted by LAQGSM03.03 used for this reaction as a stand alone code. In a similar manner, to get the units of [1/sr] for the calculated spectra, we used in our input file the Segment Divisor card **SD1** with values of the solid angles for each "segment" corresponding to the needed angles of 30, 45, 60, 90, and

130 (±5) degrees.

To get the calculated double differential spectra $d^2\sigma/dT/d\Omega$ at these angles in conventional units of [mb/sr/MeV], we still divide the tables from the MCNP6 output file at the "segments" described above to the values of the energy bins. Then, to convert such double differential spectra to the measured so called "invariant spectra," $Ed^3\sigma/d^3p$, in units of [mb/sr/GeV^2/c^{-3}] as functions of the deuteron momenta p_d in [MeV/c], we calculate the mean deuteron kinetic energy for each energy bin, T_d, and use it to get the deuteron momentum for each energy bin as $p_d = \sqrt{T_d(T_d + 2m_d)}$, where m_d is the mass of deuteron in MeV. Finally, we use the known relation $Ed^3\sigma/d^3p = (1/p)d^2\sigma/dT/d\Omega$, not forgetting to convert in this formula the deuteron momentum from [MeV/c] to [GeV/c], in order to get the calculated invariant deuteron spectra in the same units as measured. We do these transformations separately with a little post processing routine written especially for this.

To plot our invariant spectra with **xmgrace** (see file Ne800Cu_d_6REP.pdf), the final MCNP6 results obtained as described above are copied to separate files 30_d_6REP.dat, 45_d_6REP.dat, 60_d_6REP.dat, 90_d_6REP.dat, and 130_d_6REP.dat, respectively.

Besides the MCNP6 results, for comparison, we present here also results by LAQGSM03.03 used as a stand alone code (files 30_d_l.dat, 45_d_l.dat, 60_d_l.dat, 90_d_l.dat, and 130_d_l.dat, respectively).

The file Ne800Cu_d_6REP.fig is a template for plotting the figure with **xmgrace**. The pdf file for the figure with final results for this problem is Ne800Cu_d_6REP.pdf. The files with the figure are presented together with all files with calculation results and experimental data in subdirectory **/VALIDATION_LAQGSM/Experimental_data/Ne800Cu/**.

3.7. Test-Problems #7: Ne393U_REP with inp_Ne393U

This problem is to test the applicability of MCNP6 using the LAQGSM03.03 event generator to calculate production of tritium from intermediate energy heavy-ion induced reactions for different NASA, medical, FRIB (Facility for Rare Isotope Beams), and for several U.S. DOE applications.

This test calculates with MCNP6 the tritium double-differential spectra at 30, 70, 90, 110, and 150 degrees from interaction of a 393 MeV/nucleon ^{20}Ne beam with a thin ^{238}U target and compares the results with experimental data and with results by the LAQGSM03.03 event generator used as a stand alone code.

We calculate this test-problem using the **NOACT=-2** option for the 8th parameter of the **LCA** card of the MCNP6 input file. As we have presented a detailed description of the use of **NOACT=-2** option to calculate particle spectra from thin targets in the test-problem #6 of the CEM Testing Primer [5], and have provided additional examples of its use in test problems #7 and #8 of Ref. [5], we do not need to discuss in detail the input and output files for this case. Therefore, we limit ourselves to only providing the text of the input file as well as describing where to find the results in the MCNP6 output files.

The input file for this test problem is **Ne393U_REP**. It is presented in the subdirectory **/VALIDATION_LAQGSM/Inputs/** and is also shown below.

Ne393U_REP:

```
MCNP6 test with LAQGSM03.03: 393 MeV/A Ne20+U238 -> t  spectra
c at 30, 70, 90, 110, and 150 deg to compare with Sandoval's et al.
```

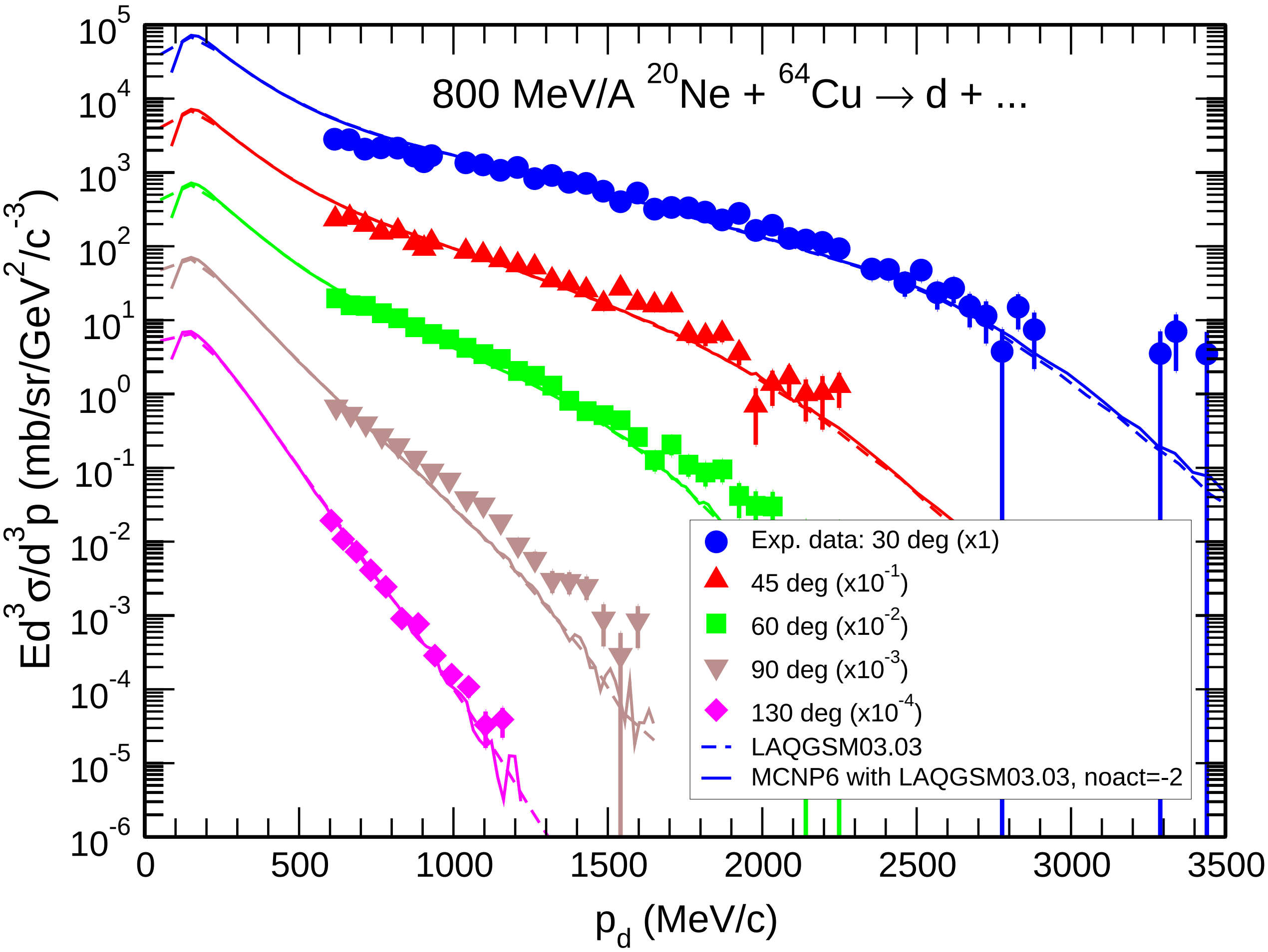

Figure 7: Experimental invariant deuteron spectra [55, 56] at 30, 45, 60, 90, and 130 degrees (symbols) from a thin Cu target bombarded with a 800 MeV/nucleon ^{20}Ne beam compared with results by LAQGSM03.03 [10] used as a stand alone code and by MCNP6 using the LAQGSM03.03 event-generator, as indicated.

```
C measurements and results by LAQGSM03.03 as a stand alone code
1   1  -10   -501       imp:h=1
2   0         501  -502  imp:h=1
99  0         502       imp:h=0

501   so 0.01
502   so 1
c
c  tally surfaces
c
5       kz    0    0.007654253     1
10      kz    0    0.031091151     1
15      kz    0    0.071796643     1
20      kz    0    0.132474088     1
25      kz    0    0.217442414     1
```

```
30     kz    0    0.333332652     1
35     kz    0    0.49028952      1
40     kz    0    0.704086505     1
45     kz    0    0.999997346     1
50     kz    0    1.420272373     1
55     kz    0    2.03959969      1
60     kz    0    2.999987744     1
65     kz    0    4.598886921     1
70     kz    0    7.548583695     1
75     kz    0    13.92808003     1
80     kz    0    32.16299385     1
85     kz    0    130.6423246     1
90     pz    0
95     kz    0    130.6503105    -1
100    kz    0    32.16399202    -1
105    kz    0    13.92837571    -1
110    kz    0    7.548708346    -1
115    kz    0    4.598950644    -1
120    kz    0    3.000024513    -1
125    kz    0    2.039622728    -1
130    kz    0    1.420287681    -1
135    kz    0    1.000007961    -1
140    kz    0    0.704094093    -1
145    kz    0    0.490295058    -1
150    kz    0    0.333336738    -1
155    kz    0    0.217445427    -1
160    kz    0    0.132476276    -1
165    kz    0    0.071798167    -1
170    kz    0    0.031092115    -1
175    kz    0    0.007654721    -1

mode n h d t s a # / * z
m1  92238 1
lca 7j -2 j 1    $ LAQGSM, no transport, only the 1st inelastic interaction
c nps 500
nps 1e6
prdmp 2j -1
sdef par=10020 erg=7860 vec=0 0 1 dir 1
phys:# 93534
phys:h 3100
phys:n 3100
phys:a 6000
phys:d 5000
phys:t 5200
phys:s 5200
phys:/ 2200
phys:* 2200
```

```
phys:z 2200
c
f1:t  502
c defining our "segments" for angles of 30, 70, 90, 110, and 150 deg
fs1 -25 -35 -65 -75 -85 95 105 115 145 155 T
c
c The following Segment Divisor card is needed to get 1/sr for p-spectra
sd1   0.58869  $ 2pi(cos0 -cos25)
      0.54762  $ 2pi(cos25 - cos35)
      2.49150  $ 2pi(cos35 - cos65)
      1.02918  $ 2pi(cos65 - cos75)
      1.07859  $ 2pi(cos75 - cos85)
      1.09523  $ 2pi(cos85 - cos95)
      1.07859  $ 2pi(cos95 - cos105)
      1.02918  $ 2pi(cos105 - cos115)
      2.49150  $ 2pi(cos115 - cos145)
      0.54762  $ 2pi(cos145 - cos155)
      0.58869  $ 2pi(cos155 - cos180)
      12.56637 $ 4pi
c
c     Boundaries of the proton energy bins: 0-1 MeV; 1-3 MeV, ...
c     tabulated exactly as used by LAQGSM03.03 as stand alone code
e1    1     3     5     7     9     11    13    15    17    19
      22    27    32    37    42    47    52    57    62    67
      72    77    82    87    92    97    105   115   125   135
      145   155   165   175   185   195   205   215   225   235
      245   255   265   275   285   295   305   315   325   335
      345   355   365   375   385   395   405   415   425   435
      445   455   465   475   485   495   505   515   525   535
      545   555   565   575   585   595   605   615   625   635
      645   655   665   675   685   695   705   715   725   735
      745   755   765   775   785   795   805   815   825   835
      845   855   865   875   885   895   905   915   925   935
      945   955   965   975   985   995   1025  1075  1125  1175
      1225  1275  1325  1375  1425  1475  1525  1575  1625  1675
      1725  1775  1825  1875  1925  1975  2025  2075  2125  2175
      2225  2275  2325  2375  2425  2475  2525  2575  2625  2675
      2725  2775  2825  2875  2925  2975  3025  3075  3125  3175
      3225  3275  3325  3375  3425  3475  3525  3575  3625  3675
      3725  3775  3825  3875  3925  3975  4025  4075  4125  4175
      4225  4275  4325  4375  4425  4475  4525  4575  4625  4675
      4725  4775  4825  4875  4925  4975  5025  5075  5125  5175
c
em1 3509.23 199r $ multiply to sig_inelastic = 3509.23 mb, as predicted by
c                  LAQGSM03.03 in Ne393Utoro.out of 06/01/2010. This is needed
c                  to get the spectra in [mb/sr/MeV], after dividig the flux
c                  to the energy bins, to get [1/MeV]; we do this for every E-bin
```

```
c
dbcn  20j  0  5j  -1  j  1  2j  0  1  $ needed to tally pi+ separately of pi-
```

The experimental data for this problem were measured at the Berkeley Bevalac by an international team and are presented and discussed in the paper [54]. The complete set of experimental data is tabulated in the 118 page AIP document No. PAPS PRVCA 21-1321-118 available upon request from the Physics Auxiliary Publication Service of the American Institute of Physics.

Experimental tritium spectra $d^2\sigma/dT/d\Omega$ in units of [mb/sr/MeV] as functions of tritium kinetic energy in [MeV] at 30, 70, 90, 110, and 150 degrees are presented in the files 30_t_e.dat, 70_t_e.dat, 90_t_e.dat, 110_t_e.dat, and 150_t_e.dat, respectively. For convenience of plotting all angles on a single figure and to compare spectra at different angles with each other, the experimental data at 70 degrees were multiplied by 10^{-1}, at 90 degrees by 10^{-2}, at 110 degrees by 10^{-3}, and at 150 degrees by 10^{-4}, as is shown on the plot (see file Ne393U_t.pdf).

The final MCNP6 output file **Ne393U_REP_3c.o** is presented in the subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**. It is calculated with the "continue" option using the auxiliary input file **inp_Ne393U**; the first MCNP6 output file calculated with the main input file, **Ne393U_REP**, is: **Ne393U_REP.o**. Tritium spectra as calculated by MCNP6 at 30, 75, 90, 110, and 150 (± 5) degrees are tabulated in units of [mb/sr/projectile] as segments for tally 1, where the segments corresponding to our angles are, respectively:
1) segment: 25 -35
2) segment: 25 35 65 -75
3) segment: 25 35 65 75 85 95
4) segment: 25 35 65 75 85 -95 -105 115
5) segment: 25 35 65 75 85 -95 -105 -115 -145 155 .

Note that to get the units of [mb] needed for the normalization of the calculated spectra to the total reaction cross section, we used the Energy Multiplier card **EM1** in our input file **Ne393U_REP** with the value 3509.23 on it for all the 200 energy bins of our tally **F1**: 3509.23 is the value of the total inelastic (reaction) cross section in [mb] as predicted by LAQGSM03.03 used for this reaction as a stand alone code. In a similar manner, to get the units of [1/sr] for the calculated spectra, we used in our input file the Segment Divisor card **SD1** with values of the solid angles for each "segment" corresponding to the needed angles of 30, 75, 90, 110, and 150 (± 5) degrees. To get the calculated double differential spectra $d^2\sigma/dT/d\Omega$ at these angles in conventional units of [mb/sr/MeV], we still divide the tables from the MCNP6 output file at the "segments" described above to the corresponding values of the energy bins. We do this separately with a little post processing routine written especially for this.

To plot our tritium spectra with **xmgrace** (see file Ne393U_t_6REP.pdf), the final MCNP6 results obtained as described above are copied to separate files 30_t_6REP.dat, 70_t_6REP.dat, 90_t_6REP.dat, 110_t_6REP.dat, and 150_t_6REP.dat, respectively. Besides the MCNP6 results, for comparison, we present here also results by LAQGSM03.03 as a stand alone code (files: 30_t_l.dat, 70_t_l.dat, 90_t_l.dat, 110_t_l.dat, and 150_t_l.dat, respectively).

The file Ne393U_t_6REP.fig is a template for plotting the figure with **xmgrace**. The pdf file for the figure with final results for this problem is Ne393U_t_6REP.pdf. The files with figure are presented together with all files with calculation results and experimental data in subdirectory **/VALIDATION_LAQGSM/Experimental_data/Ne393U/**.

Our final results for this test problem are shown below in Figure 8. We see that MCNP6

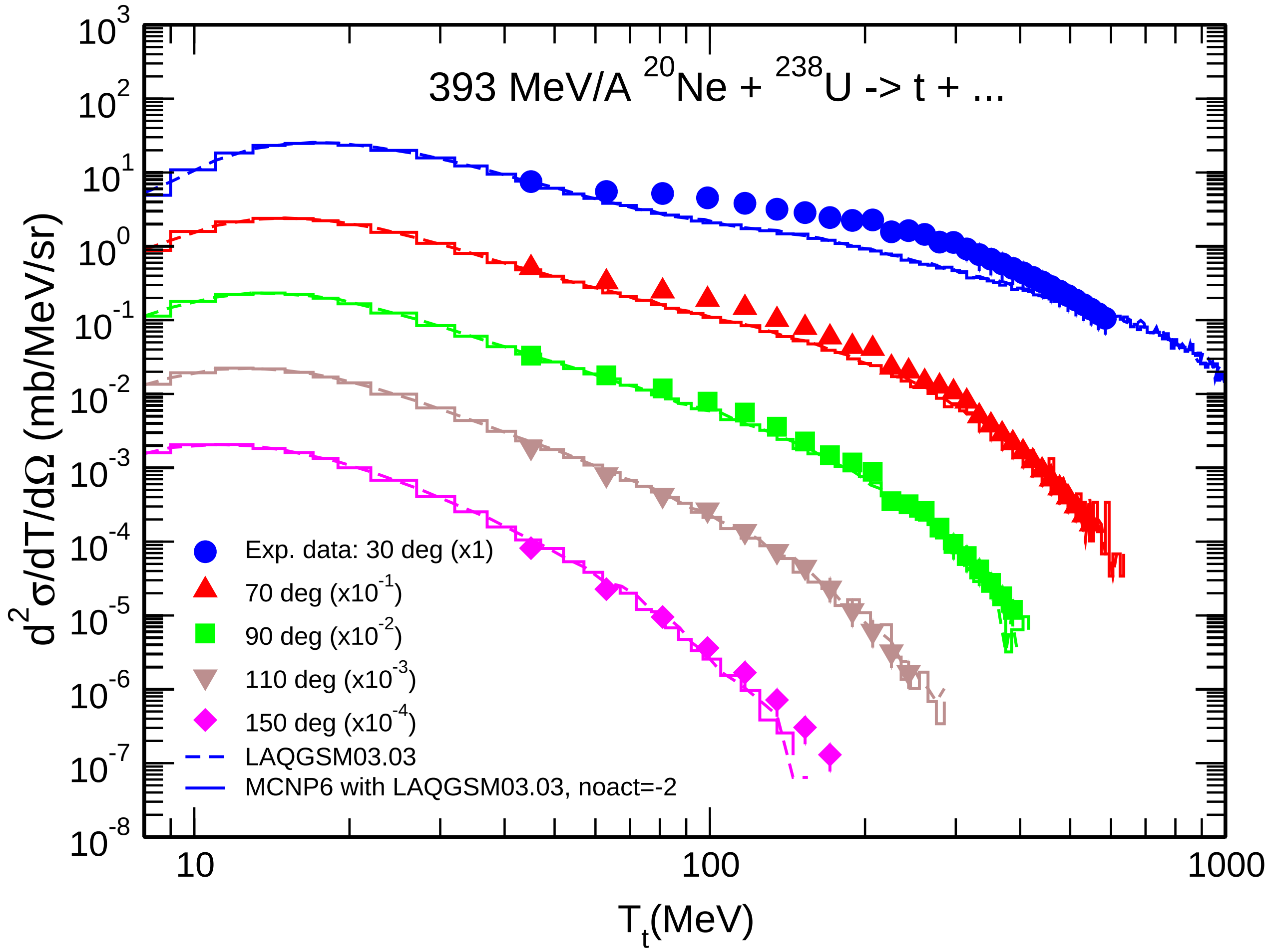

Figure 8: Experimental [54] triton spectra at 30, 70, 90, 110, and 150 degrees (symbols) from a thin ^{238}U target bombarded with a 393 MeV/nucleon ^{20}Ne beam compared with results by LAQGSM03.03 [10] used as a stand alone code and by MCNP6 using the LAQGSM03.03 event-generator, as indicated.

using LAQGSM03.03 describes well the measured triton spectra [54] and agrees very well with results obtained with the LAQGSM03.03 event generator used as a stand alone code.

3.8 Test-Problems #8: Ne241U_REP with inp_Ne241U

This problem is to test the applicability of MCNP6 using the LAQGSM03.03 event generator to calculate production of helium from intermediate energy heavy-ion induced reactions for different NASA, medical, FRIB (Facility for Rare Isotope Beams), and for several U.S. DOE applications.

This test calculates with MCNP6 the ^{3}He and ^{4}He double-differential spectra at 30, 70, 90, 110, and 150 degrees from interaction of a 241 MeV/nucleon ^{20}Ne beam with a thin ^{238}U target and compares the results with experimental data and with results by the LAQGSM03.03 event generator used as a stand alone code.

We calculate this test-problem using the **NOACT=-2** option for the 8th parameter of the

LCA card of the MCNP6 input file. As we have presented a detailed description of the use of **NOACT=-2** option to calculate particle spectra from thin targets in the test-problem #6 of the CEM Testing Primer [5], and have provided additional examples of its use in test problems #7 and #8 of Ref. [5], we do not need to discuss in detail the input and output files for this case. Therefore, we limit ourselves to only providing the text of the input file as well as describing where to find the results in the MCNP6 output files.

The input file for this test problem is **Ne241U_REP**. It is presented in the subdirectory **/VALIDATION_LAQGSM/Inputs/** and is also shown below.

Ne241U_REP:

```
MCNP6 test with LAQGSM03.03: 241 MeV/A Ne20+U238 -> He3 & He4 spectra
c at 30, 70, 90, 110, and 150 deg to compare with Sandoval's et al.
C measurements and results by LAQGSM03.03 as a stand alone code
1   1  -10   -501      imp:h=1
2   0         501  -502  imp:h=1
99  0         502      imp:h=0

501   so 0.01
502   so 1
c
c  tally surfaces
c
5      kz    0    0.007654253     1
10     kz    0    0.031091151     1
15     kz    0    0.071796643     1
20     kz    0    0.132474088     1
25     kz    0    0.217442414     1
30     kz    0    0.333332652     1
35     kz    0    0.49028952      1
40     kz    0    0.704086505     1
45     kz    0    0.999997346     1
50     kz    0    1.420272373     1
55     kz    0    2.03959969      1
60     kz    0    2.999987744     1
65     kz    0    4.598886921     1
70     kz    0    7.548583695     1
75     kz    0    13.92808003     1
80     kz    0    32.16299385     1
85     kz    0    130.6423246     1
90     pz    0
95     kz    0    130.6503105    -1
100    kz    0    32.16399202    -1
105    kz    0    13.92837571    -1
110    kz    0    7.548708346    -1
115    kz    0    4.598950644    -1
120    kz    0    3.000024513    -1
```

```
125    kz    0    2.039622728    -1
130    kz    0    1.420287681    -1
135    kz    0    1.000007961    -1
140    kz    0    0.704094093    -1
145    kz    0    0.490295058    -1
150    kz    0    0.333336738    -1
155    kz    0    0.217445427    -1
160    kz    0    0.132476276    -1
165    kz    0    0.071798167    -1
170    kz    0    0.031092115    -1
175    kz    0    0.007654721    -1

mode n h d t s a # / * z
m1  92238 1
lca 7j -2 j 1    $ LAQGSM, no transport, only the 1st inelastic interaction
c nps 200
 nps 1e6
c prdmp 2j -1
sdef par=10020 erg=4820 vec=0 0 1 dir 1
phys:# 57358
phys:h 3100
phys:n 3100
phys:a 6000
phys:d 5000
phys:t 5200
phys:s 5200
phys:/ 2200
phys:* 2200
phys:z 2200
c
f1:s  502
f11:a  502
c defining our "segments" for angles of 30, 70, 90, 110, and 150 deg
fs1 -25 -35 -65 -75 -85 95 105 115 145 155 T
fs11 -25 -35 -65 -75 -85 95 105 115 145 155 T
c
c The following Segment Divisor card is needed to get 1/sr for p-spectra
sd1   0.58869  $ 2pi(cos0 -cos25)
      0.54762  $ 2pi(cos25 - cos35)
      2.49150  $ 2pi(cos35 - cos65)
      1.02918  $ 2pi(cos65 - cos75)
      1.07859  $ 2pi(cos75 - cos85)
      1.09523  $ 2pi(cos85 - cos95)
      1.07859  $ 2pi(cos95 - cos105)
      1.02918  $ 2pi(cos105 - cos115)
      2.49150  $ 2pi(cos115 - cos145)
      0.54762  $ 2pi(cos145 - cos155)
```

```
      0.58869  $ 2pi(cos155 - cos180)
      12.56637 $ 4pi
c
sd11  0.58869  $ 2pi(cos0 -cos25)
      0.54762  $ 2pi(cos25 - cos35)
      2.49150  $ 2pi(cos35 - cos65)
      1.02918  $ 2pi(cos65 - cos75)
      1.07859  $ 2pi(cos75 - cos85)
      1.09523  $ 2pi(cos85 - cos95)
      1.07859  $ 2pi(cos95 - cos105)
      1.02918  $ 2pi(cos105 - cos115)
      2.49150  $ 2pi(cos115 - cos145)
      0.54762  $ 2pi(cos145 - cos155)
      0.58869  $ 2pi(cos155 - cos180)
      12.56637 $ 4pi
c
c     Boundaries of the proton energy bins: 0-1 MeV; 1-3 MeV, ...
c     tabulated exactly as used by LAQGSM03.03 as stand alone code
e0    1     3     5     7     9     11    13    15    17    19
      22    27    32    37    42    47    52    57    62    67
      72    77    82    87    92    97    105   115   125   135
      145   155   165   175   185   195   205   215   225   235
      245   255   265   275   285   295   305   315   325   335
      345   355   365   375   385   395   405   415   425   435
      445   455   465   475   485   495   505   515   525   535
      545   555   565   575   585   595   605   615   625   635
      645   655   665   675   685   695   705   715   725   735
      745   755   765   775   785   795   805   815   825   835
      845   855   865   875   885   895   905   915   925   935
      945   955   965   975   985   995   1025  1075  1125  1175
      1225  1275  1325  1375  1425  1475  1525  1575  1625  1675
      1725  1775  1825  1875  1925  1975  2025  2075  2125  2175
      2225  2275  2325  2375  2425  2475  2525  2575  2625  2675
      2725  2775  2825  2875  2925  2975  3025  3075  3125  3175
      3225  3275  3325  3375  3425  3475  3525  3575  3625  3675
      3725  3775  3825  3875  3925  3975  4025  4075  4125  4175
      4225  4275  4325  4375  4425  4475  4525  4575  4625  4675
      4725  4775  4825  4875  4925  4975  5025  5075  5125  5175
c
em1 3489.72 199r $ multiply to sig_inelastic = 3489.72 mb, as predicted by
c                  LAQGSM03.03 in Ne241Utoro.out of 05/28/2010. This is needed
c                  to get the spectra in [mb/sr/MeV], after dividig the flux
c                  to the energy bins, to get [1/MeV]; we do this for every E-bin
c
em11 3489.72 199r $ multiply to sig_inelastic = 3489.72 mb, as predicted by
c                  LAQGSM03.03 in Ne241Utoro.out of 05/28/2010. This is needed
c                  to get the spectra in [mb/sr/MeV], after dividig the flux
```

```
c                    to the energy bins, to get [1/MeV]; we do this for every E-bin
c
dbcn  20j  0  5j  -1  j  1  2j  0  1  $ needed to tally pi+ separately of pi-
```

The experimental data for this problem were measured at the Berkeley Bevalac by an international team and are presented and discussed in the paper [54]. The complete set of experimental data is tabulated in the 118 page AIP document No. PAPS PRVCA 21-1321-118 available upon request from the Physics Auxiliary Publication Service of the American Institute of Physics.

Experimental ^{3}He and ^{4}He spectra $d^2\sigma/dT/d\Omega$ in units of [mb/sr/MeV] as functions of particle kinetic energy in [MeV] at 30, 70, 90, and 110 degrees are presented in the files 30_he3_e.dat, 70_he3_e.dat, 90_he3_e.dat, and 110_he3_e.dat (no ^{3}He measured data available at 150 degrees, so we present for this angle only our predictions), 30_he4_e.dat, 70_he4_e.dat, 90_he4_e.dat, and 110_he4_e.dat (no ^{4}He measured data available at 150 degrees, so we present for this angle only our predictions), respectively. For convenience of plotting all angles on a single figure and to compare spectra at different angles with each other, the experimental data at 70 degrees were multiplied by 10^{-1}, at 90 degrees by 10^{-2}, and at 110 degrees by 10^{-3}, as is shown on the plot (see files Ne241U_he3_6REP.pdf and Ne241U_he4_6REP.pdf).

The final MCNP6 output file **Ne241U_REP_3c.o** is presented in the subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**. It is calculated with the "continue" option using the auxiliary input file **inp_Ne241U**; the first MCNP6 output calculated with the main input file, **Ne241U_REP**, is: **Ne241U_REP.o**. ^{3}He spectra as calculated by MCNP6 at 30, 75, 90, 110, and 150 ($\pm$5) degrees are tabulated in units of [mb/sr/projectile] as segments for **tally 1**, where the segments corresponding to our angles are, respectively:
1) segment: 25 -35
2) segment: 25 35 65 -75
3) segment: 25 35 65 75 85 95
4) segment: 25 35 65 75 85 -95 -105 115
5) segment: 25 35 65 75 85 -95 -105 -115 -145 155 .

^{4}He spectra by MCNP6 at the same angles are tabulated in similar "segments" of the same output file, but for **tally 11**.

Note that to get the units of [mb] needed for the normalization of the calculated spectra to the total reaction cross section, we used the Energy Multiplier cards **EM1** and **EM11** in our input file **Ne241_REP** with the value 3489.72 on them for all the 200 energy bins of our tallies **F1** and **F11**: 3489.72 is the value of the total inelastic (reaction) cross section in [mb] as predicted by LAQGSM03.03 used for this reaction as a stand alone code. In a similar manner, to get the units of [1/sr] for the calculated spectra, we used in our input file the Segment Divisor cards **SD1** and **SD11** with values of the solid angles for each "segment" corresponding to angles of 30, 75, 90, 110, and 150 ($\pm$5) degrees. To get the calculated double differential spectra $d^2\sigma/dT/d\Omega$ at these angles in conventional units of [mb/sr/MeV], we still divide the tables from the MCNP6 output file at the "segments" described above to the corresponding values of the energy bins. We do this separately with a little post processing routine written especially for this.

To plot our ^{3}He and ^{4}He spectra with **xmgrace** (see files Ne241U_he3_6.pdf and Ne241U_he4_6.pdf), the final MCNP6 results obtained as described above are copied to separate files 30_he3_6REP.dat, 70_he3_6REP.dat, 90_he3_6REP.dat, 110_he3_6REP.dat, and 150_he3_6REP.dat,

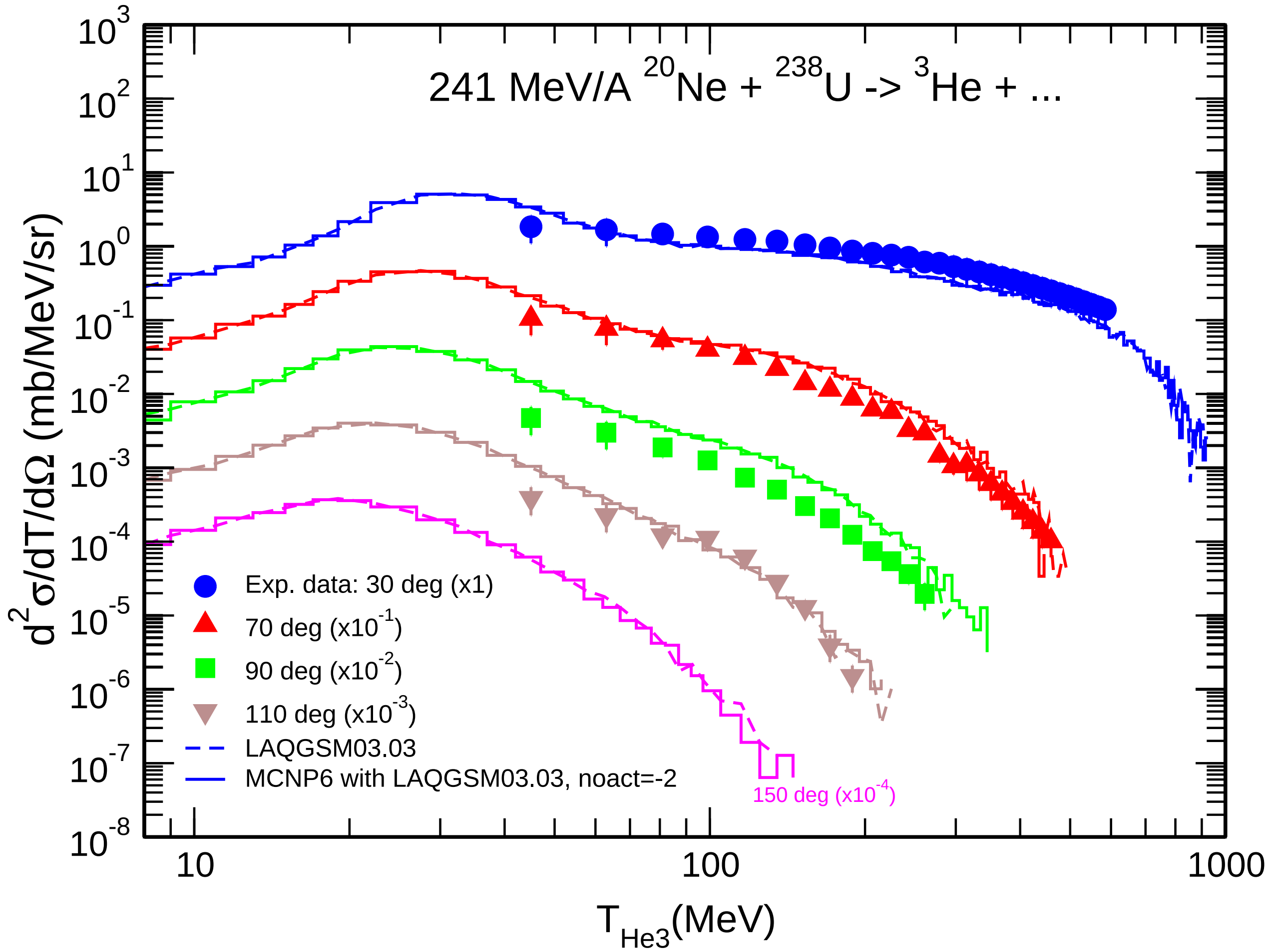

Figure 9: Experimental ^{3}He spectra [54] at 30, 70, 90, and 110 degrees (symbols) from a thin ^{238}U target bombarded with a 241 MeV/nucleon ^{20}Ne beam compared with results by LAQGSM03.03 [10] used as a stand alone code and by MCNP6 using the LAQGSM03.03 event-generator, as indicated (no ^{3}He measured data are available at 150 degrees, so we present for this angle only our predictions).

and 30_he4_6REP.dat, 70_he4_6REP.dat, 90_he4_6REP.dat, 110_he4_6REP.dat, and 150_he4_6REP.dat, respectively.

Besides the MCNP6 results, for comparison, we present here also results by LAQGSM03.03 as a stand alone code (files: 30_he3_l.dat, 70_he3_l.dat, 90_he3_l.dat, 110_he3_l.dat, and 150_he3_l.dat, and 30_he4_l.dat, 70_he4_l.dat, 90_he4_l.dat, 110_he4_l.dat, and 150_he4_l.dat, respectively).

The files Ne241U_he3_6REP.fig and Ne241U_he4_6REP.fig are templates for plotting the figures with **xmgrace**. The pdf files for the figures with final results for this problem are Ne241U_he3_6REP.pdf and Ne241U_he4_6REP.pdf. The files with both figures are presented together with all files with calculation results and experimental data in subdirectory **/VALIDATION_LAQGSM/Experimental_data/Ne241U/**.

Our final results for this test problem are shown in Figs. 9 and 10. We see that MCNP6 using LAQGSM03.03 describes well the measured ^{3}He and ^{4}He spectra [54] and agrees very well with results obtained with LAQGSM03.03 event generator used as a stand alone code.

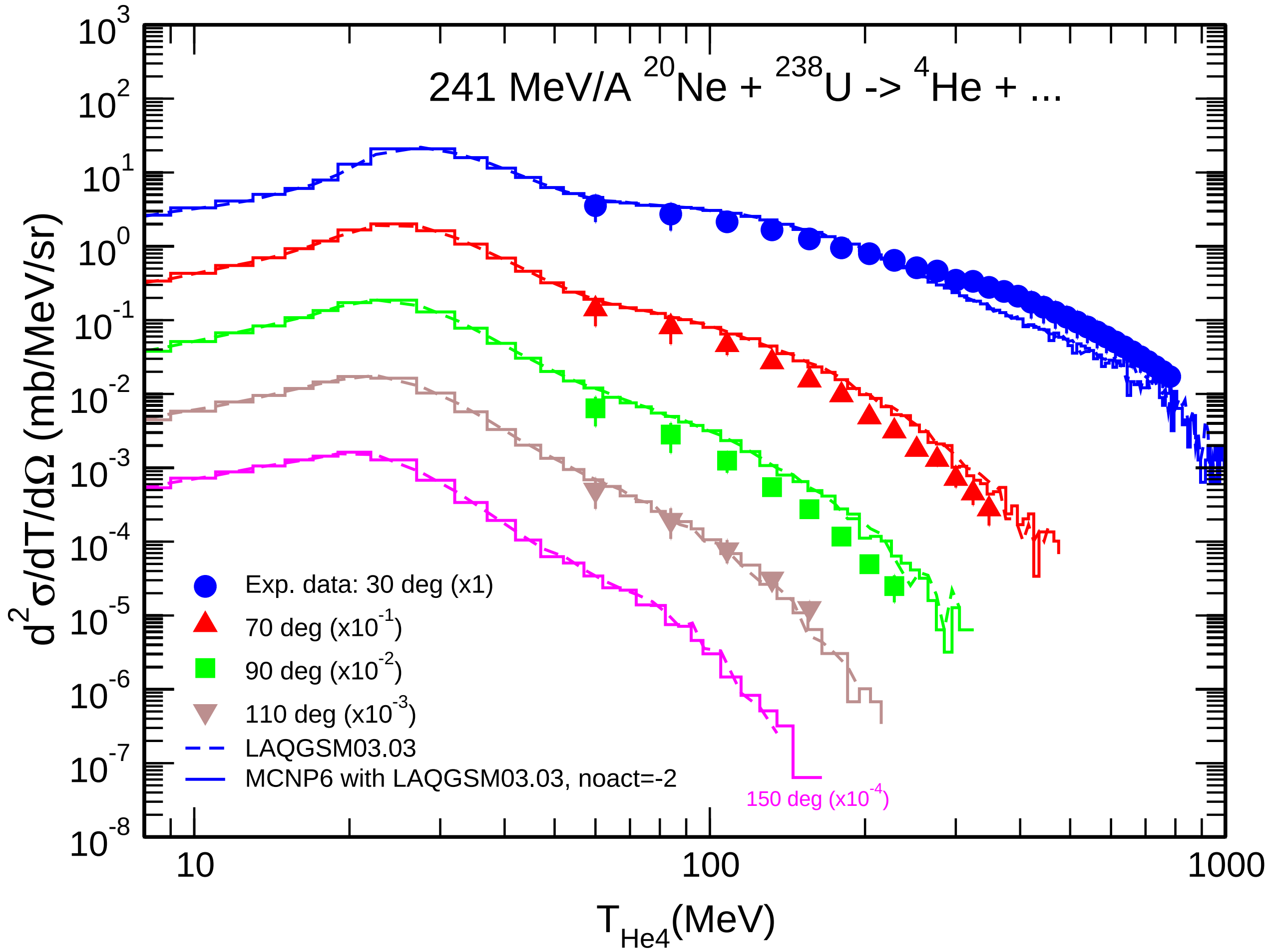

Figure 10: Experimental ^{4}He spectra [54] at 30, 70, 90, and 110 degrees (symbols) from a thin ^{238}U target bombarded with a 241 MeV/nucleon ^{20}Ne beam compared with results by LAQGSM03.03 [10] used as a stand alone code and by MCNP6 using the LAQGSM03.03 event-generator, as indicated (no ^{4}He measured data are available at 150 degrees, so we present for this angle only our predictions).

Let us note here that light charged particles, i.e., p (see Figure 6), d (see Figure 7), t (see Figure 8), ^{3}He (see Figure 9), and ^{4}He (see Figure 10) from any reactions are of a major concern for material damage, as helium can cause swelling in structure materials; tritium is often an issue from a radioprotection point of view. We see that MCNP6 describes such reactions very well.

3.9. Test-Problems #9: C800C_REP with inp_C800C

This MCNP6 problem is to test the applicability of MCNP6 using the LAQGSM03.03 event generator to calculate production of pions from intermediate energy carbon-beam induced reactions for different NASA, medical (cancer treatment with a carbon-beam), FRIB (Facility for Rare Isotope Beams), and for some other U.S. DOE applications.

This test calculates with MCNP6 the invariant spectra of π^+ at 15, 45, 70, 90, and 145 degrees and of π^- at 20, 40, 56, 90, and 145 degrees from interaction of a 800 MeV/nucleon ^{12}C beam with a thin ^{12}C target and compares the results with experimental data and with results by the LAQGSM03.03 event generator used as a stand alone code.

It has also an additional aim of testing the very recent capability of MCNP6 to tally separately production of particles and antiparticles (π^+ and π^-) using the DBCN(27) = -1 option, a feature not available in MCNPX and in earlier versions of MCNP6 (see Section 3.3 with the test problem **inp75cor_bREP**, where we discussed the absence of such a capability as a deficiency of earlier versions of MCNP6, addressed and solved by Grady Hughes in the latest version of MCNP6).

We calculate this test-problem using the **NOACT=-2** option for the 8th parameter of the **LCA** card of the MCNP6 input file. As we have presented a detailed description of the use of **NOACT=-2** option to calculate particle spectra from thin targets in the test-problem #6 of the CEM Testing Primer [5], and have provided additional examples of its use in test problems #7 and #8 of Ref. [5], we do not need to discuss in detail the input and output files for this case. Therefore, we limit ourselves to only providing the text of the input file as well as describing where to find the results in the MCNP6 output files.

The input file for this test problem is **C800C_REP**. It is presented in the subdirectory **/VALIDATION_LAQGSM/Inputs/** and is also shown below.

C800C_REP:

```
MCNP6 test with LAQGSM03.03: 800 MeV/A C12+C12 -> pi+ invariant spectra
c E^3sigma/d^3p [mb/GeV^2/c^-3/sr] at 15, 45, 70, 90, and 145 deg
c and pi- invariant spectra at at 20, 40, 56, 90, and 145 deg (+/- 2.5 deg)
c to compare with Nagamiya's et al. measurements (LBL-8463)
c and results by LAQGSM03.03 as a stand alone code
c and to check how MCNP6 tallies separately particles and antiparticles
c using the DBCN(27) = -1 option
1   1  -10   -501      imp:h=1
2   0         501  -502  imp:h=1
99  0         502      imp:h=0

501   so 0.01
502   so 1
c
c  tally surfaces
c
125    kz    0    0.049148523     1  $ tan(12.5 deg)^2
175    kz    0    0.099413326     1  $ tan(17.5 deg)^2
225    kz    0    0.171572875     1  $ tan(22.5 deg)^2
375    kz    0    0.588790706     1  $ tan(37.5 deg)^2
425    kz    0    0.83966282      1  $ tan(42.5 deg)^2
475    kz    0    1.190954245     1  $ tan(47.5 deg)^2
535    kz    0    1.826342606     1  $ tan(53.5 deg)^2
585    kz    0    2.662939929     1  $ tan(58.5 deg)^2
675    kz    0    5.828427125     1  $ tan(67.5 deg)^2
725    kz    0    10.05901359     1  $ tan(72.5 deg)^2
```

```
875    kz    0    524.5824763     1  $ tan(87.5 deg)^2
925    kz    0    524.5824763    -1  $ tan(92.5 deg)^2
1425   kz    0    0.588790706    -1  $ tan(142.5 deg)^2
1475   kz    0    0.405858517    -1  $ tan(147.5 deg)^2

mode n h d t s a # / * z
m1  06012 1
lca 7j -2 j 1    $ LAQGSM, no transport, only the 1st inelstic interaction
nps 1000
c nps 1e6
prdmp 2j -1
sdef par=06012 erg=9600 vec=0 0 1 dir 1
phys:# 9600
phys:h 3100
phys:n 3100
phys:a 6000
phys:d 5000
phys:t 5200
phys:s 5200
phys:/ 2200
phys:* 2200
phys:z 2200
c
f1:/  502
f11:*  502
c define the "segments" for pi+ at 15, 45, 70, 90, and 140 deg
fs1 -125 -175 -425 -475 -675 -725 -875 925 1425 1475 T
c define the "segments" for pi- at 20, 40, 56, 90, and 140 deg
fs11 -175 -225 -375 -425 -535 -585 -875 925 1425 1475 T
c
c The following Segment Divisor card is needed to get 1/sr for pi+ spectra
sd1   0.14894  $ 2pi(cos0 -cos12.5)
      0.14187  $ 2pi(cos12.5 - cos17.5)
      1.35993  $ 2pi(cos17.5 - cos42.5)
      0.38759  $ 2pi(cos42.5 - cos47.5)
      1.84039  $ 2pi(cos47.5 - cos67.5)
      0.51508  $ 2pi(cos67.5 - cos72.5)
      1.61532  $ 2pi(cos72.5 - cos87.5)
      0.54814  $ 2pi(cos87.5 - cos92.5)
      4.71072  $ 2pi(cos92.5 - cos142.5)
      0.31440  $ 2pi(cos142.5 - cos147.5)
      0.98400  $ 2pi(cos147.5 - cos180)
      12.56637 $ 4pi
c
c The following Segment Divisor card is needed to get 1/sr for pi- spectra
sd11  0.29080  $ 2pi(cos0 -cos17.5)
      0.18747  $ 2pi(cos17.5 - cos22.5)
```

```
      0.82012  $ 2pi(cos22.5 - cos37.5)
      0.35234  $ 2pi(cos37.5 - cos42.5)
      0.89507  $ 2pi(cos42.5 - cos53.5)
      0.45443  $ 2pi(cos53.5 - cos58.5)
      3.00889  $ 2pi(cos58.5 - cos87.5)
      0.54814  $ 2pi(cos87.5 - cos92.5)
      4.71072  $ 2pi(cos92.5 - cos142.5)
      0.31440  $ 2pi(cos142.5 - cos147.5)
      0.98400  $ 2pi(cos147.5 - cos180)
      12.56637 $ 4pi
c
c     Boundaries of the pion energy bins: 0-1 MeV; 1-3 MeV, ...
c     tabulated exactly as used by LAQGSM03.03 as stand alone code
e0    1     3     5     7     9     11    13    15    17    19
      22    27    32    37    42    47    52    57    62    67
      72    77    82    87    92    97    105   115   125   135
      145   155   165   175   185   195   205   215   225   235
      245   255   265   275   285   295   305   315   325   335
      345   355   365   375   385   395   405   415   425   435
      445   455   465   475   485   495   505   515   525   535
      545   555   565   575   585   595   605   615   625   635
      645   655   665   675   685   695   705   715   725   735
      745   755   765   775   785   795   805   815   825   835
      845   855   865   875   885   895   905   915   925   935
      945   955   965   975   985   995   1025  1075  1125  1175
      1225  1275  1325  1375  1425  1475  1525  1575  1625  1675
      1725  1775  1825  1875  1925  1975  2025  2075  2125  2175
      2225  2275  2325  2375  2425  2475  2525  2575  2625  2675
      2725  2775  2825  2875  2925  2975  3025  3075  3125  3175
      3225  3275  3325  3375  3425  3475  3525  3575  3625  3675
      3725  3775  3825  3875  3925  3975  4025  4075  4125  4175
      4225  4275  4325  4375  4425  4475  4525  4575  4625  4675
      4725  4775  4825  4875  4925  4975  5025  5075  5125  5175
c
em1 890.179 199r $ multiply to sig_inelastic = 890.179 mb, as predicted by
c                  LAQGSM03.03 in C800C2.out of 06/10/2010. This is needed
c                  to get the spectra in [mb/sr/MeV], after dividing the flux
c                  to the energy bins, to get [1/MeV]; we do this for every E-bin;
c   Then, we will multiply these double-differential spectra, d^2sigma/dT/dOmega,
c   by 1/p, to get the final invariant spectra Ed^3sigma/d^3p [mb/GeV^2/c^-3/sr],
c   coverting later also MeV^(-2) to GeV^(-2)
c
dbcn  20j  0  5j  -1  j  1  2j  0  1  $ needed to tally pi+ separately of pi-
```

The experimental data for this problem were measured at the Berkeley Bevalac by the Prof. Shoji Nagamiya's Group [55] and are tabulated in the 181 page Lawrence Berkeley National Laboratory. Report No. LBL-8463 [56].

Experimental invariant π^+ spectra at 15, 45, 70, 90, and 145 degrees and of π^- at 20, 40, 56, 90, and 145 degrees $Ed^3\sigma/d^3p$ in units of [mb/sr/GeV^2/c^{-3}] as functions of pion momentum in [MeV/c] are presented in the files 15_pip_e.dat, 45_pip_e.dat, 70_pip_e.dat, 90_pip_e.dat, and 145_pip_e.dat, and in 20_pim_e.dat, 40_pim_e.dat, 56_pim_e.dat, 90_pim_e.dat, and 145_pim_e.dat, respectively. For convenience of plotting all angles on a single figure and to compare spectra at different angles with each other, the experimental data at 45 degrees for π^+ and 40 degrees for π^- are multiplied by 10^{-1}, at 70 degrees for π^+ and 56 degrees for π^- by 10^{-2}, at 90 degrees for both π^+ and π^- by 10^{-3}, and at 145 degrees for both π^+ and π^- by 10^{-4}, as is shown on the plots (see files C800C_pip_6.pREPdf and C800C_pim_6REP.pdf).

The final MCNP6 output file **C800C_REP_3c.o** (and the MCTAL file **C800C_REP_3c.m**) is presented in the subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**. It is calculated with the "continue" option using the auxiliary input file **inp_C800C**; the first MCNP6 output file calculated with the main input file, **C800C_REP**, is: **C800C_REP.o**. Positive pion spectra as calculated by MCNP6 at 15, 45, 70, 90, and 145 ($\pm$2.5) degrees are tabulated in units of [mb/sr/projectile] as segments for **tally 1**, where the segments corresponding to our angles are, respectively:
1) segment: 125 -175
2) segment: 125 175 425 -475
3) segment: 125 175 425 475 675 -725
4) segment: 125 175 425 475 675 725 875 925
5) segment: 125 175 425 475 675 725 875 -925 -1425 1475 .

Note that to get the units of [mb] needed for normalization of the calculated spectra to the total reaction cross section, we used the Energy Multiplier card **EM1** in our input file **C800C_REP** with the value 890.179 on it for all the 200 energy bins of our tally **F1**: 890.179 is the value of the total inelastic (reaction) cross section in [mb] as predicted by LAQGSM03.03 used for this reaction as a stand alone code.

Intentionally, to demonstrate the usefulness of the Energy Multiplier card and its work for such problems, we do not use it here for the tally **F11**, i.e., we do not use a **EM11** card for negative pions. In such a case, we get the MCNP6 negative pion spectra at 20, 40, 56, 90, and 145 ($\pm$2.5) degrees tabulated in units of [pion/sr/projectile] in the same final MCNP6 output file **C800C_REP_3c.o** as segments for **tally 11**, where the segments corresponding to these angles are, respectively:
1) segment: 175 -225
2) segment: 175 225 375 -425
3) segment: 175 225 375 425 535 -585
4) segment: 175 225 375 425 535 585 875 925
5) segment: 175 225 375 425 535 585 875 -925 -1425 1475 .

Note, that in this case, to get the needed units of [mb] for the negative pion spectra, we multiply by hand the MCNP6 results to the same value of 890.179 [mb] while plotting our figure. Using a **EM11** card for π^-, analogously to **EM1** for π^+, would eliminate the necessity of this manual multiplication.

Note that in a similar manner, to get the units of [1/sr] for the calculated spectra, we used in our input file the Segment Divisor cards **SD1** and **SD11** for both π^+ and π^- with the corresponding values of the solid angles for each "segment" identifying the needed angles. To get the calculated double differential pion spectra $d^2\sigma/dT/d\Omega$ at these angles in conventional units of [mb/sr/MeV], we still divide the tables from the MCNP6 output file at the "segments" described above to the values of the energy bins.

Finally, to convert such double differential spectra to the measured so called "invariant spectra," $Ed^3\sigma/d^3p$, in units of [mb/sr/GeV^2/c^{-3}] as functions of the pion momenta p_π in [MeV/c], we calculate initially the mean pion kinetic energy for each energy bin, T_π, and then, to use it to get the pion momentum for each energy bin as $p_\pi = \sqrt{T_\pi(T_\pi + 2m_\pi)}$, where m_π is the mass of the charged pion in MeV. At the end, we use the known relation $Ed^3\sigma/d^3p = (1/p)d^2\sigma/dT/d\Omega$, not forgetting to convert in this formula the pion momentum from [MeV/c] to [GeV/c], in order to get the calculated invariant pion spectra in the same units as measured. We do these transformations separately with a little post processing routine written especially for this.

To plot our invariant spectra with **xmgrace** (see files C800C_pip_6REP.pdf and C800C_pim_6REP.pdf), the final MCNP6 results obtained as described above are copied to separate files 15_pip_6REP.dat, 45_pip_6REP.dat, 70_pip_6REP.dat, 90_pip_6REP.dat, and 145_pip_6REP.dat for π^+ and 20_pim_6REP.dat, 40_pim_6REP.dat, 56_pim_6REP.dat, 90_pim_6REP.dat, and 145_pim_6REP.dat, for π^-, respectively. Besides the MCNP6 results, for comparison, we present here also results by LAQGSM03.03 as a stand alone code (files 15_pip_l.dat, 45_pip_l.dat, 70_pip_l.dat, 90_pip_l.dat, and 145_pip_l.dat for π^+ and 20_pim_l.dat, 40_pim_l.dat, 56_pim_l.dat, 90_pim_l.dat, and 145_pim_l.dat, for π^-, respectively).

The files C800C_pip_6REP.fig and C800C_pim_6REP.fig are templates for plotting the figures with **xmgrace**. The pdf files for the figures with final results for this problem are C800C_pip_6REP.pdf and C800C_pim_6REP.pdf, with the summary file C800C_piREP.pdf showing spectra of both π^+ and π^-. The files with both figures are presented together with all files with our calculation results and with experimental data in subdirectory
/VALIDATION_LAQGSM/Experimental_data/C800C/.

Our final results for this test problem are shown below in Figures 11 and 12. We see a very good agreement between the results by MCNP6 and by LAQGSM03.03 used as a stand alone code, and a worse, especially for π^+, but still a reasonable agreement with the experimental data [55, 56].

3.10. Test-Problems #10: p300GeV_Ag_REP with inxc98

This MCNP6 problem is to test the applicability of MCNP6 using the LAQGSM03.03 event generator to describe yields of products from the ultra-relativistic reaction 300 GeV p + Ag.

To be specific, in this test problem, we calculate with MCNP6 using LAQGSM03.03 with the GENXS option the mass-number yield distribution of the products from a thin Ag target bombarded with 300-GeV protons and compare the results with available experimental data and with results by LAQGSM03.03 used as a stand alone code. Such reactions are of interest for Space Applications, for radiation shielding at high-energy accelerators, and to study the mechanisms of target fragmentation by relativistic projectiles. In addition, we have utilized this test-problem to understand and to fix a problem observed while using the GENXS option of MCNP6 at ultra-relativistic energies (a previously unobserved "bug" in the GENXS option of MCNP6 at high-energies was found and fixed recently by Dick Prael).

For this test-problem we use the GENXS option of MCNP6. As we have presented a detailed description of the use of GENXS option to calculate product yields from thin targets in test-problem #1 of the CEM Testing Primer [5], we will not discuss the input and output files for

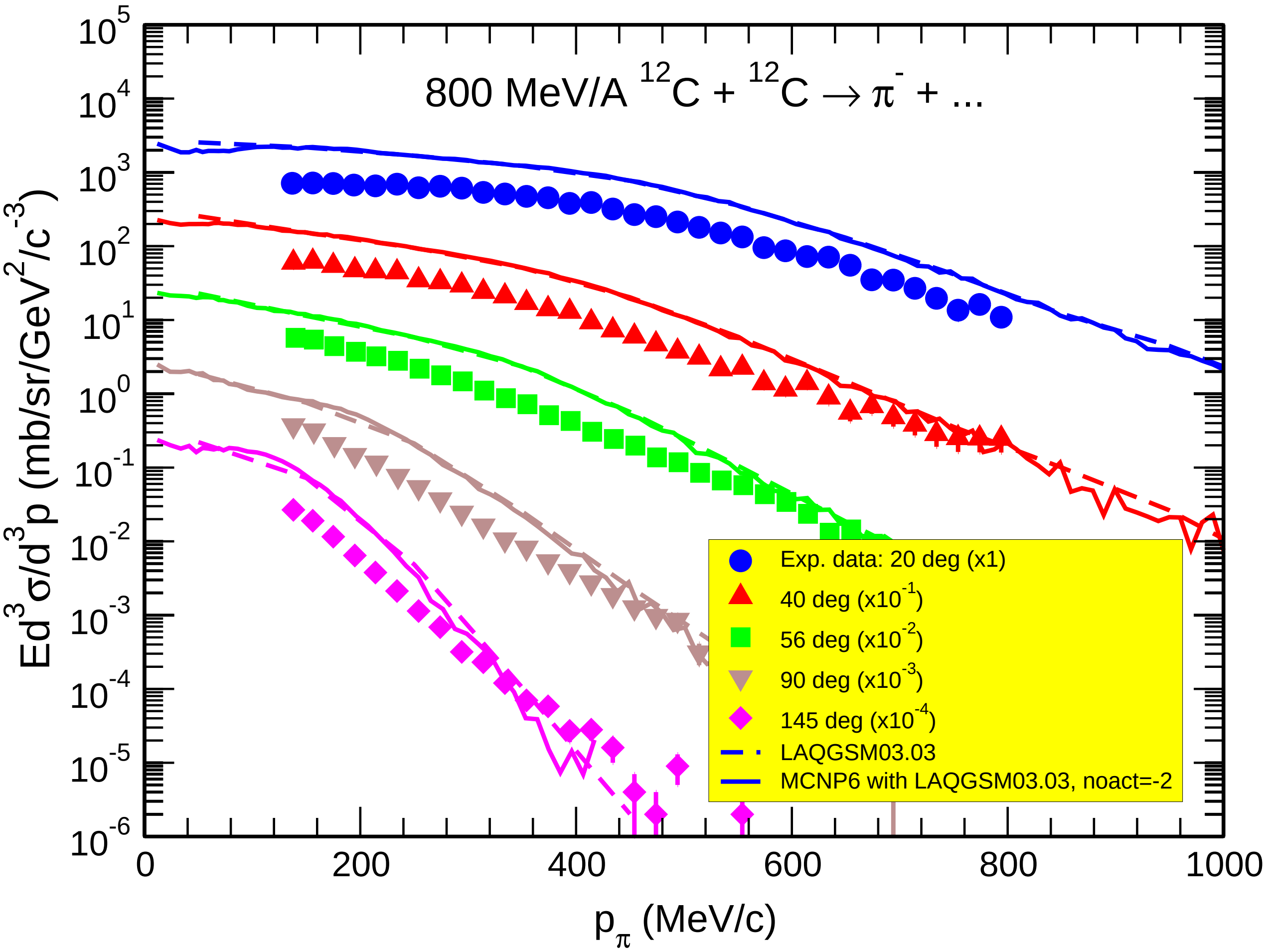

Figure 11: Experimental invariant π^- spectra [55, 56] at 20, 40, 56, 90, and 145 degrees (symbols) from a thin C target bombarded with a 800 MeV/nucleon ^{12}C beam compared with results by LAQGSM03.03 [10] used as a stand alone code and by MCNP6 using the LAQGSM03.03 event-generator, as indicated.

this case. Therefore, we limit ourselves to only providing the text of the input files (let us recall here that the GENXS option of MCNP6 requires a second, auxiliary input file in addition to the main MCNP6 input file), as well as describing where to find the results in the MCNP6 output file.

The main MCNP6 input file for the case of using the GENXS option is **p300GeV_Ag_REP**. It uses the auxiliary companion required by the GENXS option input file **inxc98**. Both of these are presented in the subdirectory **/VALIDATION_LAQGSM/Inputs/** and are also shown below.

p300GeV_Ag_REP:

```
MCNP6 test: p + Ag by LAQGSM03.03 at 300 GeV, nevtype=66
C To evaluate cosmic-ray activation of tellurium;
c These calculations are done with corrections to MCNP6 by Dick Prael(REP)
c of 12/6/10 to account all fragments (not only 3) from Fermi break-up
  1  1  1.0   -1 2 -3
```

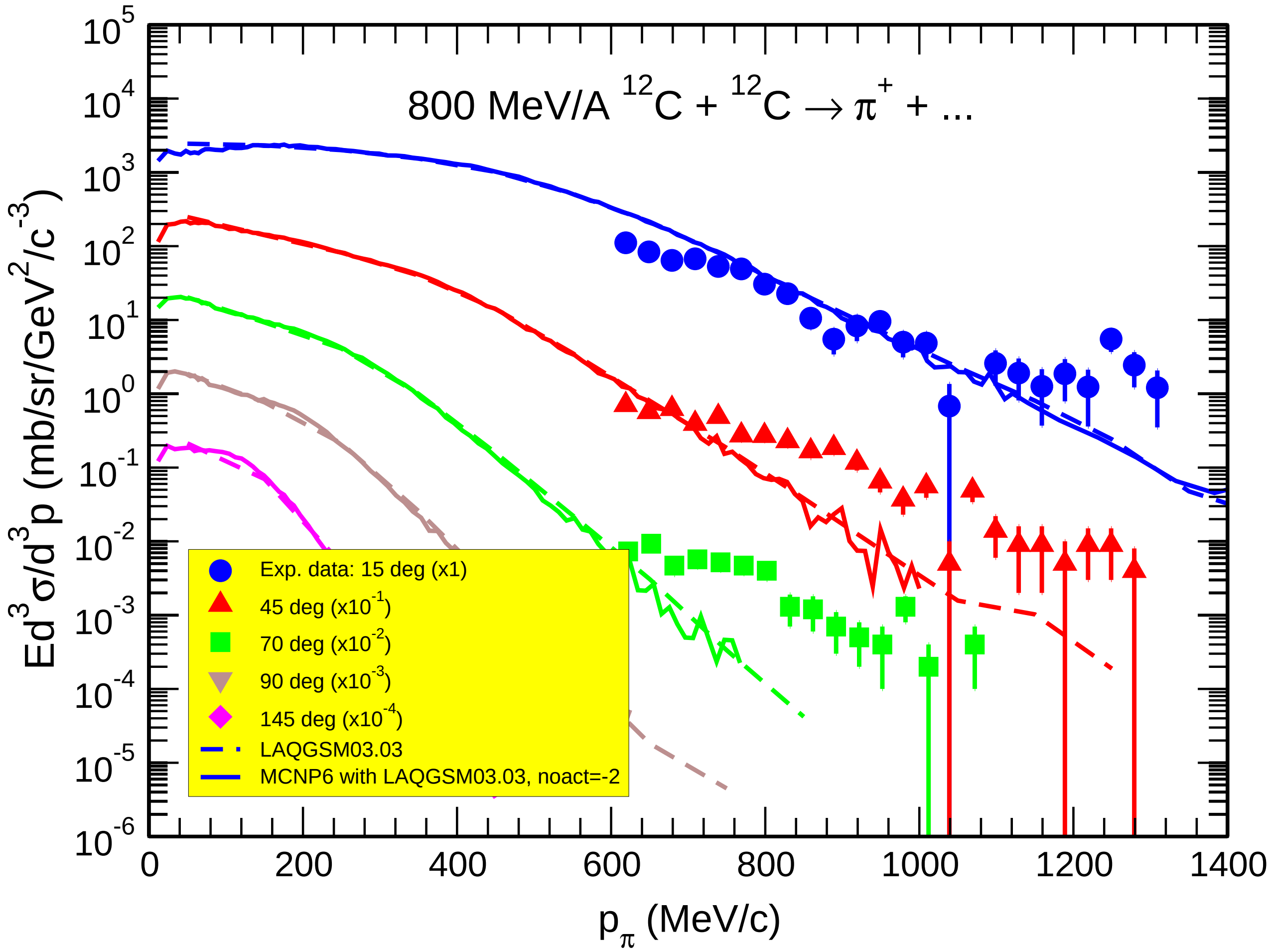

Figure 12: Experimental invariant π^+ spectra [55, 56] at 15, 45, and 70 degrees (symbols) from a thin C target bombarded with a 800 MeV/nucleon ^{12}C beam compared with results by LAQGSM03.03 [10] used as a stand alone code and by MCNP6 using the LAQGSM03.03 event-generator, as indicated (no π^+ measured data are available at 90 and 145 degrees, so we present for these angles only our predictions).

```
  2  0        -4 (1:-2:3)
  3  0         4

c ---------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c ---------------------------------------------------------------
dbcn 28j 1
  m1 47107 0.51839 47109 0.48161
  sdef erg = 300000 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:n 1 1 0
```

```
  imp:h 1 1 0
  phys:h 300100
  mode   h
LCA  2 1 5j -1 1j 1    $ use LAQGSM, nevtype = 66                   !!!
lcb  0 0 0 0 0 0
lea  2j 0
c  tropt genxs inxc98  nreact on  nescat off
  tropt genxs inxc98
c ----------------------------------------------------------------
  print 40 110 95
c  nps 1000
  nps 1000000
  prdmp 2j -1
```

inxc98:

```
MCNP6 test: p + Ag by LASQGSM03.03 at 300 GeV, nevtype=66
0 0 1 /
Cross Section Edit
```

The 300 GeV proton irradiations were performed in an external beam line at Fermilab and the measured cross section are presented in Figure 7 of the paper [57]. The file **p300000Ag_A_exp.dat** presented in the subdirectory **/VALIDATION_LAQGSM/Experimental_data/p300GeV_Ag/** shows experimental data extracted from the enlarged Figure 7 of this paper.

The mass number distribution of product yields by MCNP6 (in units of barns) is tabulated in the table entitled **Summary by mass number** of the MCNP6 output file **p300000Ag_REP.o**, presented in the Templates subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**. It is copied to a separate input file for **xmgrace**, p300000Ag_A_L_REP.dat, and the final plot appears in the file p300GeV_Au_A_sg4.pdf. The file p300000Ag_SGMno.dat presents results by LAQGSM03.03 used as a stand alone code.

A template for plotting our results with **xmgrace** is presented in the file p300GeV_Au_A_sg4.fig; the pdf file of the figure is: p300GeV_Au_A_sg4.pdf. The files with figure are presented together with all files with calculation results and experimental data in subdirectory **/VALIDATION_LAQGSM/Experimental_data/p300GeV_Ag/**.

Our final results for this test problem are shown below in Figure 13. We see that MCNP6 using LAQGSM03.03 describes well the measured yield [57] of nuclides from this reaction, except for products very near to the target, and agrees very well with results obtained with the LAQGSM03.03 event generator used as a stand alone code. The underestimation of the yield of products very near to the target by both MCNP6 using LAQGSM03.03 and by LAQGSM03.03 used as a stand alone code is probably related with the neglect by LAQGSM03.03 of the processes of electromagnetic dissociation in ultra-relativistic reactions; we may consider in the future a possible improvement of LAQGSM03.03 to address such processes.

3.11. Test-Problems #11: p800000Au_REP with inxc97

This MCNP6 problem is to test the applicability of MCNP6 using the LAQGSM03.03 event generator to describe yields of products from the ultra-relativistic reaction 800 GeV p + Au.

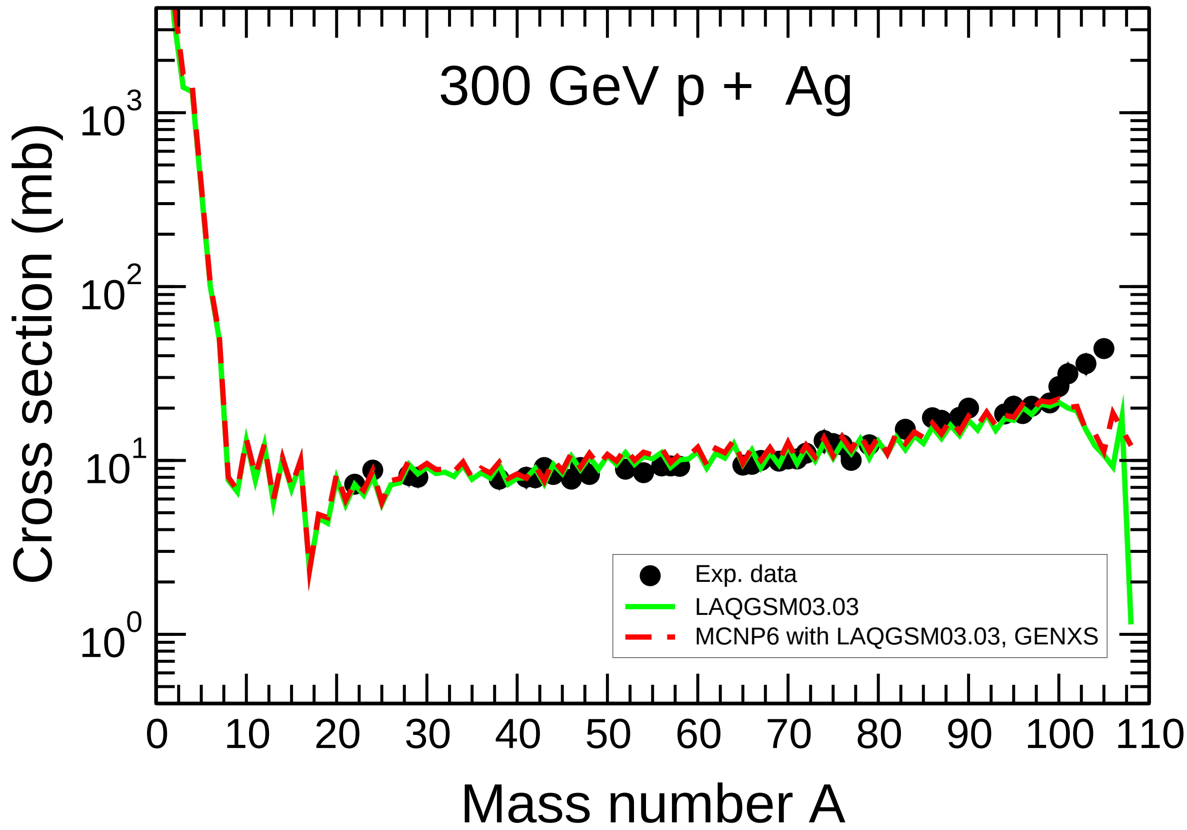

Figure 13: Experimental mass number distribution of product yields [57] (filled circles) from the 300 GeV p + Ag reaction compared with results by LAQGSM03.03 [10] used as a stand alone code and by MCNP6 using the LAQGSM03.03 event-generator, as indicated.

To be specific, in this test problem, we calculate with MCNP6 using LAQGSM03.03 with the GENXS option the mass-number yield distribution of the products from a thin Au target bombarded with 800-GeV protons and compare the results with available experimental data and with results by LAQGSM03.03 used as a stand alone code. 800 GeV is the highest energy we found experimental data at ultra-relativistic energies where LAQGSM is expected to work well, i.e., this is the highest energy we can presently V&V MCNP6 using LAQGSM against available experimental data. Such reactions are of interest for Space Applications, for radiation shielding at high-energy accelerators, and to study the mechanisms of target fragmentation by relativistic projectiles. In addition, we have utilized this test-problem to understand and to fix a problem observed while using the GENXS option of MCNP6 at ultra-relativistic energies (a previously unobserved "bug" in the GENXS option of MCNP6 at high-energies was found and fixed recently by Dick Prael).

We calculate this test-problem using the GENXS option of MCNP6. As we have presented a detailed description of the use of GENXS option to calculate product yields from thin targets in test-problem #1 of the CEM Testing Primer [5], we do not need to discuss the input and output files for this case. Therefore, we limit ourselves to only providing the text of the input files (let us recall here that the GENXS option of MCNP6 requires a second, auxiliary input file in addition to the main MCNP6 input file), as well as describing where to find the results in the MCNP6 output file.

The main MCNP6 input file for the case of using the GENXS option is **p800000Au_REP**. It uses the auxiliary companion **inxc97** required by the GENXS option. Both of these are presented in the subdirectory **/VALIDATION_LAQGSM/Inputs/** and are also shown below.

p800000Au_REP:

```
MCNP6 test: p + Au by LAQGSM03.03 at 800 GeV, nevtype=66
C To study Au fragmentation induced by very energetic projectiles;
c These calculations are done with corrections to MCNP6 by Dick Prael(REP)
c of 12/6/10 to account all fragments (not only 3) from Fermi break-up
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c ----------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c ----------------------------------------------------------------
dbcn 28j 1
  m1 79197 1.0
  sdef erg = 800000 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:n 1 1 0
  imp:h 1 1 0
  phys:h 800100
  mode   h
LCA  2 1 5j -1 1j 1    $ use LAQGSM, nevtype = 66                  !!!
lcb  0 0 0 0 0 0
lea  2j 0
c  tropt genxs inxc98  nreact on  nescat off
  tropt genxs inxc97
c ----------------------------------------------------------------
  print 40 110 95
c  nps 1000
  nps 1000000
  prdmp 2j -1
```

inxc97:

```
MCNP6 test: p + Te by LASQGSM03.03 at 23 GeV, nevtype=66
1 0 1 /
Cross Section Edit
```

```
50 0 9 /
5. 10. 15. 20. 25. 30. 35. 40. 45. 50. 55. 60. 65. 70. 75. 80.
85. 90. 95. 100. 120. /
1 5 6 7 8 21 22 23 24 /
```

The 800 GeV proton irradiations were performed in an external beam line at Fermilab and the measured cross section are presented in Table 1 and in Figure 4 of paper [58].

The mass number distribution of product yields by MCNP6 (in units of barns) is tabulated in the table entitled **Summary by mass number** of the MCNP6 output file **p800000AU_REP_c.o** presented in the subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**. It is copied to a separate input file for **xmgrace**, p800GeV_A_REP.dat, and the final plot appears in the file p800GeV_Au_A_sf4.pdf. Note that this MCNP6 calculation was done in two stages, with the "continue" option, using the auxiliary input file **inp_10e6** during the second stage. (The initial output file obtained during the first stage of calculation, **p800000AU_REP.o** is also provided.)

The file p800000Au_SGMnoGPL.dat presents results by LAQGSM03.03 used as a stand alone code.

A template for plotting our results with **xmgrace** is presented in the file p800GeV_Au_A_sf4.fig; the pdf file of the figure is: p800GeV_Au_A_sf4.pdf (see Figure 14 below). The files of figure are presented together with all files with calculation results and experimental data in subdirectory **/VALIDATION_LAQGSM/Experimental_data/p800GeV_Au/**.

Our final results for this test problem are shown in Figure 14. We see that MCNP6 using LAQGSM03.03 describes well the measured [58] yield of nuclides from this reaction, except for products very near the target, and agrees very well with results obtained with the LAQGSM03.03 event generator used as a stand alone code. The underestimation of the yield of products very near the target by both MCNP6 using LAQGSM03.03 and by LAQGSM03.03 used as a stand alone code is probably related to LAQGSM03.03 neglecting the processes of electromagnetic dissociation in ultra-relativistic reactions; we may consider in the future a possible improvement of LAQGSM03.03 to address such processes.

3.12. Test-Problems #12: p800Au_Laq with inxc97 and p800Au_CEM with inxc96

This MCNP6 problem tests the applicability of MCNP6 using the LAQGSM03.03 event generator to describe yields of products from the reaction 800 MeV p + Au.

To be specific, in this test-problem, we calculate with MCNP6 using LAQGSM03.03 with the GENXS option the mass-number yield distribution of the products from a thin Au-target bombarded with 800-MeV protons and compare the results with available experimental data and with results by LAQGSM03.03 used as a stand alone code. This test problem for MCNP6 with LAQGSM is exactly the same as the previous one (#11, p800000Au_REP), except that the incident energy of protons is one thousand times lower: 800 MeV. In fact, at 800 MeV, MCNP6 will usually never use by default LAQGSM, as LAQGSM is used by default for proton-induced reactions only at energies above 3.5 GeV; i.e., this problem tests how MCNP6 with LAQGSM works at energies below the default. We also calculate this reaction with MCNP6 using the CEM03.03 event generator, and with CEM03.03 used as a stand-alone code. This allows us to compare results by MCNP6 using the LAQGSM and CEM event-generators on the same measured data. In addition, we needed this test-problem to understand and to fix a problem

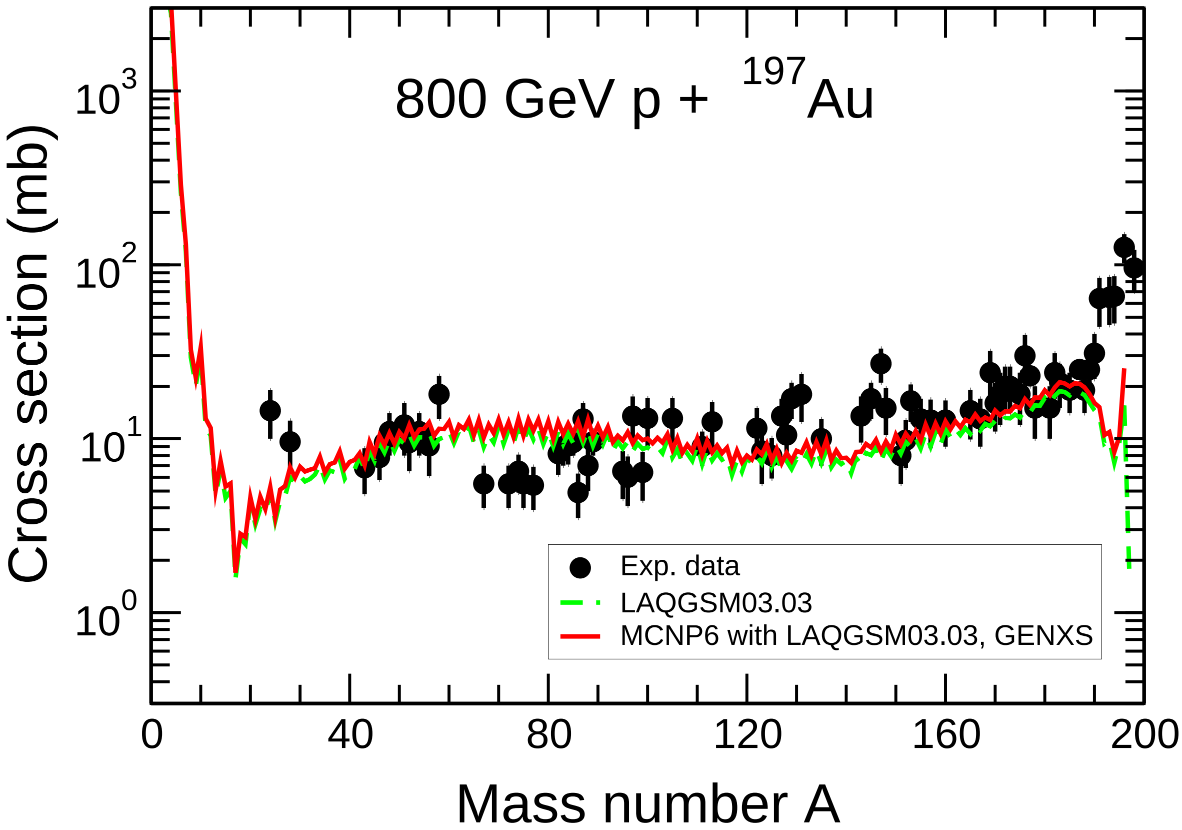

Figure 14: Experimental mass number distribution of product yields [58] (filled circles) from the 800 GeV p + Au reaction compared with results by LAQGSM03.03 [10] used as a stand alone code and by MCNP6 using the LAQGSM03.03 event-generator, as indicated.

observed while using the GENXS option of MCNP6 for several high-energy reactions (several previously unobserved "bugs" in the GENXS option of MCNP6 at high-energies were found and fixed recently by Dick Prael).

We calculate this test-problem using the GENXS option of MCNP6. As we have presented a detailed description of the use of GENXS option to calculate product yields from thin targets in test-problem #1 of the CEM Testing Primer [5], we do not need to discuss the input and output files for this case. Therefore, we limit ourselves to only providing the text of the input files (let us recall here that the GENXS option of MCNP6 requires a second, auxiliary input file in addition to the main MCNP6 input file), as well as describing where to find the results in the MCNP6 output file.

The main MCNP6 input file in the case of using the LAQGSM03.03 event generator with the GENXS option is **p800Au_Laq**. It uses the auxiliary companion input file **inxc97** required by the GENXS option. The main MCNP6 input file in the case of using the CEM03.03 event generator with the GENXS option is **p800Au_CEM**. It uses the auxiliary companion input file **inxc97** required by the GENXS option. All of these are presented in the subdirectory

/VALIDATION_LAQGSM/Inputs/ and are also shown below.

p800Au_Laq:

```
MCNP6 test: p + Au by LAQGSM03.03 at 0.800 GeV, nevtype=66
C To evaluate cosmic-ray activation of tellurium
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c ----------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c ----------------------------------------------------------------
dbcn 28j 1
  m1 79197 1.0
  sdef erg = 800 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:n 1 1 0
  imp:h 1 1 0
  phys:h 810
  mode   h
LCA  2 1 5j -1 1j 1    $ use LAQGSM, nevtype = 66                  !!!
lcb  0 0 0 0 0 0
lea  2j 0
c  tropt genxs inxc98  nreact on  nescat off
  tropt genxs inxc97
c ----------------------------------------------------------------
  print 40 110 95
c  nps 1000
  nps 1000000
  prdmp 2j -1
```

inxc97:

```
MCNP6 test: p + Te by LASQGSM03.03 at 23 GeV, nevtype=66
1 0 1 /
Cross Section Edit
50 0 9 /
5. 10. 15. 20. 25. 30. 35. 40. 45. 50. 55. 60. 65. 70. 75. 80.
85. 90. 95. 100. 120. /
1 5 6 7 8 21 22 23 24 /
```

p800Au_CEM:

```
MCNP6 test: p + Au by CEM03.02 at 800 MeV, nevtype=66
C To evaluate cosmic-ray activation of tellurium
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c -------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c -------------------------------------------------------------
  m1 79197 1.0
  sdef erg = 800 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 1000
  mode   h
LCA  8j 1    $ use CEM03.02, nevtype = 66                  !!!
  tropt genxs inxc96  nreact on  nescat off
c -------------------------------------------------------------
  print 40 110 95
c  nps 1000
  nps 1000000
  prdmp 2j -1
```

inxc96:

```
MCNP6 test: p + Te by CEM03.02 at 800 MeV, nevtype=66
1 0 1 /
Cross Section Edit
50 0 9 /
5. 10. 15. 20. 25. 30. 35. 40. 45. 50. 55. 60. 65. 70. 75. 80.
85. 90. 95. 100. 120. /
1 5 6 7 8 21 22 23 24 /
```

The measurements for this reaction were done in "inverse kinematics" at GSI, i.e., not by bombarding an Au-target with protons, but by bombarding a liquid H-target with an 800 MeV/nucleon ^{197}Au beam. As product yields are invariants regarding the system of reference, we can calculate this reaction using the "direct" kinematics, i.e., as an Au-target bombarded with an 800-MeV proton beam. The experimental data are published in Refs. [59, 60].

The mass number distribution of product yields by MCNP6 using the LAQGSM03.03 event-generator is tabulated (in units of barns) in the table entitled **Summary by mass number** of the MCNP6 output file **p800Au_Laq.o** presented in the subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**. It is copied to a separate input file for **xmgrace**, p800Au_A_M6Laq.dat, and the final plot appears in the file p800Au_A_sf4.pdf.

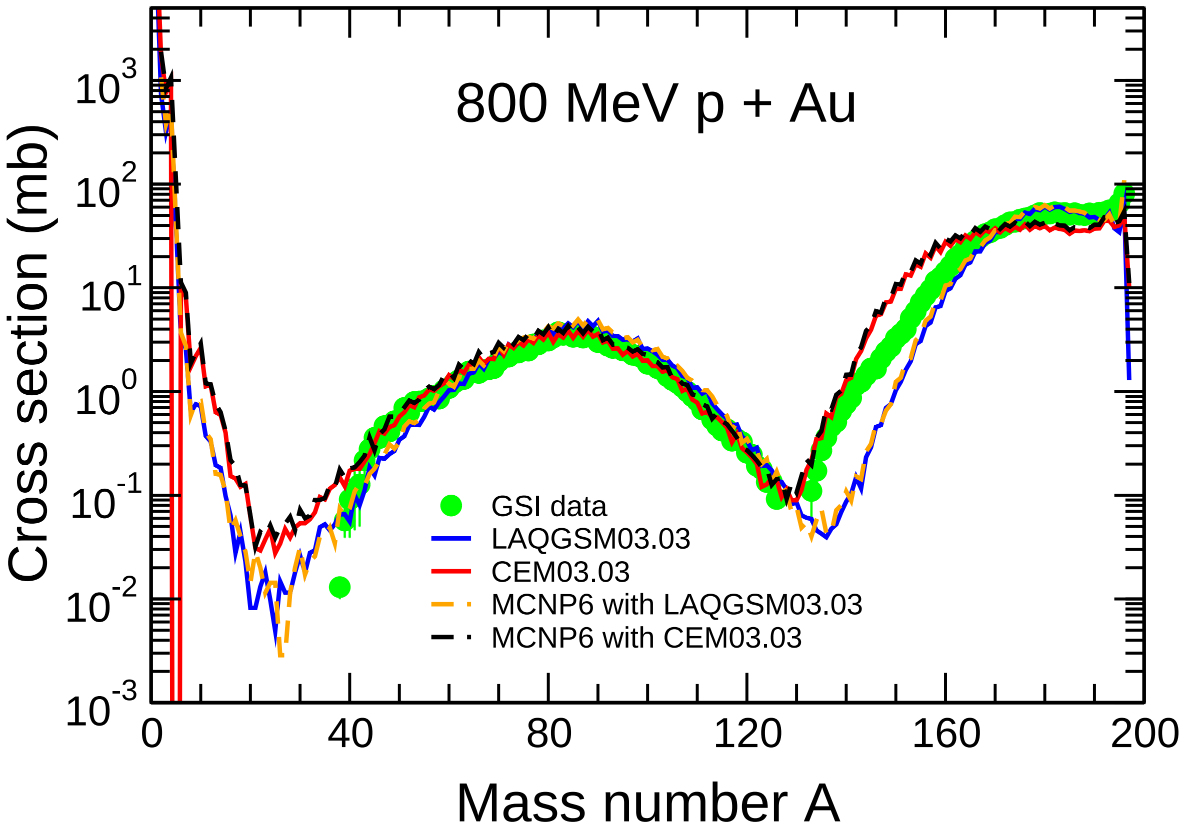

Figure 15: Experimental mass number distribution of product yields [59, 60] (filled circles) from the 800 MeV p + Au reaction compared with results by LAQGSM03.03 [10] and CEM03.03 [6] used as stand alone codes and by MCNP6 using the LAQGSM03.03 and CEM03.03 event-generators, as indicated.

Similar results by MCNP6 using the CEM03.03 event-generator are tabulated (in units of barns) in the table entitled **Summary by mass number** of the MCNP6 output file **p800AU_CEM.o** presented in the same subdirectory and is also copied here to a separate file named p800Au_A_M6CEM.dat.

The file Au800p.SGMno.dat presents results by LAQGSM03.03 used as a stand alone code, while the file ac.dat shows results by CEM03.03 used as a stand alone code. The experimental data [59, 60] for this test-problem are presented in the file ae.dat.

A template for plotting all our results with **xmgrace** is presented in the file p800Au_A_sf4.fig; the pdf file of the figure is: p800Au_A_sf4.pdf. The files with figure are presented together with all files with our calculation results and with experimental data in subdirectory **/VALIDATION_LAQGSM/Experimental_data/p800MeV_Au/**.

Our final results for this test problem are shown in Figure 15. We see that MCNP6 using LAQGSM03.03 describes well the measured [59, 60] yield of nuclides from this reaction, and agrees very well with results obtained with the LAQGSM03.03 event generator used as a stand alone code. MCNP6 using CEM03.03 describes also well the measured [59, 60] yield of nuclides from this reaction, and agrees very well with results obtained with the LAQGSM03.03 event generator used as a stand alone code. Just as expected, we can observe that for this particular problem, the agreement with the measured data is a little better for calculations using the CEM03.03 event generator than in the case of using LAQGSM03.03. This is the reason why we suggest to calculate reactions initiated by nucleons with incident energies above about 3.5 GeV with LAQGSM03.03, while at lower incident energies, to use CEM03.03.

3.13. Test-Problems #13: A) Au559MeVperA_Cu with inxc68; B) Au10600MeVperA_Cu with inxc69; C) Pb3270600Cu with inxc70

This MCNP6 problem tests the applicability of MCNP6 using the LAQGSM03.03 event generator to describe yields of products from heavy-ion induced reactions at relativistic and ultra-relativistic energies over a very large range of incident energies.

Namely, in this test problem, we calculate with MCNP6 using LAQGSM03.03 with the GENXS option the charge-number yield distribution of the products from a thin Cu-target bombarded with relativistic beams of 559 MeV/nucleon and 10.5 GeV/nucleon ^{197}Au ions and similarly with an ultra-relativistic energy of 159 GeV/nucleon beam of ^{208}Pb ions. We compare the MCNP6 results with experimental data and with results by LAQGSM used as a stand-alone code. Such capabilities of MCNP6 are needed for astrophysical applications, particularly for problems of propagation of cosmic rays through matter.

We calculate this test-problem using the GENXS option of MCNP6. As we have presented a detailed description of the use of GENXS option to calculate product yields from thin targets in test-problem #1 of the CEM Testing Primer [5], we do not need to discuss the input and output files for this case. Therefore, we limit ourselves to only providing the text of the input files (let us recall here that the GENXS option of MCNP6 requires a second, auxiliary input file in addition to the main MCNP6 input file), as well as describing where to find the results in the MCNP6 output file.

The main MCNP6 input file while using the LAQGSM03.03 event generator with the GENXS option for the case of 559 MeV/nucleon ^{197}Au + Cu is **Au559MeVperA_Cu**. It uses the auxiliary companion input file **inxc68** required by the GENXS option. The main MCNP6 input file while using the LAQGSM03.03 event generator with the GENXS option for the second case of 10.6 GeV/nucleon ^{197}Au + Cu is **Au10600MeVperA_Cu**. It uses the auxiliary companion input file **inxc69** required by the GENXS option. Finally, for the last reaction, 158 GeV/nucleon ^{208}Pb + Cu, the main MCNP6 input file is **Pb3270600Cu** and its auxiliary companion input file is **inxc70**. All of these are presented in the subdirectory **/VALIDATION_LAQGSM/Inputs/** and are also shown below.

Au559MeVperA_Cu:

```
MCNP6 test: 559 MeV/A Au197 + Cu64 by LAQGSM03.03, nevtype=66
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c --------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
```

```
  3  pz  1.0
  4  so  50.0

c ----------------------------------------------------------------
dbcn 28j 1
  m1 29064  1.0
  sdef erg=110123 par=79197 dir=1 pos=0 0 0 vec 0 0 1
  imp:n 1 1 0
  imp:h 1 1 0
  phys:h 110150
  phys:# 110150
  mode  # n a t d s h
LCA  2 1 5j -1 1j 1    $ use LAQGSM, nevtype = 66                  !!!
lcb  0 0 0 0 0 0
lea  2j 0
c  tropt genxs inxc68  nreact on  nescat off
  tropt genxs inxc68
c ----------------------------------------------------------------
  print 40 110 95
c  nps 100
  nps 100000
  prdmp 2j -1
```

inxc68:

```
MCNP6 test: 559 MeV/A Au197 + Cu64 by LASQGSM03.0, nevtype=66
1 0 1 /
Cross Section Edit
50 0 9 /
5. 10. 15. 20. 25. 30. 35. 40. 45. 50. 55. 60. 65. 70. 75. 80.
85. 90. 95. 100. 150. /
1 5 6 7 8 21 22 23 24 /
```

Au10600MeVperA_Cu:

```
MCNP6 test: 10.6 GeV/A Au197 + Cu64 by LAQGSM03.03, nevtype=66
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c ----------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0
```

```
c -----------------------------------------------------------------
dbcn 28j 1
  m1 29064  1.0
  sdef erg=2088200 par=79197 dir=1 pos=0 0 0 vec 0 0 1
  imp:n 1 1 0
  imp:h 1 1 0
  phys:g 10000
  phys:d 10000
  phys:h 10008
  phys:# 2088208
  mode  # n a t d s h
LCA  2 1 5j -1 1j 1    $ use LAQGSM, nevtype = 66                   !!!
lcb  0 0 0 0 0 0
lea  2j 0
c  tropt genxs inxc69  nreact on  nescat off
  tropt genxs inxc69
c -----------------------------------------------------------------
  print 40 110 95
c  nps 5
  nps 10000
  prdmp 2j -1
```

inxc69:

```
MCNP6 test: 10.6 GeV/A Au197 + Cu64 by LASQGSM03.0, nevtype=66
1 0 1 /
Cross Section Edit
50 0 9 /
5. 10. 15. 20. 25. 30. 35. 40. 45. 50. 55. 60. 65. 70. 75. 80.
85. 90. 95. 100. 150. /
1 5 6 7 8 21 22 23 24 /
```

Pb3270600Cu:

```
MCNP6 test: 158 GeV/A Pb207 + Cu64 by LAQGSM03.03, nevtype=66
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c -----------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0
```

```
c ----------------------------------------------------------------
dbcn 28j 1
  m1 29064  1.0
  sdef erg=32706000 par=82207 dir=1 pos=0 0 0 vec 0 0 1
  imp:n 1 1 0
  imp:h 1 1 0
  phys:g 158008
  phys:d 158008
  phys:h 158008
  phys:# 32706008
  mode  # n a t d s h
LCA  2 1 5j -1 1j 1    $ use LAQGSM, nevtype = 66                  !!!
lcb  0 0 0 0 0 0
lea  2j 0
c  tropt genxs inxc70  nreact on  nescat off
  tropt genxs inxc70
c ----------------------------------------------------------------
  print 40 110 95
  nps 10
c  nps 10000
  prdmp 2j -1
```

inxc70:

```
MCNP6 test: 158 GeV/A Pb207 + Cu64 by LASQGSM03.0, nevtype=66
1 0 1 /
Cross Section Edit
50 0 9 /
5. 10. 15. 20. 25. 30. 35. 40. 45. 50. 55. 60. 65. 70. 75. 80.
85. 90. 95. 100. 150. /
1 5 6 7 8 21 22 23 24 /
```

The measurements for these reactions were done at different laboratories by different teams of authors. So, the 559 MeV/nucleon data were measured at Lawrence Berkeley Laboratory's Bevalac accelerators and the results are published in the paper [61]. The file **559MeV_Au+Cu_exp.dat** presents the measured data for the Cu-target. The data at 10.6 GeV/nucleon were measured at the Brookhaven National Laboratory Alternating Gradient Synchrotron (AGS) accelerator and the results are published in the paper [62]. The file **10.6GeV_Au+Cu_exp.dat** presents the measured data for the Cu-target. At 158 GeV/nucleon, we compare our results with two sets of data, both measured at the CERN Super Proton Synchrotron (SPS). The 2004 data are published in the paper [63]. Part of these measurements obtained for the Cu-target are presented here in the file **PbCu158GeV_exp2004.dat**. The second set of data at 158 GeV/nucleon are published in the 2008 paper [64]. These experimental data are presented here in the file **PbCu158GeV_exp2008.dat**.

The charge number distribution of product yields calculated by MCNP6 using the LAQGSM03.03 event-generator is tabulated (in units of barns) in the table entitled **Summary by charge**

number of the MCNP6 output files **Au559MeVperA_Cu_c.o**, **Au10600MeVperA_Cu_ccc.o**, and **Pb32706000Cu_ccc.o**, at 0.559, 10.6, and 158 GeV/nucleon, respectively, all available in the subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**. Note that heavy-ion reactions at relativistic and ultra-relativistic energies require a long computing time for calculation. This is why we calculated all the three reactions from this test-problem in several steps, using the "continue" option of MCNP6, and using as "auxiliary input files" to continue the calculations the files **inp_Au559**, **inp_1e4**, and **inp_1e4** at 0.559, 10.6, and 158 GeV/nucleon, respectively; all these auxiliary input files are also presented in the subdirectory **/VALIDATION_LAQGSM/Inputs/** together with the main input files listed above. (The first output files for our reactions are **Au559MeVperA_Cu.o**, **Au10600MeVperA_Cu.o**, and **Pb32706000Cu.o**, at 0.559, 10.6, and 158 GeV/nucleon, respectively; all of them are presented in the subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**.)

To help plot our results with **xmgrace**, the MCNP6 results are copied to separate files AuCu559MeV_M6Laq.dat, AuCu10.6GeV_M6Laq.dat, and PbCu158GeV_M6Laq.dat at 0.559, 10.6, and 158 GeV/nucleon, respectively.

Results by LAQGSM03.03 used as a stand-alone code are presented here in the files AuCu559MeV_noGPL.dat, AuCu10.6GeV_noGPL.dat, and PbCu158GeV_noGPL.dat at 0.559, 10.6, and 158 GeV/nucleon, respectively.

Templates for plotting our results with **xmgrace** are presented in the files AuCu559MeV.fig, Au_Cu_10.6GeV.fig, and Pb_Cu_158GeV.fig at 0.559, 10.6, and 158 GeV/nucleon, respectively. pdf files with the final figures are AuCu559MeV.pdf, Au_Cu_10.6GeV.pdf, and Pb_Cu_158GeV.pdf at 0.559, 10.6, and 158 GeV/nucleon, respectively, with the summary file PbAu_Cu.pdf showing all three reactions in one figure. The files with figures are presented together with all files including calculation results and experimental data in subdirectory
/VALIDATION_LAQGSM/Experimental_data/Au_and_Pb_on_Cu/.

Figure 16 shows our final results for this test-problem. Let us note that the MCNP6 results shown in Figure 16 represent cross sections of the products from both the projectile and target nuclei, while the LAQGSM03.03 used as stand alone calculated only fragmentation products from the bombarding nuclei. This is why we see a good agreement between the MCNP6 and LAQGSM03.03 results and the measured projectile fragmentation cross sections (i.e., for products heavier than Cu), and a much higher MCNP6 yield of products lighter than Cu than the one calculated by LAQGSM03.03 from only the projectiles.

3.14. Test-Problems #14: C290C with inp_10e7

This MCNP6 problem tests the applicability of MCNP6 using the LAQGSM03.03 event generator to calculate production of neutrons from intermediate energy carbon-beam induced reactions for different NASA, medical (cancer treatment with a carbon-beam), FRIB (Facility for Rare Isotope Beams), and for some other U.S. DOE applications.

This test calculates with MCNP6 double-differential spectra of neutrons at 5, 10, 20, 30, 40, 60, and 80 degrees from interaction of a 290 MeV/nucleon ^{12}C beam with a thin ^{12}C target and compares the results with experimental data, with results by the LAQGSM03.03 event generator used as a stand alone code, as well as with results by the Japan version of the Quantum Molecular Dynamics (QMD) model coupled with the statistical decay model in the code JQMD [66], the Oak Ridge intranuclear cascade model HIC by Bertini *et al.* [67] followed by a standard evaporation calculation with the EVAP-4 code [51], and by a Los Alamos version

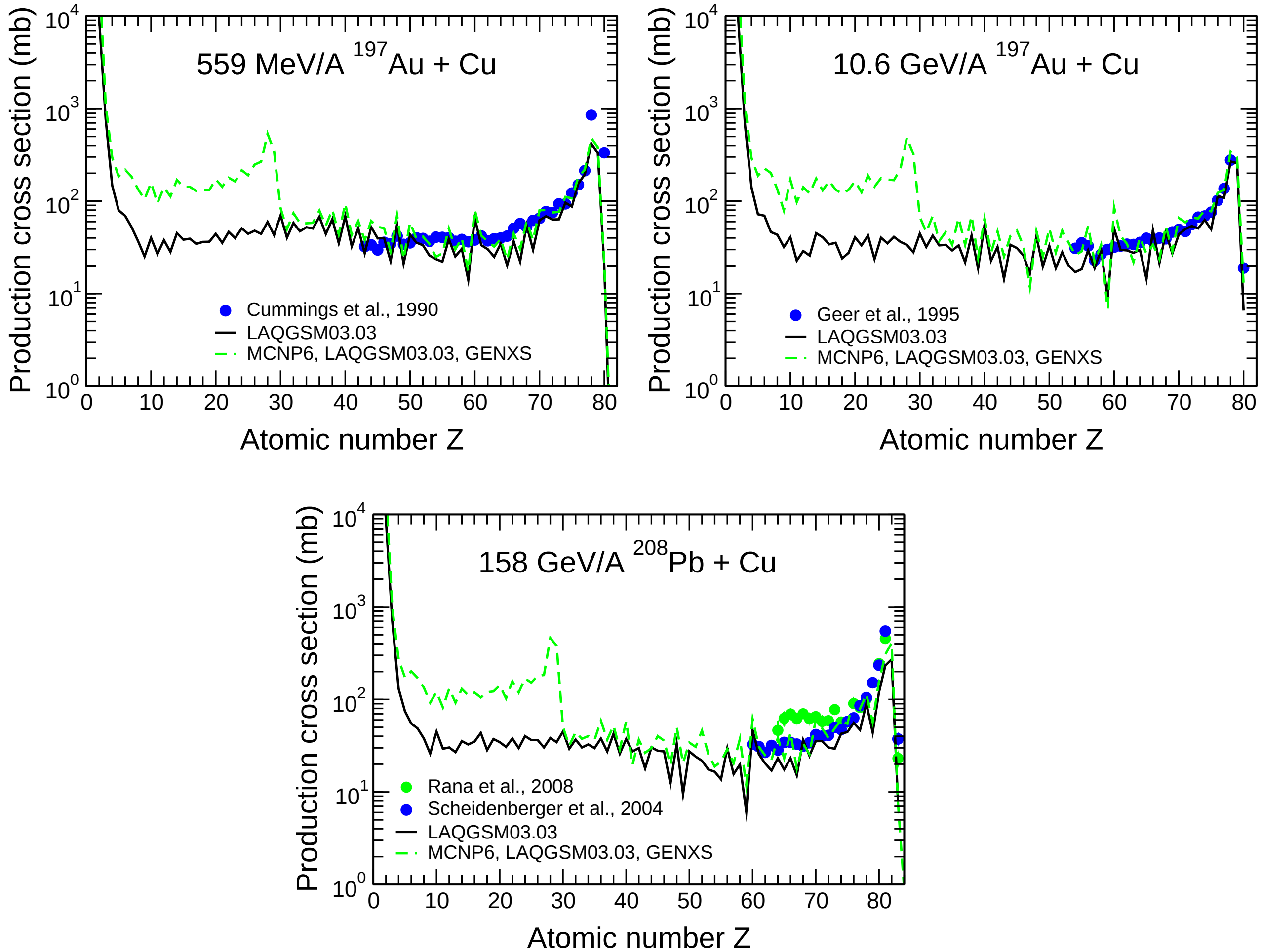

Figure 16: Experimental charge distributions of product yields [61]-[64] (color filled circles) from 559 MeV/A ^{197}Au + Cu, 10.6 GeV/A ^{197}Au + Cu, and 158 GeV/A ^{208}Pb + Cu reactions compared with results by LAQGSM03.03 [10] used as a stand alone code and by MCNP6 using the LAQGSM03.03 event-generator, as indicated.

of the Quark-Gluon String Model contained in the code LAQGSM03 [41] as published in Ref. [68]

We calculate this test-problem using the **NOACT=-2** option for the 8th parameter of the **LCA** card of the MCNP6 input file. As we have presented a detailed description of the use of **NOACT=-2** option to calculate particle spectra from thin targets in test-problem #6 of the CEM Testing Primer [5], and have provided additional examples of its use in test problems #7 and #8 of Ref. [5], we do not need to discuss in detail the input and output files for this case. Therefore, we limit ourselves to only providing the text of the input file as well as describing where to find the results in the MCNP6 output files.

The input file for this test problem is **C290C**. It is presented in the subdirectory **/VALIDATION_LAQGSM/Inputs/** and is also shown below together with the two line auxiliary input file **inp_10e7** used to perform calculations with the "continue" option of MCNP6.

C290C:

```
MCNP6 test with LAQGSM03.03: 290 MeV/A C12 + C12 -> n spectra
```

```
c as test-problem for cancer treatment with C12-ions application
1   1  -1.8  -501        imp:n=1
2   0         501  -502  imp:n=1
99  0         502        imp:n=0

501   so 0.01
502   so 1
c
c  tally surfaces
c
250    kz    0    0.001906278     1  $  2.5 deg
750    kz    0    0.017332380     1  $  7.5 deg
125    kz    0    0.049148523     1  $ 12.5 deg
175    kz    0    0.099413326     1  $ 17.5 deg
225    kz    0    0.171572875     1  $ 22.5 deg
275    kz    0    0.270990054     1  $ 27.5 deg
325    kz    0    0.405858517     1  $ 32.5 deg
375    kz    0    0.588790706     1  $ 37.5 deg
425    kz    0    0.839662820     1  $ 42.5 deg
575    kz    0    2.463912811     1  $ 57.5 deg
625    kz    0    3.690172332     1  $ 62.5 deg
775    kz    0    20.34649121     1  $ 77.5 deg
825    kz    0    57.69548054     1  $ 82.5 deg

m1  6012 1
lca 7j -2 j 1    $ LAQGSM
c nps 1000
nps 1e7
prdmp 2j -1
sdef par=6012 erg=3480 vec=0 0 1 dir 1
phys:# 3480
phys:h 2000
phys:n 2000
phys:a 2000
phys:d 2000
phys:t 2000
phys:s 2000
phys:/ 2000
phys:z 2000
mode n h # a d t s / z *
c
f1:n  502
fs1   -250 -750 -125 -175 -225 -275 -325 -375 -425 -575 -625 -775 -825 T
c The following Segment Divisor card is needed to get 1/sr for n-spectra
sd1   0.00598020  $ 2pi(cos0 -cos2.5)
      0.04777332  $ 2pi(cos2.5 - cos7.5)
      0.09518306  $ 2pi(cos7.5 - cos12.5)
```

```
      0.14186840  $ 2pi(cos12.5 - cos17.5)
      0.18747403  $ 2pi(cos17.5 - cos22.5)
      0.23165287  $ 2pi(cos22.5 - cos27.5)
      0.27406869  $ 2pi(cos27.5 - cos32.5)
      9.31439869  $ 2pi(cos32.5 - cos37.5)
      0.35233592  $ 2pi(cos37.5 - cos42.5)
      1.25649713  $ 2pi(cos42.5 - cos57.5)
      0.47470090  $ 2pi(cos57.5 - cos62.5)
      1.54132190  $ 2pi(cos62.5 - cos77.5)
      0.53980995  $ 2pi(cos77.5 - cos82.5)
      7.10330556  $ 2pi(cos82.5 - cos180)
      12.5663706  $ 4pi
c     Boundaries of the neutron energy bins: 0-1 MeV; 1-3 MeV, ...
e1    1     3     5     7     9     11    13    15    17    19
      22.5  27.5  32.5  37.5  42.5  47.5  52.5  57.5  62.5  67.5
      72.5  77.5  82.5  87.5  92.5  97.5  105   115   125   135
      145   155   165   175   185   195   205   215   225   235
      245   255   265   275   285   295   305   315   325   335
      345   355   365   375   385   395   405   415   425   435
      445   455   465   475   485   495   505   515   525   535
      545   555   565   575   585   595   605   615   625   635
      645   655   665   675   685   695   705   715   725   735
      745   755   765   775   785   795   805   815   825   835
      845   855   865   875   885   895   905   915   925   935
      945   955   965   975   985   995  1025  1075  1125  1175
     1225  1275  1325  1375  1425  1475  1525  1575  1625  1675
     1725  1775  1825  1875  1925  1975
em1 822.158 135r $ multiply to sig_inelastic = 822.158 mb, as predicted
c                by LAQGSM03.03, file C290C_n.out, Nov 30 16:30. Needed
c                to get the spectra in [mb/sr/MeV], after dividig the flux
c                to the energy bins, to get [1/MeV]
c
c
e0   2000
f11:n   502
f21:h   502
f31:d   502
f41:t   502
f51:s   502
f61:a   502
f71:/   502
f81:z   502
f91:*   502
dbcn  20j  0  7j  1  2j  0  1
```

inp_10e7:

```
continue
nps 10000000
```

The experimental data for this problem were measured at the Heavy Ion Medical Accelerator in Chiba (HIMAC) facility of the National Institute of Radiological Sciences (NIRS), Japan and are published in the paper [65].

Experimental spectra of neutrons at 5, 10, 20, 30, 40, 60, and 80 degrees, $d^2\sigma/dT/d\Omega$, in units of [mb/MeV/sr] as functions of the neutron energy in [MeV] are presented in the files 11.dat, 12.dat, 13.dat, 14.dat, 15.dat, 16.dat, and 17.dat, respectively.

The final MCNP6 output file **C290C_c.o** is presented in the subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**. Neutron spectra as calculated by MCNP6 at 5, 10, 20, 30, 40, 60, and 80 ($\pm$2.5) degrees are tabulated in units of [mb/sr/projectile] as segments for tally 1, where the segments corresponding to our angles are, respectively:
1) segment: 250 -750
2) segment: 250 750 -125
3) segment: 250 750 125 175 -225
4) segment: 250 750 125 175 225 -325
5) segment: 250 750 125 175 225 325 375 -425
6) segment: 250 750 125 175 225 325 375 425 575 -625
7) segment: 250 750 125 175 225 325 375 425 575 625 775 -825 .

Let us mention that **C290C_c.o** was calculated with the "continue" option, using the auxiliary two-line input file **inp_10e7**; the first MCNP6 output file calculated with the main input file, **C290C**, is: **C290C.o**.

Note that to get the units of [mb] needed for the absolute normalization of the MCNP6 spectra to the total reaction cross section, we used the Energy Multiplier card **EM1** in our input file **C290C** with the value 822.158 on it for all the 136 energy bins of our tally **F1**: 822.158 is the value of the total inelastic (reaction) cross section in [mb] as predicted by LAQGSM03.03 used for this reaction as a stand alone code.

Note that in a similar manner, to get the units of [1/sr] for the calculated spectra, we used in our input file the Segment Divisor card **SD1** with the corresponding values of the solid angles for each "segment" identifying the needed angles. Finally, to get the calculated double differential neutron spectra $d^2\sigma/dT/d\Omega$ at these angles in conventional units of [mb/sr/MeV], we divide the tables from the MCNP6 output file at the "segments" described above to the values of the energy bins; we do this after all the MCNP6 calculations are completed with a little routine we wrote especially for this division.

The final MCNP6 neutron spectra at 5, 10, 20, 30, 40, 60, and 80 degrees obtained as described above are copied here to separate files noact_5.dat, noact_10.dat, noact_20.dat, noact_30.dat, noact_40.dat, noact_60.dat, and noact_80.dat, respectively.

Besides the MCNP6 results, for comparison, we present here also results by LAQGSM03.03 used as a stand alone code (files L0303_5.dat, L0303_10.dat, L0303_20.dat, L0303_30.dat, L0303_40.dat, L0303_60.dat, L0303_80.dat, respectively).

In addition, for comparison, we present here also results by the Japan version of the Quantum Molecular Dynamics (QMD) model coupled with the statistical decay model in the code JQMD [66], the Oak Ridge intranuclear cascade model HIC by Bertini *et al.* [67] followed by a standard evaporation calculation with the EVAP-4 code [51], and by a Los Alamos version of the Quark-Gluon String Model contained in the code LAQGSM03 [41] as published in Ref. [68]. Neutron spectra at 5, 10, 20, 30, 40, 60, and 80 degrees by QMD, HIC, and LAQGSM03 codes as published in the listed above paper are presented here in the files: Q11.dat, Q12.dat, Q13.dat, Q14.dat, Q15.dat, Q16.dat, Q17.dat (for QMD), H11.dat, H12.dat, H13.dat, H14.dat, H15.dat, H16.dat, H17.dat (for HIC) L11.dat, L12.dat, L13.dat, L14.dat, L15.dat, L16.dat, and L17.dat (for LAQGSM03), respectively.

The file C290C_n_noact.fig is a template for plotting the figure of comparison with **xmgrace**. The pdf file for the figure is C290C_n_noact.pdf. The files with figure are presented together with all files with the calculation results and with experimental data in subdirectory **/VALIDATION_LAQGSM/Experimental_data/c290c/**.

Our final results for this test problem are shown in Figure 17. We see that MCNP6 using LAQGSM03.03 describes well the measured [65] neutron spectra from this C+C reaction, and agrees very well with results obtained with the LAQGSM03.03 event generator used as a stand alone code and with published [68] results obtained with the code JQMD [66], the Oak Ridge intranuclear cascade model HIC by Bertini *et al.* [67] followed by a standard evaporation calculation with the EVAP-4 code [51], and by a Los Alamos version of the Quark-Gluon String Model contained in the code LAQGSM03 [41]

3.15. Test-Problems #15: p400GeVTa_GENXSREP with inxc3

This MCNP6 problem is to test the applicability of MCNP6 using the LAQGSM03.03 event generator to describe double-differential spectra of particles produced in the ultra-relativistic reaction 400 GeV p + ^{181}Ta. Such reactions are of interest to several astrophysical and space applications. Note that, to the best of our knowledge, the spectra tested here at 400 GeV represent published experimental data at the highest energy where we expect LAQGSM03.03 to still work reliably, i.e., below $\sim$ 1 TeV/nucleon: We do not know of any experimental spectra at incident energies above 400 GeV but below 1 TeV. Such reactions are also of great academic interest in studying the production of so called **cumulative particles** at ultra-relativistic energies, i.e., energetic particles at backward angles in the kinematic region forbidden in interactions of the projectile with free stationary nucleons of the target nucleus. It is believed that **cumulative particles** contain information needed for the study of the high momentum component of nuclear wave functions, or of collective phenomena in nuclei, or of quark and gluon degrees of freedom.

We have utilized this test-problem to understand and to fix a problem observed while using the GENXS option of MCNP6 at ultra-relativistic energies (a previously unobserved "bug" in the GENXS option of MCNP6 at high-energies was found and fixed recently by Dick Prael; see Section 2.3 in Ref. [20] for more details).

The current problem has also an additional aim of testing the very recent capability of MCNP6 to tally separately production of particles and antiparticles (π^+ and π^-) using the DBCN(27) = -1 option, a feature not available in MCNPX and in earlier versions of MCNP6 (see Section 3.3 with the test problem **inp75cor_bREP**, where we discussed the absence of such a capability as a deficiency of earlier versions of MCNP6, addressed and solved by Grady Hughes in the latest version of MCNP6).

This test calculates with MCNP6, using LAQGSM03.03, spectra of p, π^+, π^-, K^+, K^-, anti-protons, d, t, ^{3}He, and ^{4}He at 70, 90, 118, 137, and 160 degrees from interactions of 400 GeV protons with ^{181}Ta. It compares the MCNP6 results with experimental data [69, 70] and with results by the LAQGSM03.03 event generator used as a stand alone code and with several published results [71] by an older version of LAQGSM, LAQGSM03.01 [7].

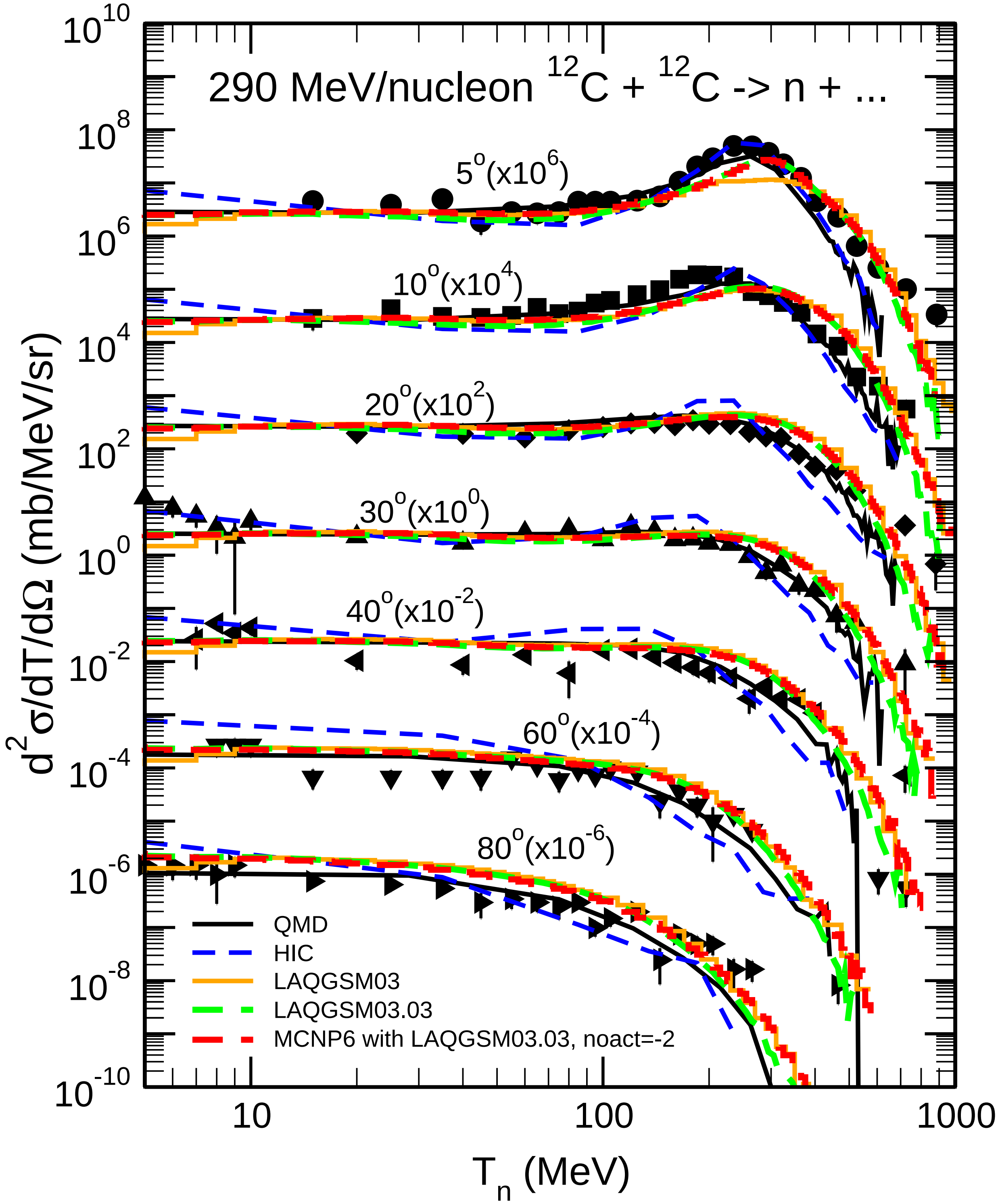

Figure 17: Experimental neutron spectra [65] at 5, 10, 20, 30, 40, 60, and 80 degrees (symbols) from a thin ^{12}C target bombarded with a 290 MeV/nucleon ^{12}C beam compared with results by the Japan version of the Quantum Molecular Dynamics (QMD) model coupled with the statistical decay model in the code JQMD [66], the Oak Ridge intranuclear cascade model HIC by Bertini *et al.* [67] followed by a standard evaporation calculation with the EVAP-4 code [51], and by a Los Alamos version of the Quark-Gluon String Model contained in the code LAQGSM03 [41] as published in Ref. [68], as well as with our current calculations by LAQGSM03.03 [10] used as a stand alone code and by MCNP6 using the LAQGSM03.03 event-generator, as indicated.

We calculate this test-problem using the GENXS option of MCNP6. As we have presented a detailed description of the use of the GENXS option to calculate particle spectra from thin targets in test-problem #5 of the CEM Testing Primer [5], we do not need to discuss the input and output files for this case. Therefore, we limit ourselves to only providing the text of the input files (let us recall here that the GENXS option of MCNP6 requires a second, auxiliary input file in addition to the main MCNP6 input file), as well as describing where to find the results in the MCNP6 output file.

The main MCNP6 input file for the case of using the GENXS option is **p400GeVTa_GENXSREP**. It uses the auxiliary companion input file **inxc388** required by the GENXS option. Both of these are presented in the subdirectory **/VALIDATION_LAQGSM/Inputs/** and are also shown below.

p400GeVTa_GENXSREP:

```
MCNP6 test: 400 GeV p + Ta181 by LAQGSM03.03, nevtype=66
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c --------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c --------------------------------------------------------------
dbcn 28j 1
  m1 73181  1.0
  sdef erg=400000 par=h dir=1 pos=0 0 0 vec 0 0 1
  imp:n 1 1 0
  imp:h 1 1 0
  phys:n 400008
  phys:h 400008
  phys:/ 400008
  phys:* 400008
  phys:z 400008
  phys:k 400008
  phys:? 400008
  phys:q 400008
  phys:g 400008
  phys:d 400008
  phys:t 400008
  phys:s 400008
  phys:a 400008
  phys:# 400008
  mode  n h / * z k ? q g d t s a #
LCA  2 1 5j -1 1j 1    $ use LAQGSM, nevtype = 66                  !!!
```

```
lcb  0 0 0 0 0 0
lea  2j 0
  tropt genxs inxc38  nreact on  nescat off
c  tropt genxs inxc38
c -----------------------------------------------------------------
  print 40 110 95
  nps 1000
c  nps 700000
  prdmp 2j -1
```

inxc38:

```
MCNP6 test: invariant particle spectra from 400 GeV p+Ta181 by LAQGSM03.03
1 0 0 /
Cross Section Edit
150 -11 10 /
   1.     3.     5.     7.     9.    11.    13.    15.    17.    19.
  22.    27.    32.    37.    42.    47.    52.    57.    62.    67.
  72.    77.    82.    87.    92.    97.   105.   125.   135.   145.
 155.   165.   175.   185.   195.   205.   215.   225.   235.   245.
 255.   265.   275.   285.   295.   305.   315.   325.   335.   345.
 355.   365.   375.   385.   395.   405.   415.   425.   435.   445.
 455.   465.   475.   485.   495.   505.   515.   525.   535.   545.
 555.   565.   575.   585.   595.   605.   615.   625.   635.   645.
 655.   665.   675.   685.   695.   705.   715.   725.   735.   745.
 755.   765.   775.   785.   795.   805.   815.   825.   835.   845.
 855.   865.   875.   885.   895.   905.   915.   925.   935.   945.
 955.   965.   975.   985.   995.  1025.  1075.  1125.  1175.  1225.
1275.  1325.  1375.  1425.  1475.  1525.  1575.  1625.  1675.  1725.
1775.  1825.  1875.  1925.  1975.  2025.  2075.  2125.  2175.  2225. /
163. 157. 140. 134. 121. 115. 93. 87. 73. 67. 0./
5 6 7 15 16 19 21 22 23 24 /
```

The experimental data for this problem were measured at the Fermi National Accelerator Laboratory and are published in Refs. [69, 70].

For brevity sake, here, we compare our results with the measured spectra of only K^+, t, π^+, and π^-, although we calculated spectra of several other particles from this reaction, as mentioned above. Experimental K^+ invariant spectra per nucleon of the target, i.e., $(1/A)Ed^3\sigma/d^3p$ in units of [mb c^3/sr/GeV^2/nucleon] as functions of K^+ momentum in [GeV/c] at 90 and 118 degrees are presented here in the files ptakp90e.dat and ptakp118e.dat, respectively. Experimental invariant spectra of tritons, in the same units, at 70, 90, 118, 137, and 160 degrees are presented here in the files ptat70e.dat, ptat90e.dat, ptat118e.dat, ptat137e.dat, and ptat160e.dat, respectively. Experimental invariant spectra of π^+, in the same units, at 70, 90, 118, 137, and 160 degrees are presented here in the files ptapip70e.dat, ptapip90e.dat, ptapip118e.dat, ptapip137e.dat, and ptapip160e.dat, respectively. Finally, experimental invariant spectra of π^-, in the same units, at 70, 90, 137, and 160 degrees are presented here in the files ptapim70e.dat, ptapim90e.dat, ptapim137e.dat, and ptapim160e.dat, respectively.

K^+ double-differential spectra calculated by MCNP6 using LAQGSM03.03 with the GENXS option at 160, 137, and 118 (±3) degrees are tabulated in units of [b/sr/MeV] in the 2nd, 4th, and 6th pairs of columns of the first part of the **k_plus production cross section** table of the final MCNP6 output file **p400GeVTa_GENXSREP_8c.o** (after the K^+ energy tabulated in the 1st column) and for 40 and 20 degrees, in the 1st and 3rd pairs of columns of the second part of the same tables, following the K^+ energy tabulated in the 1st column. We present the final MCNP6 output file in the subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**. Note that the MCNP6 calculations for this test-problem were performed in several steps, using the "continue" option. The first MCNP6 output file is **p400GeVTa_GENXSREP.o**; it is presented in the same Templates subdirectory.

Triton, positive pion, and negative pion spectra by MCNP6 are tabulated in exactly the same manner in the same output file in the tables labeled as **triton production cross section**, **pi_plus production cross section**, and **pi_minus production cross section**, respectively. To convert the MCNP6 double-differential spectra tabulated in the output file in units of [b/sr/MeV] into "invariant spectra", $(1/A)Ed^3\sigma/d^3p$ in units of [mb c^3/sr/GeV^2/nucleon], we wrote a short auxiliary routine especially for this purpose and have performed the conversion separately, after all MCNP6 calculations were completed. To help plotting the invariant spectra with **xmgrace** (see files pTa_Kp.pdf, pTa_t.pdf, pTa_pip.pdf, and pTa_pim.pdf), the MCNP6 "invariant spectra", i.e., already after the conversion, are copied here to separate files ptakp70_GREP.dat, ptakp90_GREP.dat, ptakp118_GREP.dat, ptakp137_GREP.dat, ptakp160_GREP.dat, for MCNP6 invariant spectra of K^+ at 70, 90, 118, 137, and 160 (±3) degrees, respectively. In a similar manner, the MCNP6 invariant spectra of t, π^+, and π^- at 70, 90, 118, 137, and 160 (±3) degrees are copied in the separate files: ptat70_GREP.dat, ptat90_GREP.dat, ptat118_GREP.dat, ptat137_GREP.dat, ptat160_GREP.dat, ptapip70_GREP.dat, ptapip90_GREP.dat, ptapip118_GREP.dat, ptapip137_GREP.dat, ptapip160_GREP.dat, ptapim70_GREP.dat, ptapim90_GREP.dat, ptapim118_GREP.dat, ptapim137_GREP.dat, and ptapim160_GREP.dat, respectively.

Besides the MCNP6 results, for t, π^+, and π^- we show here also recent calculations by LAQGSM03.03 used as a stand alone code, while for K^+, for comparison, we show the 2005 results by an older version of LAQGSM, LAQGSM03.01 [7] as published in Ref. [71].

Invariant spectra of t, π^+, and π^- by LAQGSM03.03 used as a stand alone code at 70, 90, 118, 137, and 160 degrees are presented here in the files: ptat70_03.dat, ptat90_03.dat, ptat118_03.dat, ptat137_03.dat, ptat160_03.dat, ptapip70_03.dat, ptapip90_03.dat, ptapip118_03.dat, ptapip137_03.dat, ptapip160_03.dat, ptapim70_03.dat, ptapim90_03.dat, ptapim118_03.dat, pta pim137_03.dat, and ptapim160_03.dat, respectively. The 2005 LAQGSM03.01 invariant spectra of K^+ at 70, 90, 118, 137, and 160 degrees are presented here in the files: ptakp70_01.dat, ptakp90_01.dat, ptakp118_01.dat, ptakp137_01.dat, and ptakp160_01.dat, respectively.

The files pTa_Kp.fig, pTa_t.fig, pTa_pip.fig, and pTa_pim.fig are templates for plotting the K^+, t, π^+, and π^- invariant spectra with **xmgrace**. The pdf files of figures with these spectra are pTa_Kp.pdf, pTa_t.pdf, pTa_pip.pdf, and pTa_pim.pdf. The summary file p400GeV_Ta.pdf shows all invariant spectra, of K^+, t, π^+, and π^- on a single plot. The files with our figures are presented together with all files with calculation results and with experimental data in subdirectory **/VALIDATION_LAQGSM/Experimental_data/p400GeV_Ta/**.

Our final results for this test problem are shown in Figure 18. We see that after a "bug" in the initial version of MCNP6 affecting the results from such reactions was fixed by Dr. Dick Prael (see Section 2.4 of Ref. [20] for more details) MCNP6 using LAQGSM03.03 describes well the measured spectra of cumulative particles from this ultra-relativistic reaction, and agrees

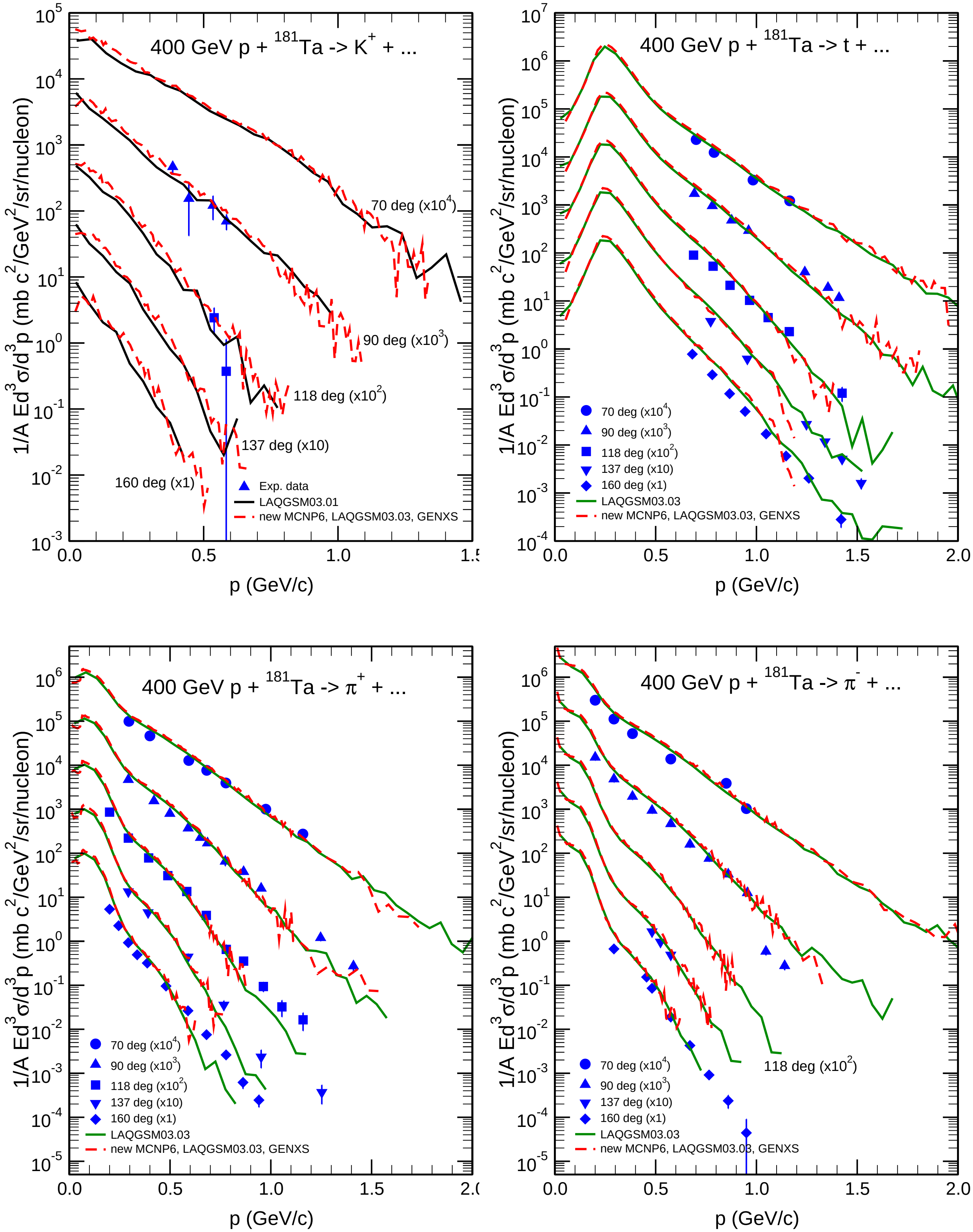

Figure 18: Experimental invariant spectra [69, 70] of K^+, t, π^+, and π^- from the reaction 400 GeV $p+^{181}$Ta (symbols) compared with the current results by LAQGSM03.03 [10] used as a stand alone code and by MCNP6 using the LAQGSM03.03 event-generator, and with our 2005 results by LAQGSM03.01 [7] from Ref. [71], as indicated.

well with results by the LAQGSM03.03 event generator used as a stand alone code and by the older LAQGSM03.01 [7]. In addition, we see that after the problem of MCNP6 tallying particles separately from antiparticles was solved by Dr. Grady Hughes, as discussed above in Section 3.3, the current version of MCNP6 is able to describe spectra of π^+ separately from those of π^-; that was not possible in the initial version of MCNP6.

3.16. Test-Problems #16: Ca140MeVperA_Be with inxc69

This MCNP6 problem is to test the applicability of MCNP6 using the LAQGSM03.03 event generator to describe yields of products from heavy-ion induced reactions of interest for different applications, including the Facility for Rare Isotope Beams (FRIB), an update and continuation of the initial U.S. DOE project known as "Rare Isotope Production" (RIA).

Namely, in this test problem, we calculate with MCNP6 using LAQGSM03.03 with the GENXS option the mass-number yield distribution of the Si-ions from a thin ^{9}Be target bombarded with a beams of 140 MeV/nucleon ^{40}Ca ions. We compare our MCNP6 results with calculations by LAQGSM03.03 used as a stand alone code (presented here in the file LAQ.dat) and with the recent experimental data published in the PhD thesis of Dr. Michal Mocko [72] (presented here in the file exp.dat).

In addition, we compare our MCNP6 calculations also with results by several other models as published in Michal Mocko's PhD thesis by namely, with calculations using the known and widely used systematics EPAX of K. Summerer and B. Blank [73] (presented here in the file epax.dat); the semi-phenomenological model ABRABLA by J.-J. Gaimard and K.-H. Schmidt [74] (presented here in the file aa.dat); the Heavy-Ion Phase-Space Exploration (HIPSE) model by Denis Lacroix *et al.* [75] (presented here in the file hipse.dat); and the Antisymmetrized Molecular Dynamics (AMD) model by Akira Ono and Hisashi Horiuchi [76] (presented here in the file amd.dat).

We calculate this test-problem using the GENXS option of MCNP6. As we have presented a detailed description of the use of GENXS option to calculate product yields from thin targets in test-problem #1 of the CEM Testing Primer [5], we do not need to discuss the input and output files for this case. Therefore, we limit ourselves to only providing the text of the input files (let us recall here that the GENXS option of MCNP6 requires a second, auxiliary input file in addition to the main MCNP6 input file), as well as describing where to find the results in the MCNP6 output file.

The main MCNP6 input file while using the LAQGSM03.03 event generator with the GENXS option is **Ca140MeVperA_Be**. It uses the auxiliary companion input file **inxc69** required by the GENXS option. Both of these are presented in the subdirectory **/VALIDATION_LAQGSM/Inputs/** and are also shown below.

Ca140MeVperA_Be:

```
MCNP6 test: 140 MeV/A Ca40 + Be9 by LAQGSM03.03, nevtype=66
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c --------------------------------------------------------------
  1  cz  4.0
```

```
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c -----------------------------------------------------------------
dbcn 28j 1
  m1 04009  1.0
  sdef erg=5600 par=20040 dir=1 pos=0 0 0 vec 0 0 1
  imp:n 1 1 0
  imp:h 1 1 0
  phys:g 200
  phys:d 200
  phys:h 200
  phys:# 5600
  mode  # n a t d s h
LCA  2 1 5j -1 1j 1    $ use LAQGSM, nevtype = 66                  !!!
lcb  0 0 0 0 0 0
lea  2j 0
  tropt genxs inxc69  nreact on  nescat off
c  tropt genxs inxc69
c -----------------------------------------------------------------
  print 40 110 95
c  nps 1000
  nps 10000000
  prdmp 2j -1
```

inxc69:

```
MCNP6 test: 10.6 GeV/A Au197 + Cu64 by LASQGSM03.0, nevtype=66
1 0 1 /
Cross Section Edit
50 0 9 /
5. 10. 15. 20. 25. 30. 35. 40. 45. 50. 55. 60. 65. 70. 75. 80.
85. 90. 95. 100. 150. /
1 5 6 7 8 21 22 23 24 /
```

The MCNP6 output file, **Ca140MeVperA_Be.o** in presented in the subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**. The cross sections for the production of different isotopes of Si are printed (in barns) in the Z=14 portion of the table entitled **Distribution of residual nuclei**, and, to help plot these results with **xmgrace**, are also copied here to a separate file named M6GENXS.dat.

A template for plotting all these results with **xmgrace** is presented in the file 140MeV_Ca40Be9_SiREP.fig. The file 140MeV_Ca40Be9_SiREP.pdf shows the final figure obtained with **xmgrace**. The files with figure are presented together with all files with calculation results and with the measured data in subdirectory **/VALIDATION_LAQGSM/Experimental_data/Ca140 MeVperA_Be/**.

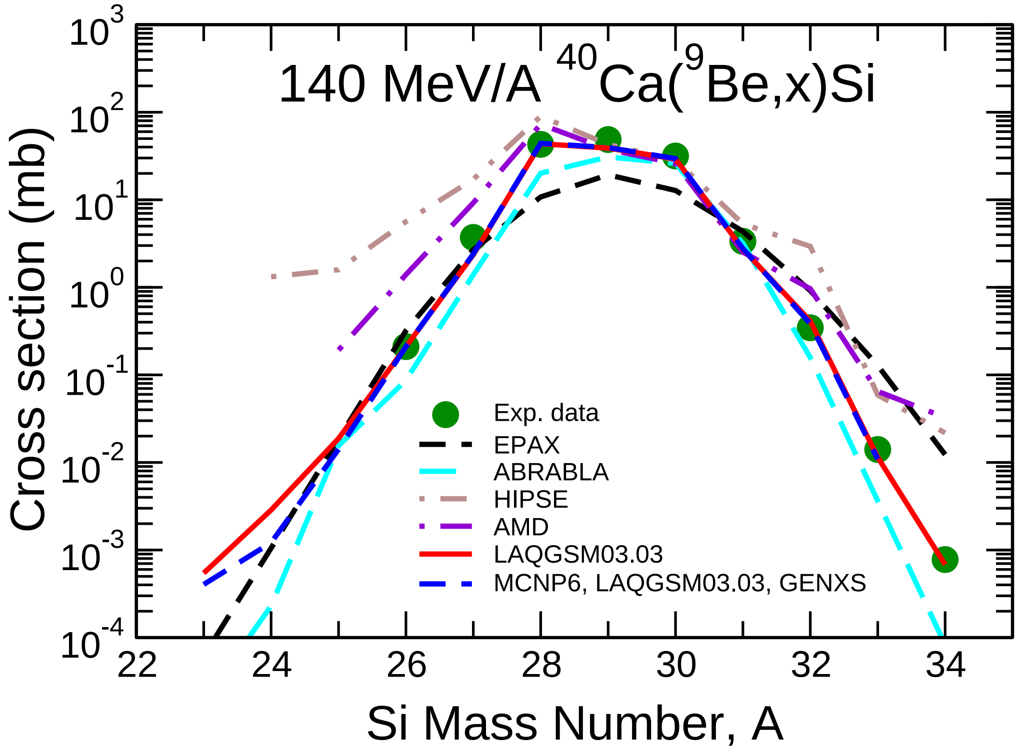

Figure 19: Experimental mass number distribution of the Si ions yields [72] (green filled circles) from the 140 MeV/A ^{40}Ca + ^{9}Be reaction compared with results by EPAX [73], ABRABLA [74], HIPSE [75], and AMD [76] from [72], as well as with the predictions by LAQGSM03.03 [10] used as a stand alone code and by MCNP6 using the LAQGSM03.03 event-generator, as indicated.

Our final results for this test problem are shown in Figure 19. We see that MCNP6 using LAQGSM03.03 describes well the measured yield of Si-ions [72] and agrees very well with results obtained with the LAQGSM03.03 event generator used as a stand alone code and with results by EPAX [73], ABRABLA [74], HIPSE [75], and AMD [76] published in Ref. [72].

3.17. Test-Problems #17: bg4.5C_pi_Laq with inxs025

This MCNP6 problem is to test a very recent extension of MCNP6 by Dick Prael using the LAQGSM03.03 event generator to describe double-differential spectra of particles produced in reactions induced by high-energy bremsstrahlung photons on thin targets. Such reactions are of interest to several astrophysical and space applications, as well as for the Continuous Electron Beam Accelerator Facility (CEBAF) in Newport News, VA, upgraded recently to be able to accelerate electron beams to energies up to 12 GeV.

This test calculates with MCNP6 using LAQGSM03.03 spectra of p, π^+, and π^-, at 30 (20, for pions), 60, 90, 120, and 160 (for protons) degrees from interactions of bremsstrahlung photons with the maximum energy of $E_0 = 4.5$ GeV with ^{12}C. It compares the MCNP6 results with available experimental data and with results by the LAQGSM03.03 event generator used as a stand alone code. Note that, to the best of our knowledge, the particle spectra tested here at $E_0 = 4.5$ GeV represent actually examples of experimental spectra of particles from reactions induced by bremsstrahlung gammas on nuclei with the highest energy, as available in the literature now. This is, the current problem tests MCNP6 against measured spectra of particles from reactions induced by bremsstrahlung gammas with the highest maximum energy published so far in the literature.

We calculate this test-problem using the GENXS option of MCNP6. As we have presented a detailed description of the use of the GENXS option to calculate particle spectra from thin targets in test-problem #5 of the CEM Testing Primer [5], we do not need to discuss the input and output files for this case. Therefore, we limit ourselves to only providing the text of the input files (let us recall here that the GENXS option of MCNP6 requires a second, auxiliary input file in addition to the main MCNP6 input file), as well as describing where to find the results in the MCNP6 output file.

The main MCNP6 input file for the case of using the GENXS option is **bg4.5C_pi_Laq**. It uses the auxiliary companion input file **inxs025** required by the GENXS option. Both of these are presented in the subdirectory **/VALIDATION_LAQGSM/Inputs/** and are also shown below.

bg4.5C_pi_Laq:

```
4.5 GeV max bremstrahlung on C12 particle calculation
c ---------------------------------------------------------------
c Uses LAQGSM and dbcn(29)/=0
c ---------------------------------------------------------------
c Cells
c ---------------------------------------------------------------
11  1  -18.7  -40
31  0          40

c ---------------------------------------------------------------
c Surfaces
c ---------------------------------------------------------------
40  so  1.

c ---------------------------------------------------------------
c Materials
c ---------------------------------------------------------------
m1     6012 1
c ---------------------------------------------------------------
c Source
c ---------------------------------------------------------------
sdef   erg=4500 par=p vec=1 0 0 dir=1
c ---------------------------------------------------------------
c Options
c ---------------------------------------------------------------
imp:p 1 0
mode p
lca    7j -1 0 1 $ First interaction only
mx1:p    model
```

```
phys:p 3j 1 $ Turn on photonuclear
c ---------------------------------------------------------------
c nps    1000
nps    1000000
prdmp  1000000 100000 1 2
tropt  genxs inxs025
dbcn   28j 1 2j 1 $ For MCNP6, E_min=30 MeV (default)
c dbcn   28j 1 2j 1 4j 10 $ For MCNP6, E_min=10 MeV (DBCN(37)=10)
```

inxs025:

```
4.5 GeV max bremstrahlung on C12 particle spectra calculation
1 0 1
Uses LAQGSM and dbcn(29)/=1
150, -17, 4, 1000000.0/
   1.    3.    5.    7.    9.   11.   13.   15.   17.   19.
  22.   27.   32.   37.   42.   47.   52.   57.   62.   67.
  72.    77.    82.    87.    92.    97.   105.   125.   135.   145.
 155.   165.   175.   185.   195.   205.   215.   225.   235.   245.
 255.   265.   275.   285.   295.   305.   315.   325.   335.   345.
 355.   365.   375.   385.   395.   405.   415.   425.   435.   445.
 455.   465.   475.   485.   495.   505.   515.   525.   535.   545.
 555.   565.   575.   585.   595.   605.   615.   625.   635.   645.
 655.   665.   675.   685.   695.   705.   715.   725.   735.   745.
 755.   765.   775.   785.   795.   805.   815.   825.   835.   845.
 855.   865.   875.   885.   895.   905.   915.   925.   935.   945.
 955.   965.   975.   985.   995.  1025.  1075.  1125.  1175.  1225.
1275.  1325.  1375.  1425.  1475.  1525.  1575.  1625.  1675.  1725.
1775.  1825.  1875.  1925.  1975.  2025.  2075.  2125.  2175.  2225. /
165. 155. 145. 135. 125. 115. 95. 85. 75. 65. 55. 51. 41. 35. 25. 15. 0./
5, 6, 7, 21/
```

The main difference of the current MCNP6 input file using the GENXS option for reactions induced by bremsstrahlung gammas from all the other examples we provided above is in the **DBCN** card. Let us address this point here again (though we discussed it already in test-problems # 16 and #17 of the CEM Testing Primer [5]), as it is a new MCNP6 feature introduced very recently by Dick Prael and it is not documented yet. As we can see from our input file, the last card is **DBCN** (let us recall again that the most detailed description of the MCNP6 **DBCN** input card is presented in the recent document by Grady Hughes [46], but this paper was written by Dr. Hughes before Dr. Prael introduced the very recent bremsstrahlung capability in MCNP6 using GENXS; therefore, it was not described in [46]). So, the last two cards of the current input file **bg4.5C_pi_Laq** are:

```
dbcn   28j 1 2j 1 $ For MCNP6, E_min=30 MeV (default)
c dbcn   28j 1 2j 1 4j 10 $ For MCNP6, E_min=10 MeV (DBCN(37)=10) .
```

On the **DBCN** card we have **1** for its 32nd parameter. The use of a **non-zero** value for the 32nd parameter of the **DBCN** card is the main instruction for MCNP6 **to calculate a**

reaction induced by bremsstrahlung gammas. The maximum value of the energies of bremsstrahlung gammas, E^{max}, or, as it is often noted in the literature, E_0, is defined on the **SDEF** card:

```
sdef   erg=4500 par=p vec=1 0 0 dir=1 .
```

We see that is is equal to 4500 MeV, for this test-problem. The minimum energy for bremsstrahlung gammas is set in MCNP6 by default to be equal to E_{min} = 30 MeV (as is in our test-problem). But users can change the value of the E_{min}, providing the needed value (in MeV) as the value for the 37th parameter on the **DBCN** card. In our input file, we have a commented **DBCN** card where we chose the values of the minimum energy of bremsstrahlung gammas to be equal to 10 MeV: To calculate with this option, MCNP6 users need only to comment the first **DBCN** card in our input file and to uncomment the second one.

Finally, let us mention that the current version of MCNP6 with GENXS for bremsstrahlung induced reactions **allows only one isotope as the material of the problem**, in contrast to reactions induced by other types of projectiles, where we can have a complex material of several isotopes (see, *e.g.*, test-problem #10 of the CEM Testing Primer [5], where we use the GENXS option for a reaction induced by protons on a ^{nat}Ti target composed of 5 different isotopes).

The experimental data for this problem were measured at the Yerevan electron synchrotron of the Yerevan Physics Institute, Armenia, former USSR. The proton spectra are published in the paper [77], while the pion spectra are from the work [78].

Note that all the experimental characteristics for reactions induced by bremsstrahlung photons are usually normalized per "equivalent quanta", $Q =< E > /E_0$, where $< E >$ is the mean energy of the bremsstrahlung photons and E_0 is the "end-point" or the maximum energy of the bremsstrahlung photons.

Experimental double-differential spectra of protons $d^2\sigma/dT/d\Omega/Q$ at 30, 60, 90, 120, and 160 degrees are presented here in units of [mub/MeV/sr/Q] in the files p30e.dat, p60e.dat, p90e.dat, p120e.dat, and p160e.dat, respectively. Measured double-differential spectra of positive pions $d^2\sigma/dT/d\Omega/Q$ at 20, 60, 90, and 120 degrees are presented here in units of [mub/MeV/sr/Q] in the files pip20e.dat, pip60e.dat, pip90e.dat, and pip120e.dat, respectively. Similar experimental spectra of negative pions are presented here in the files pim20e.dat, pim60e.dat, pim90e.dat, and pim120e.dat, respectively.

Proton double-differential spectra by MCNP6 using LAQGSM03.03 with the GENXS option at 160, and 120 ($\pm$5) degrees are tabulated in units of [mub/sr/MeV] in the 2nd and 6th pairs of columns of the first part of the **proton production cross section** table of the MCNP6 output file **bg4.5C_pi_Laq.o** (after the proton energy tabulated in the 1st column); for 90 and 60 degrees, in the 1st and 4th pairs of columns of the second part of the same table, following the proton energy tabulated in the 1st column; and for 30 degrees, in the 1st pair of columns of the third part of the same table. We present the MCNP6 output file in the subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**. Note that the MCNP6 results for reactions induced by bremsstrahlung photons are not normalized per "equivalent quanta". This is, in order to compare our MCNP6 results with the measured spectra we need to estimate separately the value of the "equivalent quanta", $Q =< E > /E_0$, or to use its value from other calculations. We have calculated our spectra also with CEM03.03 and LAQGSM03.03 used as a stand alone codes; both of them provide the value of Q in their output. Here, while plotting our figures, we normalize the MCNP6 results to the value of the "equivalent quanta", Q = 0.1341099, as calculated by CEM03.03 for this reaction for bremsstrahlung photons with energies between E_{min} = 30 MeV and E^{max} = 4500 MeV (= E_0).

Positive pion spectra by MCNP6 with the GENXS option at 120 (± 5) degrees are tabulated in units of [mub/sr/MeV] in the 6th pair of columns of the first part of the **pi_plus production cross section** table of the same output file; (after the pion energy tabulated in the 1st column); for 90 and 60 degrees, in the 1st and 4th pairs of columns of the second part of the same table, following the pion energy tabulated in the 1st column; and for 20 degrees, in the 2nd pair of columns of the third part of the same table. Negative pion spectra by MCNP6 are tabulated in exactly the same manner in the same output file in the table labeled as **pi_minus production cross section**, respectively.

To help plot the MCNP6 p, π^+, and π^- spectra with **xmgrace** (see files gb4_5C_p_Laq.pdf, gb4_5C_pip_Laq.pdf, and gb4_5C_pim_Laq.pdf), the MCNP6 double-differential spectra are copied here to separate files p30_M6Laq.dat, p60_M6Laq.dat, p90_M6Laq.dat, p120_M6Laq.dat, and p160_M6Laq.dat, for protons, pip20_M6Laq.dat, pip60_M6Laq.dat, pip90_M6Laq.dat, and pip120_M6Laq.dat, for positive pions, and pim20_M6Laq.dat, pim60_M6Laq.dat, pim90_M6Laq.dat, and pimp120_M6Laq.dat, for negative pions, respectively. Let us note one more time that while plotting our figures, we normalize the MCNP6 results to the value of the "equivalent quanta", $Q = 0.1341099$, as calculated by CEM03.03 for this reaction.

Besides the MCNP6 results, for comparison, we show here also calculations by LAQGSM03.03 used as a stand alone code. Spectra of p, π^+, and π^- by LAQGSM03.03 used as a stand alone code at 30, 60, 90, 120, and 160 degrees for protons and at 20, 60, 90, and 120 degrees for pions are presented here in the files: p30l.dat, p60l.dat, p90l.dat, p120l.dat, and p160l.dat, for protons; pip20l.dat, pip60l.dat, pip90l.dat, and pip120l.dat, for positive pions; and pim20l.dat, pim60l.dat, pim90l.dat, and pim120l.dat, for negative pions, respectively.

The files gb4_5C_p_Laq.fig, gb4_5C_pip_Laq.fig, and gb4_5C_pim_Laq.fig are templates for plotting the p, π^+, and π^- spectra with **xmgrace**. The pdf files of figures with these spectra are gb4_5C_p_Laq.pdf, gb4_5C_pip_Laq.pdf, and gb4_5C_pim_Laq.pdf. The summary file gb4.5C.pdf shows all spectra of p, π^+, and π^- on a single plot. The files with figures are presented together with all files with the calculation results and with experimental data in subdirectory **/VALIDATION_LAQGSM/Experimental_data/gb4.5GeV_C/**.

Our final results for this test problem are shown in Figure 20. We see that MCNP6 using LAQGSM03.03 describes well the measured [77, 78] p, π^+, and π^- spectra from from interaction of bremsstrahlung γ quanta of maximum energy $E^{max} = 4.5$ GeV with a thin ^{12}C target and agrees very well with results obtained with the LAQGSM03.03 event generator used as a stand alone code.

3.18. Test-Problems #18: Ne2.1GeVPb with inxc38

This MCNP6 problem tests the applicability of MCNP6 using the LAQGSM03.03 event generator to describe invariant double-differential spectra of K^+ produced in the relativistic reaction 2.1 GeV/nucleon ^{20}Ne + ^{208}Pb. Such reactions may provide a means of studying nuclear matter under conditions of high density or high temperature. The threshold energy for K^+ production in free nucleon-nucleon collisions is 1.56 GeV. Kaons have comparatively low interaction cross section corresponding to the mean free path at normal nuclear density of about 6-8 fm which provides a possibility to gather information on compressed zone of nuclear matter. Another interest in such reactions is to gain insight into the production mechanism of the kaons.

For us, this test-problem has also a special aim in testing a new MCNP6 capability of

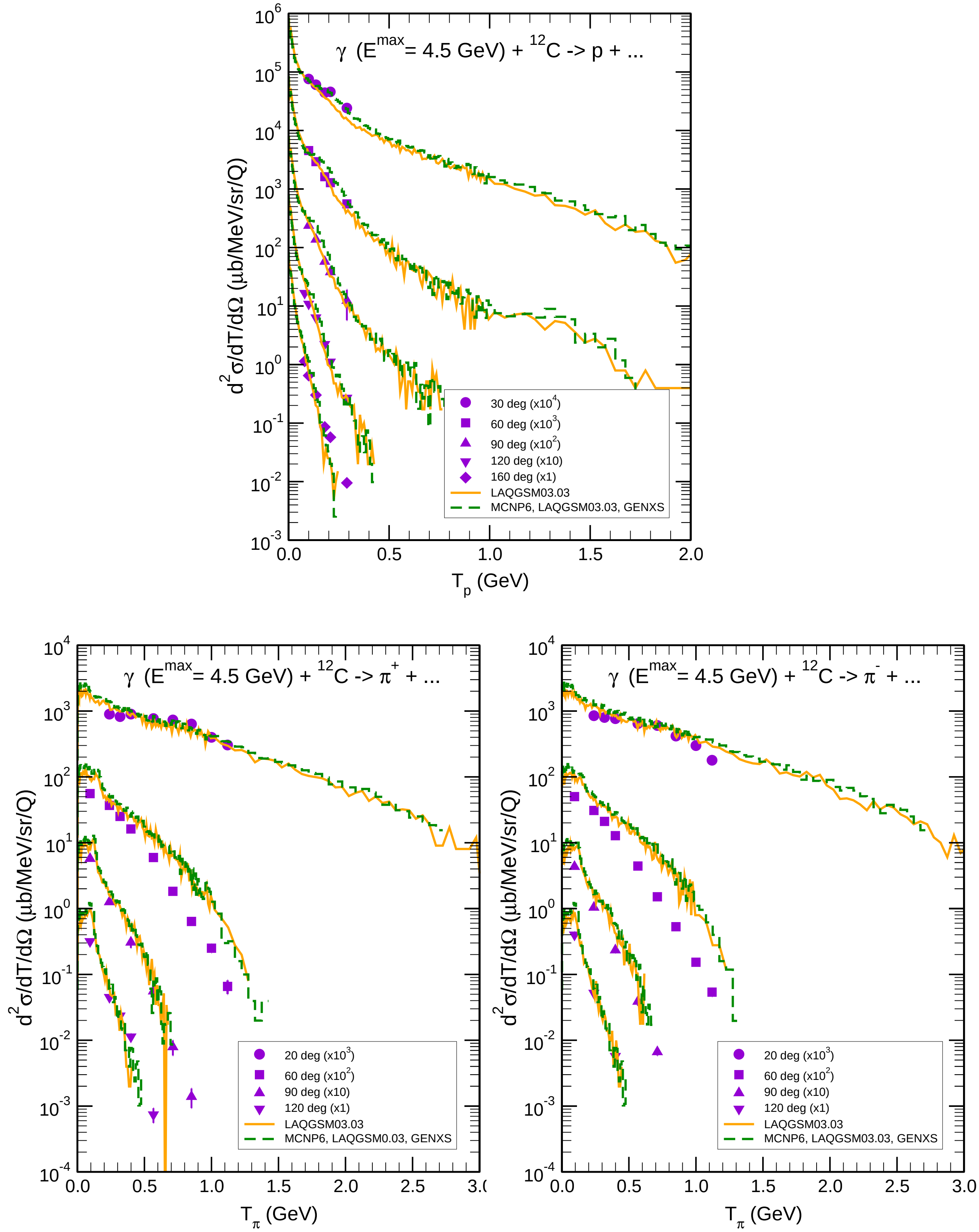

Figure 20: Experimental proton spectra [77, 78] at 30, 60, 90, 120, and 160 degrees and π^+ and π^- spectra at 20, 60, 90, and 120 degrees (symbols) from interaction of bremsstrahlung γ quanta of maximum energy $E^{max} = 4.5$ GeV with a thin ^{12}C target compared with results LAQGSM03.03 [10] used as a stand alone code and by MCNP6 using the LAQGSM03.03 event-generator, as indicated.

changing the number of the particle and light fragment types, **nevtype**, which should be taken into account in evaporation calculations (with a parameter defined on the 11th position of the **LCA** MCNP6 input file). The default MCNP6 value of the parameter **nevtype** is equal to **66**. Here, we are not interested in any fragments and need to calculate only spectra of K^+. We can perform these calculations with the lowest value for **nevtype** accepted at present by MCNP6, **nevtype=6**, saving a lot of computing time in comparison with using the default value of **nevtype=66**.

We calculate this test-problem using the GENXS option of MCNP6. As we have presented a detailed description of the use of the GENXS option to calculate particle spectra from thin targets in test-problem #5 of the CEM Testing Primer [5], we do not need to discuss the input and output files for this case. Therefore, we limit ourselves to only providing the text of the input files (let us recall here that the GENXS option of MCNP6 requires a second, auxiliary input file in addition to the main MCNP6 input file), as well as describing where to find the results in the MCNP6 output file.

The main MCNP6 input file for the case of using the GENXS option is **Ne2.1GeVPb**. It uses the auxiliary companion input file **inxc88** required by the GENXS option. Both of these are presented in the subdirectory **/VALIDATION_LAQGSM/Inputs/** and are also shown below.

Ne2.1GeVPb:

```
MCNP6 test: 2.1 GeV/A  Ne20 + Pb208 by LAQGSM03.03, nevtype=6
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c --------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c --------------------------------------------------------------
dbcn 28j 1
  m1 82208  1.0
  sdef erg=42000 par=10020 dir=1 pos=0 0 0 vec 0 0 1
  imp:n 1 1 0
  imp:h 1 1 0
  phys:n 42008
  phys:h 42008
  phys:/ 42008
  phys:* 42008
  phys:z 42008
  phys:k 42008
  phys:? 42008
  phys:q 42008
  phys:g 42008
```

```
  phys:d 42008
  phys:t 42008
  phys:s 42008
  phys:a 42008
  phys:# 42008
  mode  n h / * z k ? q g d t s a #
LCA  2 1 5j -1 1j 1 6   $ use LAQGSM, nevtype = 6: LCA(11)=6        !!!
lcb  0 0 0 0 0 0
lea  2j 0
  tropt genxs inxc88  nreact on  nescat off
c  tropt genxs inxc38
c -----------------------------------------------------------------
  print 40 110 95
  nps 1000
c  nps 700000
  prdmp 2j -1
```

inxc88:

```
MCNP6 test: invariant K+ spectra from 2.1 GeV Ne20+Pb208 by LAQGSM03.03
1 0 0 /
Cross Section Edit
150 -9 10 /
   1.     3.     5.     7.     9.    11.    13.    15.    17.    19.
  22.    27.    32.    37.    42.    47.    52.    57.    62.    67.
  72.    77.    82.    87.    92.    97.   105.   125.   135.   145.
 155.   165.   175.   185.   195.   205.   215.   225.   235.   245.
 255.   265.   275.   285.   295.   305.   315.   325.   335.   345.
 355.   365.   375.   385.   395.   405.   415.   425.   435.   445.
 455.   465.   475.   485.   495.   505.   515.   525.   535.   545.
 555.   565.   575.   585.   595.   605.   615.   625.   635.   645.
 655.   665.   675.   685.   695.   705.   715.   725.   735.   745.
 755.   765.   775.   785.   795.   805.   815.   825.   835.   845.
 855.   865.   875.   885.   895.   905.   915.   925.   935.   945.
 955.   965.   975.   985.   995.  1025.  1075.  1125.  1175.  1225.
1275.  1325.  1375.  1425.  1475.  1525.  1575.  1625.  1675.  1725.
1775.  1825.  1875.  1925.  1975.  2025.  2075.  2125.  2175.  2225. /
85. 75. 60. 50. 40. 30. 20. 10. 0./
5 6 7 15 16 19 21 22 23 24 /
```

The experimental data for this problem were measured at the Bevalac accelerator of the Lawrence Berkeley Laboratory and were published in the paper [79].

Experimental K^+ invariant spectra, i.e., $Ed^3\sigma/d^3p$ in units of [mb c^3/sr/GeV^2] as functions of K^+ momentum in [GeV/c] at 15, 25, 35, 45, 55, and 80 degrees are presented here in the files 15e.dat, 25e.dat, 35e.dat, 45e.dat, 55e.dat, and 80e.dat, respectively.

K^+ double-differential spectra by MCNP6 using LAQGSM03.03 with the GENXS option at 80, 55, 45, 35, and 25 ($\pm$5) degrees are tabulated in units of [b/sr/MeV] in the 2nd, 4th, 5th, 6th, and 7th pairs of columns of the first part of the **k_plus production cross section** table of the final MCNP6 output file **Ne2.1GeVPb_4c.o** (after the K^+ energy tabulated in the 1st column) and for 15 degrees, in the 1st pair of columns of the second part of the same tables, following the K^+ energy tabulated in the 1st column.

Note that we performed the MCNP6 calculations for this test-problem in several steps, using the "continue" option; the first, initial MCNP6 output file is **Ne2.1GeVPb.o**. We have used the two-line auxiliary input file **inp_10e6** to continue the calculations; it is provided in the subdirectory **/VALIDATION_LAQGSM/Inputs/**.

We present the initial and the final MCNP6 output files in the Templates subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**.

To convert the MCNP6 double-differential spectra tabulated in the output file in units of [b/sr/MeV] into "invariant spectra", $Ed^3\sigma/d^3p$ in units of [mb c^3/sr/GeV^2], we wrote a short auxiliary routine and have performed the conversion separately, after all MCNP6 calculations are completed. To help plot the invariant spectra with **xmgrace** (see file Ne2100Pb_K+.pdf) the MCNP6 "invariant spectra" of K^+ at 15, 25, 35, 45, 55, and 80 degrees, i.e., already after conversion, are copied to separate files M6kp15.dat, M6kp25.dat, M6kp35.dat, M6kp45.dat, M6kp55.dat, and M6kp80.dat, respectively.

Besides the MCNP6 results, we show also recent calculations by LAQGSM03.03 used as a stand alone code. Invariant spectra of K^+ at 15, 25, 35, 45, 55, and 80 degrees by LAQGSM03.03 used as a stand alone code are presented here in the files 15l.dat, 25l.dat, 35l.dat, 45l.dat, 55l.dat, and 80l.dat, respectively.

The file Ne2100Pb_K+.fig is a template for plotting the K^+ invariant spectra with **xmgrace**. The pdf file of the figure with these spectra is Ne2100Pb_K+.pdf. The files with figure are presented together with all files with the calculation results and with experimental data in subdirectory **/VALIDATION_LAQGSM/Experimental_data/Ne2.1GeVPb/**.

Our final results for this test problem are shown in Figure 21. We see that MCNP6 using LAQGSM03.03 describes well the measured [79] K^+ spectra from such heavy-ion induced reactions and agrees very well with results obtained with the LAQGSM03.03 event generator used as a stand alone code.

4. Conclusion

MCNP6, the latest and most advanced LANL Monte Carlo transport code representing a recent merger of MCNP5 and MCNPX, has been validated and verified against a variety of intermediate and high-energy experimental data and against calculations by different versions of MCNPX and results by several other codes. In the present primer, we show 18 examples of test-problems for MCNP6 using mostly the latest modifications of the Los Alamos version of the Quark-Gluon String Model (LAQGSM) event-generator LAQGSM03.03. Another 18 problems for MCNP6 with the Cascade-Exciton Model (CEM) event-generator, CEM03.03 are presented in a separate, first primer of this series [5].

We found that MCNP6 describes reasonably well various reactions induced by particles and heavy-ions (see also Refs. [5, 20]) at incident energies from 18 MeV to about 1 TeV/nucleon measured on both thin and thick targets and agrees very well with similar results obtained with MCNPX and calculations by other codes. Most of several computational bugs and more serious physics problems observed in MCNP6/X during our V&V have been fixed. We continue our work to solve all the known problems before the official distribution of MCNP6 to the public via RSICC at Oak Ridge, TN, USA planned for the year 2011. From the results presented

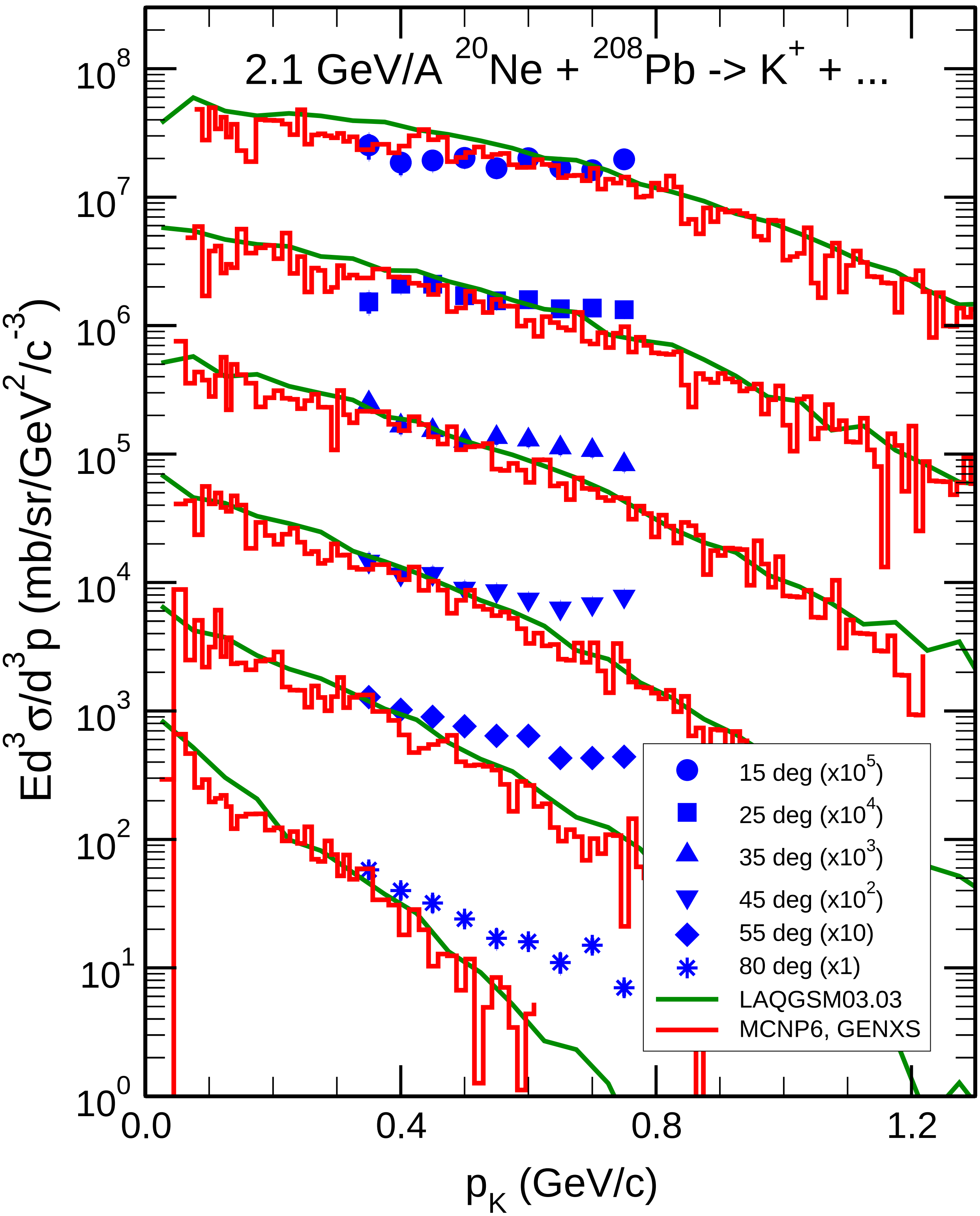

Figure 21: Experimental invariant K^+ spectra [79] at 15, 25, 35, 45, 55, and 80 degrees (symbols) from a thin ^{208}Pb target bombarded with a 2.1 GeV/nucleon ^{20}Ne beam compared with results LAQGSM03.03 [10] used as a stand alone code and by MCNP6 with the GENXS option [36] using the LAQGSM03.03 event-generator, as indicated.

here as well as in Refs. [5, 20], we can conclude that MCNP6 is a reliable and useful Monte Carlo transport code for different applications involving reactions induced by almost all types of elementary particles and heavy-ions, in a very broad range of incident energies. We hope that the current primer will help future users of MCNP6 construct their input files and better understand the final MCNP6 results for their applications at intermediate and high energies.

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References

[1] Tim Goorley, "Eolus L2: MCNP MCNPX merger (U)," LANL Report LA-UR-09-06034, Los Alamos (2009); H. Grady Hughes, John S. Hendricks, Forrest B. Brown, Gregg W. McKinney, Jeffrey S. Bull, Michael R. James, John T. Goorley, Michael L. Fensin, Thomas E. Booth, Laurie S. Waters, Robert A. Forster, Stepan G. Mashnik, Richard E. Prael, Joseph W. Durkee, Avneet Sood, Roger L. Martz, Anthony J. Zukaitis, Denise B. Pelowitz, Russell C. Johns, Jeremy E. Sweezy, "Recent Developments in MCNP and MCNPX," LA-UR-08-01065, Los Alamos (2008), Proc. workshop on Uncertainty Assessment in Computational Dosimetry Bologna, Italy, October 8-10, 2007; G. Gualdrini and P. Ferrari, (editors), (ISBN 978-3-9805741-9-8), 2008.

[2] T. Goorley, M. James, T. Booth, F. Brown, J. Bull, L. J. Cox, J. Durkee, J. Elson, M. Fensin, R. A. Forster, J. Hendricks, H. G. Hughes, R. Johns, B. Kiedrowski, R. Martz, S. Mashnik, G. McKinney, D. Pelowitz, R. Prael, J. Sweezy, L. Waters, T. Wilcox, T. Zukaitis, "MCNP6 initial release notes," LANL Report LA-UR-11-01765, Los Alamos (2011); "Initial MCNP6 Release Notes," LANL Report LA-UR-11-02352, Los Alamos (2011).

[3] X-5 Monte Carlo Team, "MCNP — A General Monte Carlo N-Particle Transport Code, Version 5, Volume I: Overview and Theory" LANL Report LA-UR-03-1987; Volume II: "User's Guide," LANL Report LA-CP-03-0245; Volume III: "Developer's Guide," LANL Report LA-CP-03-0284.

[4] H. G. Hughes, R. E. Prael, and R. C. Little, "MCNPX — The LAHET/MCNP Code Merger," LANL Report LA-UR-97-4891, Los Alamos (1997); L. S. Waters, Ed., "MCNPX User's Manual, Version 2.3.0," LANL Report LA-UR-02-2607 (April, 2002); more recent references and many useful details on MCNPX may be found at the Web page http://mcnpx.lanl.gov/.

[5] Stepan G. Mashnik, "Validation and Verification of MCNP6 against High-Energy Experimental Data and Calculations by other Codes. I. The CEM Testing Primer," LANL Report LA-UR-11-05129, Los Alamos (2011).

[6] S. G. Mashnik, K. K. Gudima, R. E. Prael, A. J. Sierk, M. I. Baznat, and N. V. Mokhov, "CEM03.03 and LAQGSM03.03 Event Generators for the MCNP6, MCNPX, and MARS15 Transport Codes," Invited lectures presented at the Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions, February 4–8, 2008, ICTP, Trieste, Italy, IAEA Report INDC(NDS)-0530, Distr. SC, Vienna, Austria, August 2008, p. 51; LANL Report LA-UR-08-2931, Los Alamos (2008); E-print: arXiv:0805.0751v2 [nucl-th].

[7] S. G. Mashnik, K. K. Gudima, M. I. Baznat, A. J. Sierk, R. E. Prael, and N. V. Mokhov, "CEM03.01 and LAQGSM03.01 Versions of the Improved Cascade-Exciton Model (CEM) and Los Alamos Quark-Gluon String Model (LAQGSM) Codes," LANL Research Note X-5-RN (U) 05-11, LANL Report LA-UR-05-2686, Los Alamos (2005).

[8] Stepan G. Mashnik, Konstantin K. Gudima, Arnold J. Sierk, Mircea I. Baznat, and Nikolai V. Mokhov, "CEM03.01 User Manual," LANL Report LA-UR-05-7321, Los Alamos (2005); RSICC Code Package PSR-532; http://www-rsicc.ornl.gov/codes/psr/psr5/psr532.html; http://www.nea.fr/abs/html/psr-0532.html.

[9] S. G. Mashnik, R. E. Prael, and K. K. Gudima, "Implementation of CEM03.01 into MCNP6 and its Verification and Validation Running through MCNP6. CEM03.02 Upgrade," Research Note X-3-RN(U)-07-03, LANL Report LA-UR-06-8652, Los Alamos (2007).

[10] S. G. Mashnik, K. K. Gudima, N. V. Mokhov, and R. E. Prael, "LAQGSM03.03 Upgrade and Its Validation," Research Note X-3-RN(U)07-15, August 27, 2007; LANL Report LA-UR-07-6198; E-print: arXiv:0709.173v1 [nucl-th] 12 Sep 2007.

[11] N. V. Mokhov, K. K. Gudima, C. C. James, M. A. Kostin, S. G. Mashnik, E. Ng, J.-F. Ostiguy, I. L. Rakhno, A. J. Sierk, S. I. Striganov, "Recent Enhancements to the MARS15 Code," Radiation Protection Dosimetry, 2005, vol. 116, No. 104, pp. 99-103; LA-UR-04-3047, Los Alamos (2004); E-print: nucl-th/0404084; more recent references and many useful details on MARS may be found at the Web page http://www-ap.fnal.gov/MARS/.

[12] Denise B. Pelowitz, John S. Hendricks, Joe W. Durkee, Michael R. James, Michael L. Fensin, Gregg W. McKinney, Stepan G. Mashnik, and Laurie S. Waters, "MCNPX 2.7.A Extensions," LANL Report LA-UR-08-07182, Los Alamos, November 6, 2008.

[13] Denise B. Pelowitz, Michael R. James, Gregg W. McKinney, Joe W. Durkee, Michael L. Fensin, John S. Hendricks, Stepan G. Mashnik, and Laurie S. Waters, "MCNPX 2.7.B Extensions," LA-UR-09-04150, July 6, 2009.

[14] Denise B. Pelowitz, Michael R. James, Gregg W. McKinney, Joe W. Durkee, Michael L. Fensin, John S. Hendricks, Stepan G. Mashnik, Jerome M. Verbeke, Laurie S. Waters, and Jerome M. Verbeke, "MCNPX 2.7.C Extensions," LANL Report LA-UR-10-00481, Los Alamos, January 28, 2010 (Revised February 17, 2010), https://mcnpx.lanl.gov/.

[15] Denise B. Pelowitz, Joe W. Durkee, Jay S. Elson, Michael L. Fensin, John S. Hendricks, Michael R. James, Russell C. Johns, Gregg W. McKinney, Stepan G. Mashnik, Jerome M. Verbeke, and Laurie S. Waters, "MCNPX 2.7.D Extensions," LANL Report LA-UR-10-07031, October 20, 2010.

[16] Denise B. Pelowitz, Joe W. Durkee, Jay S. Elson, Michael L. Fensin, John S. Hendricks, Michael R. James, Russell C. Johns, Gregg W. McKinney, Stepan G. Mashnik, Jerome M. Verbeke, Laurie S. Waters, and Trevor A. Wilcox, "MCNPX 2.7.E Extensions," LANL Report LA-UR-11-01502, Los Alamos, March 10, 2011.

[17] Denise B. Pelowitz, Joe W. Durkee, Jay S. Elson, Michael L. Fensin, John S. Hendricks, Michael R. James, Russell C. Johns, Gregg W. McKinney, Stepan G. Mashnik, Jerome M. Verbeke, Laurie S. Waters, Trevor A. Wilcox, "MCNPX 2.7.0 Extensions," LANL Report LA-UR-11-02295, Los Alamos, April 2011.

[18] Robert A. Weller, Marcus H. Mendenhall, Robert A. Reed, Ronald D. Schrimpf, Kevin M. Warren, Brian D. Sierawski, Lloyd W. Massengill, "Monte Carlo Simulation of Single Event Effects," IEEE Transactions on Nuclear Science, vol. 57, No. 4, (Aug 2010) 1726–1746; Michael Andrew Clemens, Nicholas C.Hooten, Vishwa Ramachandran, Nathaniel A. Dodds, Robert A. Weller, Marcus H. Mendenhall, Robert A. Reed, Paul E. Dodd, Marty R. Shaneyfelt, James R. Schwank, Ewart W. Blackmore, "The Effect of High-Z Materials on Proton-Induced Charge Collection," IEEE Transactions on Nuclear Science, vol. 57, No. 6, (Dec 2010) 3212–3218.

[19] *Benchmark of Spallation Models* organized at the International Atomic Energy Agency during 2008-2009 by Detlef Filges, Sylvie Leray, Jean-Christophe David, Gunter Mank, Yair Yariv, Alberto Mengoni, Alexander Stanculescu, Mayeen Khandaker, and Naohiko Otsuka, IAEA Vienna, Austria, http://nds121.iaea.org/alberto/mediawiki-1.6.10/index.php/Main_Page.

[20] Stepan G. Mashnik, "Validation and Verification of MCNP6 Against Intermediate and High-Energy Experimental Data and Results by Other Codes," LANL Report LA-UR-10-07847, Los Alamos (2010); arXiv:1011.4978; Eur. Phys. J. Plus **126**: 49 (2011).

[21] S. Furihata, "Statistical Analysis of Light Fragment Production from Medium Energy Proton-Induced Reactions," Nucl. Instr. Meth. B **171** (2000) 252–258; "The Gem Code — the Generalized Evaporation Model and the Fission Model," Proc. MC2000, Lisbon, Portugal, 2000, edited by A. Kling, F. J. C. Barão, M. Nakagawa, L. Távora, and P. Vaz, Springer, Berlin, (2001), pp. 1045–1050; *The Gem Code Version 2 Users Manual*, Mitsubishi Research Institute, Inc., Tokyo, Japan (November 8, 2001).

[22] S. Furihata, K. Niita, S. Meigo, Y. Ikeda, and F. Maekawa, "The Gem Code—a Simulation Program for the Evaporation and Fission Process of an Excited Nucleus," JAERI-Data/Code 2001-015, JAERI, Tokai-mura, Naka-gam, Ibaraki-ken, Japan (2001).

[23] S.Furihata, *Development of a Generalized Evaporation Model and Study of Residual Nuclei Production*, Ph.D. thesis, Tohoku University, March, 2003; S. Furihata and T. Nakamura, "Calculation of Nuclide Production from Proton Induced Reactions on Heavy Targets with INC/GEM," J. Nucl. Sci. Technol. Suppl. **2** (2002) 758–761.

[24] I. Dostrovsky, Z. Frankel, and G. Friedlander, "Monte Carlo Calculations of Nuclear Evaporation Processes. II. Application to Low-Energy Reactions," Phys. Rev. **116** (1959) 683–702.

[25] R. E. Prael and H. Lichtenstein, *User guide to LCS: The LAHET Code System*, LANL Report LA-UR-89-3014, Los Alamos (1989); http://www-xdiv.lanl.gov/XTM/lcs/lahet-doc.html.

[26] F. Atchison, "Spallation and Fission in Heavy Metal Nuclei under Medium Energy Proton Bombardment," in Proc. Meeting on Targets for Neutron Beam Spallation Source, Julich, June 11–12, 1979, pp. 17–46, G. S. Bauer, Ed., Jul-Conf-34, Kernforschungsanlage Julich GmbH, Germany (1980).

[27] F. Atchison, "A Treatment of Fission for HETC," in *Intermediate Energy Nuclear Data: Models and Codes*, pp. 199–218 in: Proc. of a Specialists's Meeting, May 30–June 1, 1994, Issy-Les-Moulineaux, France, OECD, Paris, France (1994).

[28] F. Atchison, "A treatment of medium-energy particle induced fission for spallation-systems' calculations," Nucl. Instrum. Methods B **259** (2007) 909–932.

[29] V. F. Weisskopf and D. H. Ewing, "On the Yield of Nuclear Reactions with Heavy Elements," Phys. Rev. **57** (1940) 472–483.

[30] G. Audi and A. H. Wapstra, "The 1995 Update to the Atomic Mass Evaluation," Nucl. Phys. **A595** (1995) 409–480.

[31] P. Möller, J. R. Nix, W. D. Myers, and W. J. Swiatecki, "Nuclear Ground-States Masses and Deformations," Atomic Data and Nuclear Data Tables, **59** (1995) 185–381.

[32] P. E. Haustein, "An Overview of the 1986–1987 Atomic Mass Predictions," Atomic Data and Nuclear Data Tables **39** (1988) 185–393.

[33] A. G. W. Cameron, "A Revised Semiempirical Atomic Mass Formula," Can. J. Phys. **35** (1957) 1021–1032.

[34] S. G. Mashnik, K. K. Gudima, R. E. Prael, and A. J. Sierk, "Analysis of the GSI A+p and A+A Spallation, Fission, and Fragmentation Measurements with the LANL CEM2k and LAQGSM Codes," in Proc. TRAMU@GSI, Darmstadt, Germany, 2003, Eds. A. Kelic and K.-H. Schmidt, ISBN 3-00-012276-1, http://ww-wnt.gsi.de/tramu; E-print: nucl-th/0404018.

[35] Denise B. Pelowitz, editor, *MCNPX^{TM} User's Manual, Version 2.6.0*, LA-CP-07-1473, Los Alamos, April 2008.

[36] R. E. Prael, "Tally Edits for the MCNP6 GENXS Option," LANL Research Note X-5-RN(U)04-41, Los Alamos, 23 August, 2004; LANL Report LA-UR-11-02146, Los Alamos (2011).

[37] L. Heilbronn, C. J. Zeitlin, Y. Iwata, T. Murakami, H. Iwase, T. Nakamura, T. Nunomiya, H. Sato, H. Yashima, R. M. Ronningen, and K. Ieki, "Secondary Neutron-Production Cross Sections from Heavy-Ion Interactions Between 230 and 600 MeV per Nucleon," Nucl. Sci. Eng. **157** (2007) 142–158; numerical values of measured spectra were obtained from the authors of the experiment performed at the Heavy Ion Medical Accelerator in Chiba (HIMAC) facility of the National Institute of Radiological Science (NIRS), Japan via Dr. Igor Remec of the Oak Ridge National Laboratory.

[38] Hiroshi Iwase, Yoshiyuki Iwata, Takashi Nakamura, Konstantin Gudima, Stepan Mashnik, Arnold Sierk,and Richard Prael, "Neutron Spectra from Intermediate-Energy Nucleus-Nucleus Reactions," LANL Report LA-UR-05-0367, Los Alamos (2005); E-print: nucl-th/0501066; Proc. Int. Conf. on Nuclear Data for Sci. Techn. (ND2004), September

26 - October 1, 2004, Santa Fe, NM, USA, edited by R. C. Haight, M. B. Chadwick, T. Kawano, and P. Talou, (AIP Conference Proceedings, Volume 769, Melville, New York, 2005), pp. 1066–1069.

[39] H. Sato, T. Kurosawa, H. Iwase, T. Nakamura, Y. Uwamino, and N. Nakao, "Measurements of double differential neutron production cross sections by 135 MeV/nucleon He, C, Ne and 95 MeV/nucleon Ar ions," Phys. Rev. C **64** (2001) 034607.

[40] Takahashi Nakamura and Lawrence Heilbronn, *Handbook on Secondary Particle Production and Transport by High-Energy Heavy Ions*, World Scientific, Singapore, 2006.

[41] S. G. Mashnik, K. K. Gudima, A. J. Sierk, R. E. Prael, "Improved Intranuclear Cascade Models for the Codes CEM2k and LAQGSM," LANL Report LA-UR-05-0711, Los Alamos (2005); E-print: nucl-th/0502019; Proc. Int. Conf. on Nuclear Data for Sci. & Techn. (ND2004), September 26 - October 1, 2004, Santa Fe, NM, USA, edited by R. C. Haight, M. B. Chadwick, T. Kawano, and P. Talou, (AIP Conference Proceedings, Volume 769, Melville, New York, 2005), pp. 1188-1192.

[42] Y. Yariv and Z. Frankel, "Intranuclear Cascade Calculation of High-Energy Heavy-Ion Interactions," Phys. Rev. C **20** (1979) 2227–2243; Y. Yariv and Z. Frankel, "Inclusive Cascade Calculation of High Energy Heavy Ion Collisions: Effect of Interactions between Cascade Particles," Phys. Rev. C **24** (1981) 488–494; Y. Yariv, "ISABEL — INC Model for High-Energy Hadron-Nucleus Reactions," Proc. Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions, ICTP Trieste, Italy, 4-8 February 2008, INDC(NDS)-0530 Distr. SC, IAEA, Vienna, August 2008, pp. 15–28.

[43] Itacil C. Gomes, private communication, April 2006.

[44] L. Bandura, B. Erdelyi, and J. Nolen, "An integrated high-performance beam optics-nuclear processes framework with hybrid transfer map-Monte Carlo particle transport and optimization," Nucl. Instr. Meth. in Phys. Res. **B268** (2010) 3485–3497.

[45] John S. Hendricks, Gregg W. McKinney, Michael L. Fensin, Michael R. James, Joe W. Drukee, Denise B. Pelowitz, Laurie S. Waters, and Russel C. Johns, "New Monte Carlo advances for radiation modeling," presentation (viewgraphs) at the ICRS-11/RPSD 2008 Conference, Pine Mountain, GA, USA, April 13-18, 2008, LANL Report LA-UR-08-2218, Los Alamos (2008).

[46] H. Grady Hughes, "Controlling MCNP6 Transport with DBCN Options," LANL Report LA-UR-11-01887, Los Alamos (2011).

[47] A. M. Baldin, "A Scaled Invariance of Hadron Collisions and a Possibility of High-Energy Particle Beam Production via Relativistic Acceleration of Multi-Charged Ions," Kratkie Soobshcheniya po Fizike FIAN **1** (1971) 35–39 [in Russian]; V. I. Komarov, G. E. Kosarev, H. Muller, D. Netzband, V. D Toneev, T. Stiehler, S. Tesch, K. K. Gudima, and S. G. Mashnik, "Proton-Nucleus Interactions at 640 MeV Accompanied by Backward Emission of Energetic Protons," Nucl. Phys. **A326** (1979) 297–324; L. L. Frankfurt and M. I. Strikman, "High-Energy Phenomena, Short-Range Nuclear Structure and QCD," Phys. Rep. **76** (1981) 215–347; V. B. Kopeliovich, "Long and Intermediate Range Phenomena; Selected Topics in High Energy Nuclear Physics," Phys. Rep. **139** (1986) 51–157; S. G. Mashnik, "Neutron-Induced Particle Production in the Cumulative and Noncumulative Regions at Intermediate Energies," Nucl. Phys. **A568** (1994) 703–726; M. V. Tokarev and I. Zborovsky, "Self-similarity of high p_T hadron production in cumulative processes

and violation of discrete symmetries at small scales (suggestion for experiment)," Phys. Part. Nucl. Lett. **6** (2010) 160–170.

[48] I. L. Azhgirey, V. I. Belyakov-Bodin, I. I. Degtyarev, V. A. Sherstnev, S. G. Mashnik, F. X. Gallmeier, and W. Lu, "CTOF measurements and Monte Carlo analyses of neutron spectra for the backward direction from a lead target irradiated with 200 to 1000 MeV protons," LANL Report LA-UR 10-04265, Los Alamos (2010); E-print: arXiv:1006.4899]; Nucl. Instr. Meth. in Phys. Res. **B268** (2010) 3426–3433.

[49] H. W. Bertini, "Low-Energy Intranuclear Cascade Calculation," Phys. Rev. **131** (1963) 1801–1871; "Intranuclear Cascade Calculation of the Secondary Nucleon Spectra from Nucleon-Nucleus Interactions in the Energy Range 340 to 2900 MeV and Comparison with Experiment", Phys. Rev. **188** (1969) 1711–1730.

[50] R. E. Prael and M. Bozoian, "Adaptation of the Multistage Preequilibrium Model for the Monte Carlo Method," LANL Report LA-UR-88-3238, Los Alamos (September 1988).

[51] L. Dresner, *EVAP – A Fortran Program for Calculation the Evaporation of Various Particles from Excited Compound Nuclei*, Oak Ridge National Laboratory Report ORNL-TM-196, 1962; Miraim P. Guthrie *EVAP-2 and EVAP-3: Modifications of a Code to Calculate Particle Evaporation from Excited Compound Nuclei*, Oak Ridge National Laboratory Report ORNL-4379, 1969 March, 36 pp. M. P. Guthrie, *EVAP-4: Another Modification of a Code to Calculate Particle Evaporation from Excited Compound Nuclei*, Oak Ridge National Laboratory Report ORNL-TM-3119, 1970; P. Cloth, D. Filges, G. Sterzenbach, T. W. Armstrong, and B.L. Colborn, *The KFA-Version of the High-Energy Transport Code HETC and the Generalized Evaluation Code SIMPEL*, Kernforschungsanlage Jülich Report Jül-Spez-196, 1983.

[52] J. Cugnon, C. Volant, and S. Vuillier, "Improved Intranuclear Cascade Model for Nucleon-Nucleus Interactions,"Nucl. Phys. **A620** (1997) 475–509; A. Boudard, J. Cugnon, S. Leray, and C. Volant, "Intranuclear Cascade Model for a Comprehensive Description of Spallation Reaction Data," Phys. Rev. C **66** (2002) 044615.

[53] A. R. Junghans, M. de Jong, H.-G. Clerc, A. V. Ignatyuk, G. A. Kudyaev, and K.-H. Schmidt, "Projectile-Fragment Yields as a Probe for the Collective Enhancement in the Nuclear Level Density," Nucl. Phys. A **629** (1998) 635–655; J.-J. Gaimard, and K.-H. Schmidt, "A reexamination of the abrasion-ablation model for the description of the nuclear fragmentation reaction," Nucl. Phys. A **531** (1991) 709–745.

[54] A. Sandoval, H. H. Gutbrod, W. G. Meyer, R. Stock, Ch. Lukner, A. M. Poskanzer, J. Gosset, J. -C. Jourdain, C. H. King, G. King, Nguyen Van Sen, G. D. Westfall, and K. L. Wolf, "Spectra of p, d, and t from relativistic nuclear collisions," Phys. Rev. C **21** (1980) 1321–1343; all measured spectra are tabulated in 118 pages of data tables published in the AIP document No. PAPS PRVCA 21-132-118 which can be ordered from the Physics Auxiliary Publications Service of the American Institute of Physics.

[55] S. Nagamiya, M. -C. Lemaire, E. Moeller, S. Schnetzer, G. Shapiro, H. Steiner, and I. Tanihata, "Production of pions and light fragments at large angles in high-energy nuclear collisions," Phys. Rev. C **24** (1981) 971–1009; all measured spectra are tabulated in 181 pages of data tables published in [56].

[56] M.-C. Lemaire, S. Nagamiya, O. Chamberlain, G. Shapiro, S. Schnetzer, H. Steiner, I. Tanihata, "Tables of light-fragment inclusive cross sections in relativistic heavy ion

collisions. Part I. C + C, C + Pb, Ne + NaF, Ne + Cu, Ne + Pb → $\pi^{\pm}$, p, d, t, ^{3}He; E_{BEAM} = 800 MeV/A, Lawrence Berkeley National Laboratory. Report No. LBL-8463, Nov. 1978, 181 pages.

[57] N. T. Porile, G. D. Cole, and C. R. Rudy, "Nuclear reactions of silver with 25.2 GeV C12 ions and 300 GeV protons," Phys. Rev. C **19** (1079) 2288–2304.

[58] L. Sihver, K. Aleklett, W. Loveland, P. L. McGaughey, D. H. E. Gross, and H. R. Jaqaman, "Gold target fragmentation by 800 GeV protons," Nucl. Phys. **A543** (1992) 703–721.

[59] F. Rejmund, B. Mustapha, P. Armbruster, J. Benlliure, M. Bernas, A. Boudard, J. P. Dufour, T. Enqvist, R. Legrain, S. Leray, K.-H. Schmidt, C. Stephan, J. Taieb, L. Tassan-Got, and C. Volant, "Measurement of Isotopic Cross Sections of Spallation Residues in 800 A MeV 197-Au + p Collisions," Nucl. Phys. **A683** (2001) 540–565.

[60] J. Benlliure, P. Armbruster, M. Bernas, A. Boudard, J. P. Dufour, T. Enqvist, R. Legrain, S. Leray, B. Mustapha, F. Rejmund, K.-H. Schmidt, C. Stephan, L. Tassan-Got, and C. Volant, "Isotopic Production Cross Sections of Fission Residues in 197-Au-on-Proton Collisions at 800 A MeV," Nucl. Phys. **A683** (2001) 513–539.

[61] J. R. Cummings, W. R. Binns, T. L. Garrard, M. H. Israel, J. Klarmann, E. C. Stone, and C. J. Waddington, "Determination of the cross sections for the production of fragments from relativistic nucleus-nucleus interactions. I. Measurements," Phys. Rev. C **42** (1990) 2508.

[62] L. Y. Geer, J. Klarmann, B. S. Nilsen, C. J. Waddington, W. R. Binns, J. R. Cummings, and T. L. Garrard, "Charge-changing fragmentation of 10.6 GeV/nucleon ^{197}Au nuclei," Phys. Rev. C **52** (1995) 334.

[63] C. Scheidenberger, I. A. Pshenichnov, K. Smmerer, A. Ventura, J. P. Bondorf, A. S. Botvina, I. N. Mishustin, D. Boutin, S. Datz, H. Geissel, P. Grafstrm, H. Knudsen, H. F. Krause, B. Lommel, S. P. Mller, G. Mnzenberg, R. H. Schuch, E. Uggerhj, U. Uggerhj, C. R. Vane, Z. Z. Vilakazi, and H. Weick, "Charge-changing interactions of ultrarelativistic Pb nuclei," Phys. Rev. C **70** (2004) 014902.

[64] Mukhtar Ahmed Rana and Shahid Manzoor, "Examining the fragmentation of 158 A GeV lead ions on copper target: Charge-changing cross sections," Radiation Measurements **43** (2008) pp. 1383–1389.

[65] Y. Iwata, T. Murakami, H. Sato, H. Iwase, T. Nakamura, T. Kurosawa, L. Heilbronn, R. M. Ronningen, K. Ieki, Y. Tozawa, and K. Niita, "Double-differential cross sections for the neutron production from heavy-ion reactions at energies E/A 290-600 MeV," Phys. Rev. C **64** (2001) 054609.

[66] Koji Niita, Satoshi Chiba, Toshiki Maruyama, Tomoyuki Maruyama, Hiroshi Takada, Tokio Fukahori, Yasuaki Nakahara, and Akira Iwamoto, "Analysis of the (N, xN') reactions by quantum molecular dynamics plus statistical decay model," Phys. Rev. C **52** (1995) 2620–2635.

[67] H. W. Bertini, T. A. Gabriel, R. T. Santoro, O. W. Hermann, N. M. Larson, and J. M. Hunt, "HIC-1: A First Approach to the Calculation of Heavy-Ion Reactions at Energies $\geq$ 50 MeV/Nucleon," ORNL-TM-4134, Oak Ridge (1974).

[68] Hiroshi Iwase, Yoshiyuki Iwata, Takashi Nakamura, Konstantin Gudima, Stepan Mashnik, Arnold Sierk, and Richard Prael, "Neutron Spectra from Intermediate-Energy Nucleus-Nucleus Reactions," LANL Report LA-UR-05-0367, Los Alamos (2005); E-print: nucl-th/0501066; Proc. Int. Conf. on Nuclear Data for Sci. & Techn. (ND2004), September 26 - October 1, 2004, Santa Fe, NM, USA, edited by R. C. Haight, M. B. Chadwick, T. Kawano, and P. Talou, (AIP Conference Proceedings, Volume 769, Melville, New York, 2005), pp. 1066–1069.

[69] N. A. Nikiforov, Y. D. Bayukov, V. I. Efremenko, G. A. Leksin, V. I. Tchistilin, Y. M. Zaitsev, S. Frankel, W. Frati, M. Gazzaly, and C. F. Perdrisat, "Backward production of pions and kaons in the interactions of 400 GeV protons with nuclei," Phys. Rev. C **22** (1980) 700–710.

[70] S. Frankel, W. Frati, M. Gazzaly, Y. D. Bayukov, V. I. Efremenko, G. A. Leksin, N. A. Nikiforov, V. I. Tchistilin, Y. M. Zaitsev, and C. F. Perdrisat, "Backward production of light ions in the interactions of 400 GeV protons with nuclei," Phys. Rev. C **20** (1979) 2257–2266.

[71] S. G. Mashnik, K. K. Gudima, R. E. Prael, A. J. Sierk, M. I. Baznat, and N. V. Mokhov, "Overview and Validation of the CEM03.01 and LAQGSM03.01 Event Generators for MCNP6, MCNPX, and MARS15," LANL Report LA-UR-06-5998 Los Alamos (2006); Presentation (slides) at the *Hadronic Shower Simulation Workshop (HSSW06), Fermi National Accelerator Laboratory, Batavia, IL, USA, September 6–8, 2006*, http://indico.cern.ch/conferenceOtherViews.py?view=standard&confId=3734.

[72] Michal Mocko, "Rare Isotope Production," PhD thesis, Michigan State University, 2006, http://groups.nscl.msu.edu/nscl_library/Thesis/index.htm.

[73] K. Summerer and B. Blank, "Modified empirical parameterization of fragmentation cross sections," Phys. Rev. C **61** (2000) 034607.

[74] J.-J. Gaimard and K.-H. Schmidt, "A reexamination of the abrasion-ablation model for the description of the nuclear fragmentation," Nucl. Phys. **A531** (1991) 709.

[75] Denis Lacroix, Aymeric Van Lauwe, and Dominique Durand, "Event generator for nuclear collisions at intermediate energies," Phys. Rev. C **69** (2004) 054604.

[76] Akira Ono, Hisashi Horiuchi, "Antisymmetrized molecular dynamics for heavy ion collisions," Prog. Part. Nucl. Phys. **53** (2004) 501.

[77] K. V. Alanakian, M. Dj. Amarian, R. A. Demirchian, K. Sh. Egiyan, M. S. Ogandjanian, and Yu. G. Sharabian, "On the Angular Dependence of Photoprotons from Nuclei Irradiated by gamma-Quanta with Maximum Energy 4.5 GeV," (in Russian) Report EPI-386(44)-79, Yerevan Physics Institute, Yerevan (1979).

[78] K. V. Alanakian, M. Dj. Amarian, R. A. Demirchian, K. Sh. Egiyan, Dj. V. Kaumian, Zh. L. Kocharova, M. S. Ogandjanian, and Yu. G. Sharabian, "$\pi^{\pm}$ - Meson Spectra in the Inclusive Reaction gamma $C \rightarrow \pi X$ Caused by Bremsstrahlung gamma-quanta with the Maximum Energy 4.5 GeV," Report EPI-450(57)-90, Yerevan Physics Institute, Yerevan (1981).

[79] S. Schnetzer, R. M. Lombard, M.-C. Lemaire, E. Moeller, S. Nagamiya, G. Shapiro, H. Steiner, and I. Tanihata, "Inclusive production of K^+ mesons in 2.1-GeV/nucleon nuclear collisions," Phys. Rev. C **40** (1989) 640-653.