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The Preliminary Validation and Verification of GSM

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1 INTRODUCTION

The Generalized Spallation Model, or GSM, simulates hadron-nucleus and nucleus-nucleus collisions at intermediate to high incident energies. It is recommended that use of GSM be limited to interactions for particles and nuclei with kinetic energies greater than ~ 100 MeV, up to ~ 1 TeV/A. GSM was developed to investigate the deprecation of the Los Alamos Quark-Gluon String Model (LAQGSM), as implemented in the event generator LAQGSM03.03. The deprecation of LAQGSM will allow for a simplification of the high energy physics models utilized within the Monte Carlo N-Particle[®] (MCNP[®]) transport code¹. MCNP applies simulated data from the Cascade Exciton Model (CEM), as implemented in the CEM03.03 event generator, and the LAQGSM event generator for most high energy reactions, by default, for its simulations.

The purpose of the work presented here is to provide information regarding the preliminary verification and validation (V&V) of GSM, in particular regarding its use of the modified Dubna cascade model and quark-gluon string model. Successful V&V of GSM will provide a technical basis for the inclusion of the GSM event generator to MCNP, and the subsequent removal of the CEM and LAQGSM event generators from MCNP.

These event generators are most useful regarding accelerator-driven, medical, and space applications. Some such applications include the accelerator transmutation of nuclear wastes, neutron spallation sources, proton radiography, radiation therapy via proton and heavy-ion beams, shielding of equipment in the presence of galactic cosmic rays (GCRs), single event upsets (SEUs), and many others. The successful validation of GSM will allow for the removal of both the CEM and LAQGSM event generators within MCNP. The simplifications GSM can provide to MCNP have potential to significantly curtail the amount of code within MCNP itself, making MCNP more efficient and economically maintainable. GSM also utilizes an upgraded version of the Modified Exciton Model (MEM), where the MEM was expanded to include emission of ejectiles up to ^{28}Mg [1]. Upgrades to other models utilized by GSM have taken place prior to its creation. LAQGSM does not have these updates available to it at present.

Both the CEM and LAQGSM event generators have a physics-rich history. The spallation physics being modeled by these, and other event generators created throughout the world, was originally proposed more than 30 years ago. The models implemented within CEM were first proposed at the Laboratory of Theoretical Physics, JINR, Dubna, USSR, by Gudima, Mashnik, and Toneev [2]. Many codes, modifications, and upgrades to these models have since been developed and validated. The primary difference between the various models lie mainly in the assumptions used within the models, in addition to the depth of calculations utilized within the event generators employing the models. The majority of the differences in the codes stem from those of the simulation of the reaction's IntraNuclear Cascade (INC) process. Sec. 2 further

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discusses the physics utilized within GSM.

2 A BRIEF SURVEY OF NUCLEAR SPALLATION PHYSICS

The GSM event generator simulates spallation reactions by estimating fragment emissions via Monte-Carlo techniques. The estimation of fragment emission during the spallation reaction is split into three primary phases, being the IntraNuclear Cascade (INC), the equilibration of the excited residual nucleus, often referred to as preequilibrium, and the evaporation of particles from, or the fission² of, the compound nucleus. The physics simulated by GSM is completed similarly to its predecessors, CEM and LAQGSM [3]. GSM is a recent development utilizing the INC models of both CEM and LAQGSM, where the excited residual nuclei's equilibration and subsequent evaporation or break-up calculations use the same models that are employed within CEM. The INC models available to GSM are the standard version of the Dubna cascade model [4, 5], as incorporated in the event generator CEM03.03 [6], and a coupling of the modified version of the standard Dubna cascade model with the quark gluon string model, as utilized in the LAQGSM event generator, LAQGSM03.03 [7]. Following the INC process, the residual nucleus and associated fragments undergo coalescence, preequilibrium emission, and evaporation or fission prior to reaching a stable state. Smaller, energetic fragments will undergo the INC and Fermi break-up processes. The spallation process is typically regarded as two separate stages, each based on the state of the nucleus. These stages are called the precompound and compound stages. The precompound stage consists of the particle cascade, coalescence of emitted nucleons, and equilibration of the excited nucleus. The compound stage of the reaction occurs once the nucleus has become compound, meaning it has de-excited, upon which it may undergo evaporation or fission. Fig. 1 depicts the flow of the calculations for spallation physics within GSM.

2.1 Primary Assumptions

The various assumptions used in GSM, and other event generators, primarily lie within the INC model. The INC process can typically be regarded as a series of successive quasi-free collisions of the fast primary particle with the individual nucleons of the nucleus, according to the ideas of Serber [8]. The main assumption typically used within most INC models is that the DeBroglie wavelength of the participant particles is sufficiently small, being smaller than the distance between internuclear nucleons [9]. This requirement effectively requires large kinetic energies, being on the order of several tens of MeV or greater. Additionally, the time in which an intranuclear collision between two nucleons occurs must be less than the time interval between such consecutive interactions, allowing for statistically *independent* intranuclear collisions [9].

²Note if the compound nucleus fissions, the resulting fission fragments may also undergo evaporation depending on their excited states.

Fig. 1. Flow chart of CEM, GSM, and LAQGSM spallation physics calculations.

2.2 The INC Model

The INC process of the nuclear reaction will produce many secondary particles. The secondary particles will likely move in a similar direction to the incident beam, and may create more secondary particles throughout the INC process [10], creating a cascade of particles. The culmination of all primary and secondary particles characterizes the INC process, also referred to as a hadronic cascade [10]. This process will create numerous neutrons and protons outside the nucleus, leaving behind an excited residual nucleus. The emitted cascade nucleons may coalesce while the excited residual nucleus concurrently de-excites.

GSM has available to it two slightly differing INC models, one being the standard, non-time dependent, Dubna Cascade Model (DCM) [6] and the other being a modified version of the standard DCM³ coupled with the Quark-Gluon String Model (QGSM) [7]. Details on these cascade models can be found in Ref. [3–5] and Ref. [11–16], respectively. The DCM depicts the energetic reaction as a high-energy particle passing through a gas of free nucleons, producing a cascade of secondary particles, which may leave the nucleus or be absorbed in the nucleus, exciting it to some high energy [3]. The use of each of the DCMs within GSM is based on the kinetic energy of the incident particle and its atomic and mass numbers. Incident nucleons, pions, and photons below $\sim 4.5 \text{ GeV}$ are currently simulated in GSM with the use of the standard DCM, as is done in CEM [6]. Incident nucleons, pions, and photons above $\sim 4.5 \text{ GeV}$, including all incident light- and heavy-ions, are simulated using the coupled non-standard DCM and QGSM, as is done in LAQGSM [7]. It is suggested that use of the non-standard DCM be restricted to particles with kinetic energies between $\sim 4.5 \text{ GeV}/A$ and $\sim 1 \text{ TeV}/A$.

Both of the INC models used within GSM follow the flow depicted in Fig. 2 [3]. Fig. 2 depicts the

³This version of the DCM will herein be referred to as the non-standard DCM.

various calculations (blue boxes) and branching conditions (yellow boxes) throughout the simulation. At the start of the simulation, both the DCM models employed by GSM determine a change in momentum of the incident particle (box 1), the interacting partner nucleon (box 2) and if the partner nucleon is inside the nucleus (box 3). If the partner is outside the nucleus then the incident particle is assumed to have passed through the nucleus (box 10). If the interaction is inside the nucleus, then the nature of the collision is determined as elastic or inelastic (box 4), and the resulting secondary particle's characteristics are determined (box 5). Both of the INC models within GSM test, for each secondary particle, if the interaction is allowed by the Pauli exclusion principle (box 6). Failure to meet the Pauli principle assumes the incident particle transports into the nucleus further before interacting (box 2). This check ensures only physically allowed processes occur. After satisfying the Pauli principle, depending on the energy of the produced secondary particle (box 7), the secondary particle will either be absorbed or be tracked (box 8) as a new particle in the INC, and interact further (box 9, then 2). This process is repeated until the primary and all secondary particles no longer interact, having been absorbed or leaving the nucleus (box 11), upon which the INC simulation is completed and the residual nuclei's equilibration is simulated (box 12) after simulating the coalescence of emitted cascade nucleons (not shown in Fig. 2). Ref. [3] contains more detailed information regarding Fig. 2.

Fig. 2. Flow chart of CEM, GSM, and LAQGSM INC physics calculations.

The standard version of the DCM within GSM utilizes requires several assumptions. Apart from those stated above, the standard DCM assumes 7 concentric and constant nuclear density zones [6] and assumes

time-independence of collisions during the INC process. This version of the DCM approximates the collision of the incident particle with the target nucleus as a series of successive quasi-free collisions of the fast cascade particles with the intranuclear nucleons [3], accounting for various scatter and absorption mechanisms. Note also the standard DCM applies different physics for photonuclear reactions (incident γ -particles). Emission of secondary particles is assumed isotropic azimuthally, and randomly sampled along the θ angle⁴. The Pauli principle is checked in the DCM by assuming target nucleons occupy all energy levels, up to the Fermi energy, and considers if the produced secondary has an energy smaller than that of the Fermi energy [6]. Detailed information on the standard version of the DCM may be found in Ref. [3, 9], particularly in Ref. [4, 17, 18], and references therein.

The non-standard version of the DCM used in GSM considers the interactions of fast cascade particles, or participants, with nucleon spectators of both the incident and target nuclei in addition to the potential interaction between participants [9]. The non-standard DCM [11], coupled with the QGSM [12–16], that GSM employs eliminates some of the assumptions used in its INC calculation. A continuous nuclear matter density, following that of a Fermi distribution, instead of 7 concentric zones, is used [7]. Unlike the standard version of the DCM employed by GSM, reflection and refraction of the incident particle is not calculated due to the use of a continuous nuclear density. The “trawling” effect, or depletion of nuclear density, is also tracked in addition to the time of intranuclear collisions throughout the development of the cascade. The non-standard DCM accounts for the time between participant and spectator collisions and particle formation times. This hybrid version of the DCM is said to use experimental cross sections below, and the QGSM above (for relativistic hadron-hadron collisions), energies of $\sim 4.5 \text{ GeV}/A$ to simulate the angular and energy distributions of cascade particles [7, 9]. The QGSM used within GSM approximates the nuclear collisions as many independent quark-gluon strings [12–16], and the quark dynamics calculations required are minimized by further simplification of the quark-gluon string [7]. Physics regarding QGSM can be found in Ref. [7, 12–16], and references therein.

2.3 The Coalescence Model

Emitted cascade nucleons may coalesce to create high-energy fragments via final state interactions among emitted cascade nucleons [19, 20]. The coalescence model used by GSM assumes that all emitted cascade nucleons must have a small momentum difference and appropriate isotopic content to form a high-energy composite particle [9]. The coalescence process relies on the overlap in a quantum mechanical wave of the emitted cascade nucleons [20], and GSM uses an approximation to this. GSM also utilizes a recent improvement to the coalescence model, where it was expanded to include emission of light fragments up to ${}^7\text{Be}$ [21, 22]. This expansion provides GSM with greater predictive power for high-energy light fragments.

⁴Note both the standard and non-standard DCM used by GSM utilize a spherical 3-dimensional geometry for its simulations.

2.4 The Preequilibrium Model

The residual nucleus will attempt to de-excite proceeding the INC process, likely emitting fragments as it de-excites. The preequilibrium model used in the CEM, GSM, and LAQGSM event generators simulates the equilibration of the residual nucleus. GSM, like CEM, uses an expanded version of the modified Exciton Model (MEM) to calculate this de-excitation [23, 24]. The expanded version of the MEM will simulate this de-excitation via nuclear transitions and track emittance of fragments, ranging from d , t , ${}^3\text{He}$, etc., up to ${}^{28}\text{Mg}$ [1]. Additionally, the MEM uses energy-*dependent* condensation probabilities, in addition to tracking fragments larger than ${}^4\text{He}$ [25], providing improvements to the preequilibrium emission probabilities calculated in GSM versus those of LAQGSM.

2.5 The Evaporation and Fission Models

Once in an equilibrated state, after the “fast” or precompound stage of the reaction, the resulting compound nucleus will continue to de-excite. GSM considers evaporation or fission of the compound residual nucleus once it reaches this state. GSM uses an extension of the Generalized Evaporation Model (GEM), implemented in a code called GEM2, for its evaporation and fission models, much like its predecessors [6, 9]. GEM2, developed by Furihata [26–29], is based on Atchison’s model [30, 31], commonly referred to as the Rutherford Appleton Laboratory (RAL) fission model, using the Weisskopf-Ewing approach [10] to determine the probability of evaporation. Within GEM2, both evaporation and fission of the compound residual nucleus can occur, where fission “competes” with evaporation during neutron emission [3]. The mass distribution of fissioning isotopes depends on the type of fission, and the charge and kinetic energy distributions are assumed to follow a Gaussian distribution [3, 9]. GEM2 has been modified within GSM and its predecessors [9], namely that it was extended to include fission of isotopes with atomic numbers $Z \geq 65$, and parameters modified [32, 33] to better described fission when used in conjunction with the INC and equilibration models in GSM and its predecessors [9]. Note that GEM2 systematics rely heavily on experimental data, not fundamental physics, as suggested by Ref. [34]. This method of calculation then requires a re-parameterization of the level density parameters within GSM, and other models, when upgrades are made to either, or both, of the INC and equilibration models (if present) [9].

2.6 The Fermi Break-Up Model

Fermi break-up is considered in GSM for fragments at all stages and residual nuclei with mass numbers smaller than 13, *e.i.* $A_{fr} \leq 12$. Fermi break-up is used for these fragments and residual nuclei in place of preequilibrium and/or evaporation and fission for several reasons [9]. Fermi break-up, instead of evaporation and fission, is used for these nuclides to account for the unique nuclear structure of these smaller nuclides

and potential α -particle clustering these smaller nuclei may have, such as in isotopes like carbon and oxygen. The use of Fermi break-up also prevents the use of poor statistical assumptions made with such a minuscule number of nucleons [35]. Fermi break-up follows the idea that two particles, when incident upon each other with large kinetic energies, will suddenly break up and release a large amount of energy. The assumption is then made that the energy is dissipated into the surrounding nucleons, creating smaller high energy fragments proportional to the particle's weight [35, 36].

2.7 The Random Number Generator

GSM, like many other event generators, relies heavily on the Monte Carlo method and underlying statistical assumptions, such as assuming the unique structure of large nuclei can be neglected due to a large sample of resulting nuclei. The random number generator (RNG) used within GSM is the same as that of CEM, or MCNP, code version 5 [37]. Additionally, GSM can use the RNG of LAQGSM instead within the modified DCM/QGSM code. GSM uses the MCNP5 RNG by default. The RNGs available to GSM uniformly produce random numbers on the interval of $[0, 1)$, much like most standard RNGs typically used. The default RNG used by GSM is of the linear-congruential generator type, meaning that it can efficiently generate random numbers, and in addition can “skip ahead” in the random number sequence, a useful feature for parallel calculations⁵. The default RNG in GSM produces random numbers with a precision equal to that of 63 bits, and a period on the order of 10^{18} [37]. The other RNG available to parts of GSM was adopted from an RNG created by F. James around 1987. The RNG created by James was based on a lagged Fibonacci sequence, producing random numbers with a 24-bit precision and a period on the order of 10^{43} [38]. Both RNGs utilized by GSM have been extensively analyzed and used in several other codes, providing reassurance of their reliability.

3 VERIFICATION OF GSM

GSM, as mentioned previously, is a coupling of the INC model of LAQGSM and the CEM event generators. GSM was constructed such that the INC routines used for the spallation reaction in LAQGSM were made available for the main routines of CEM to use. The fragment and residual nuclei information was then transferred to the appropriate variables that CEM uses to store and tally fragment and residual data. Minor modifications have been made to the routines following the INC calculation in the code to allow for larger residual projectile data to be obtained.

GSM has been verified to include the same physics models that both CEM and LAQGSM use. The code used for the modified DCM version in GSM was taken directly from the code of LAQGSM, with minor modifications and upgrades completed since. The underlying CEM code within GSM has remained as-is,

⁵Note that GSM cannot simulate spallation reactions in parallel at this time.

apart from minor modifications. Both of GSM's predecessors, CEM and LAQGSM, have been extensively verified throughout the years based on fundamental physics by several scientists, namely S. Mashnik, K. Gudima, and A. Sierk. The combination of CEM and LAQGSM physics to create GSM implies that GSM models the physics that both CEM and LAQGSM model in a similar manner, meaning GSM has few known errors within its underlying physics models. Results of simulations in GSM, as seen in Sec. 4, lead to the conclusion that GSM incorporates the various physical models into its simulations correctly, and that the models utilized by GSM are sufficient for the reactions observed. Additionally, GSM has been verified to produce consistent results between simulations, modifications of various non-physics related options in GSM, and between various calculational media.

The creation of GSM has allowed for significantly more maintainable code. GSM is more maintainable than CEM and LAQGSM for several reasons, namely that GSM reduces the logical complexity of using two separate, but related, models, and because the reduction of GSM's logical complexity will result in fewer errors between the models, requiring less time and maintenance than previously necessary to resolve errors. Minor modifications made to GSM have also made GSM less prone to errors. The addition of a verbosity filter to GSM, coupled with the inclusion of terminal output, aids users and developers in the discovery of errors. The reduction in the various physical models used also aids future development and enhancement of the GSM event generator. The reduction in the number of physical models coded into GSM also reduces the overall size of the event generator and the effort required to maintain it.

The reduction in the number of physical models used in GSM allows it to be $\sim 85\%$ the size of CEM and LAQGSM when combined. The reduction allowed by the use of GSM is roughly $\sim 10\,000$ lines of Fortran66/77 code, further aiding in its ease of maintainability. The individual routines used within GSM, particularly for the code transferred from the LAQGSM event generator, have also been split into multiple files and significant comments added. Although this process creates more files to manage when compiling GSM, it aids future developers by describing the physics of the simulation more clearly, logically, and coherently. Shorter files allow developers to quickly understand the process being underwent in the routine of interest, and in addition results in shorter coded routines. Shorter routines within the code further simplify the use and understanding of what a specific routine is attempting to model. Much of the code required for the modified DCM to function properly was contained in two files, each being more than 10 000 lines long. The main physics routines that are commonly used by the modified DCM were removed from these files, among others, to aid in simplifying the overall code and its potential modernization. The reduction in length significantly boosts the maintainability of the GSM code in the authors' opinion. The complexity of the physics within GSM matches that of the pre-existing CEM and LAQGSM codes. The modernization of the GSM code is highly recommended, such that the portions of GSM utilizing the Fortran66 and Fortran77 standards be modified to use that of Fortran90 or higher. This much needed upgrade has potential to noticeably reduce the complexity of the underlying logic (see Fig. 2⁶) within GSM and its comprehension.

⁶Although the logic of Fig. 2 is clearly presented, the logic within the code is difficult to decipher, heavily utilizing the

Many comments were added to the routines of GSM to help improve the readability of the code when modified by future developers regarding this issue.

GSM in addition is more flexible than either CEM or LAQGSM. This is due to the nature of the physics coupling and additional modifications. The physics simulated within both CEM and LAQGSM are tightly coupled, and as such are as tightly coupled in GSM. GSM, however, has a list of variables by which users and developers can insert, or remove, various physics models when the modified DCM code is used in GSM. This variable list aided in the development of GSM by ensuring it modeled spallation physics correctly via the inclusion, or exclusion, of various physics, and in finding errors, both pre-existing and not, within the code of the underlying physics models in GSM. GSM offers additional flexibility to developers and users via its terminal output, informing them of assumptions or misgivings of a simulation, in addition to both mathematical and programmatic errors, which aid in the use and further development of GSM.

Logical decoupling of the code in the modified DCM physics models was also explored during GSM's development, however has not been verified at this time, and is thus not used in GSM at present. The logical decoupling and modernization of this code has the ability to make GSM more flexible, and in addition will make GSM significantly more human readable and less error prone. Error resolution methods were placed into GSM, primarily regarding input parameter errors, where GSM will assume the user is requesting as much detail as allowable within GSM on a given calculation to ensure the user is obtaining the desired data⁷. There are several segments of code within GSM that can be further simplified and decoupled to aid in its simplification, primarily in the routine simulating post-cascade physics. Some of these recommended improvements, while not deficiencies, are listed in Appendix A for completeness.

Coding standards were employed during the development of GSM. Where possible, no new *common blocks* were created in GSM when coupling the non-standard DCM model with CEM, and instead modules were used according to the Fortran2003 and Fortran2008 standards. Comments were heavily used within the modified portions of code in GSM, such that non-scientists could easily modify the program as instructed if necessary. General, and very basic, guidelines for “good” programming have also been employed in most all additions of code to GSM. Several warnings occur during compilation of GSM regarding the size of the common blocks containing large amounts of data. It is recommended to resolve these warnings for consistency and good programming practice. It is also recommended to remove the use of common blocks, a heavily used (among scientific codes) Fortran66 and Fortran77 feature, and replace with modules or other appropriate mechanism to better control the use of the variables within the common blocks. Although these warnings have no observable affect on the simulation and results of GSM, they present opportunities within GSM for inconsistencies, allowing GSM to have potential, unknown errors within itself. These common blocks are likely those from the transfer of the non-standard DCM code into CEM, resulting in

Fortran66 standard, in particular the non-standard DCM code's heavy use of *go to* statements.

⁷Most codes with this kind of error protection will assume the user is *not* asking for the highest level of detail, however the opposite is assumed in GSM due to the time required for most simulations, in particular light- and heavy-ion induced reactions.

inconsistencies of the variables utilized.

GSM satisfies well the requirements for spallation physics calculations. The functionalities of GSM are the same as both CEM and LAQGSM, but are held within a more robust and comprehensive programmatic framework. The physics models within GSM check for conservation of several tracked particle characteristics, and correct or eliminate data as necessary if the various applicable conservation laws are not met. GSM, as will be seen in the proceeding sections, also reproduces well simulated data agreeable to that of experiment. This is anticipated considering the extensive validation efforts that have been made on CEM and LAQGSM. Internal code reviews informally occurred throughout the GSM development process.

The non-standard DCM code used in GSM follows the calculation outlined by Fig. 2, modeling the introduction of high-energy participant particles into the nucleus and the participant's subsequent collisions and resulting particle cascade. The DCM, both the standard and non-standard versions available to GSM, models the physics that were briefly outlined in Sec. 2.2. The physics parameters used by both DCM versions in GSM for spallation simulations are declared prior to the simulation of any physics models. Fragment data is tracked in two main arrays within both versions of the DCM during simulation, namely the *pmemo* and *imemo* arrays. The data stored in these arrays is used to store fragment data in two different arrays in GSM, namely the *parz* and *spt* arrays⁸. The *parz* and *spt* arrays are used for the remainder of the simulation. Various conservation laws and comparisons of fragment energies to cutoff potentials are examined prior to collecting the fragment data.

Note that when simulating light- and heavy-ion interactions in GSM with the non-standard DCM, the size of the GSM fragment data arrays was often exceeded, allowing for no new fragments to be counted from other physical processes. This deficiency was resolved by assuming that only a few cascade nucleons available to coalesce will not much interact with other cascade nucleons that may coalesce⁹. This assumption allows for the coalescing of the appropriate cascade nucleons and tallying the fragments then, up to the size of the internal GSM arrays, and subsequently emptying the particle bank and filling it with the remaining fragments. The process will repeat until the fragment particle “bank” is no longer filled, upon which the cascade nucleons within the fragment “bank” may coalesce with each other. The error introduced by this assumption is assumed to be small given that the array is not often filled by the INC process alone for most interactions. More information on this assumption may be found in Appendix A, however the size of the internal GSM fragment bank arrays can be increased to remove this memory requirement.

The standard DCM code available to GSM has remained unchanged, while the non-standard version of the DCM code, from LAQGSM, has had minor changes made to it which simply transfer fragment and residual nuclei data to the main data arrays within GSM at the completion of the INC calculation. The transfer of fragment data from the non-standard DCM code to the appropriate variables in GSM was done

⁸The *sptr* array contains information about the fragments physical position.

⁹This assumption seems reasonable for the production of less than ~ 200 cascade fragments, where not all of the fragments will coalesce.

via the use of the *pmemo* and *imemo* arrays within both the standard and non-standard versions of the DCM. Table 3 depicts the information stored within each of these arrays for each version of the DCM available to GSM. Note that the angles, θ and ϕ , in Table 3 for the fragment are those of its direction of motion (in spherical geometry). Fragment data from the standard DCM version did not need to be transformed for use in GSM, however the data, namely that of the fourth through seventh elements of the *pmemo* array, of the non-standard DCM version did need to be transformed prior to its use in GSM. This was done by simple ratios of the fragments' momenta, whose equations are shown below. Note that the fifth element of the *imemo* array is used during the INC simulation only, and therefore no longer contributes to the overall simulation at the completion of the cascade process.

$$\begin{aligned} \cos(\theta) &= \frac{p_z}{|\vec{p}|} \\ \sin(\theta) &= \sqrt{1 - \cos^2(\theta)} \\ \cos(\phi) &= \frac{p_x}{|\vec{p}| \sin(\theta)} \\ \sin(\phi) &= \frac{p_y}{|\vec{p}| \sin(\theta)} \end{aligned}$$

TABLE I. Fragment Data Storage within the GSM INC Models

Variable Name	Standard DCM Description	Non-Standard DCM Description
<i>pmemo</i> (1, <i>k</i>)	Normalized x-position, <i>x</i>	Normalized x-position, <i>x</i>
<i>pmemo</i> (2, <i>k</i>)	Normalized y-position, <i>y</i>	Normalized y-position, <i>y</i>
<i>pmemo</i> (3, <i>k</i>)	Normalized z-position, <i>z</i>	Normalized z-position, <i>z</i>
<i>pmemo</i> (4, <i>k</i>)	$\sin(\theta)$	X Momentum, p_x
<i>pmemo</i> (5, <i>k</i>)	$\cos(\theta)$	Y Momentum, p_y
<i>pmemo</i> (6, <i>k</i>)	$\sin(\phi)$	Z Momentum, p_z
<i>pmemo</i> (7, <i>k</i>)	$\cos(\phi)$	Formation Time in the INC, t_f^c
<i>pmemo</i> (8, <i>k</i>)	Kinetic Energy, E_k	Kinetic Energy, E_k
<i>pmemo</i> (9, <i>k</i>)	Rest Mass, E_0	Rest Mass, E_0
<i>imemo</i> (1, <i>k</i>)	Atomic Number, <i>Z</i>	Atomic Number, <i>Z</i>
<i>imemo</i> (2, <i>k</i>)	Gamma ID (0 or 1)	Gamma ID (0 or 1)
<i>imemo</i> (3, <i>k</i>)	Strangeness (Decay Number)	Strangeness (Decay Number)
<i>imemo</i> (4, <i>k</i>)	Mass Number, <i>A</i>	Mass Number, <i>A</i>
<i>imemo</i> (5, <i>k</i>)	Nuclear Zone	Time Parameter

Known deficiencies, including some brief recommendations and suggested investigations for improvements to the GSM code architecture, are listed and described in Appendix A. The suggested resolution to the deficiency is given in Appendix A when sufficient investigation on the deficiency was done. External

code reviews of GSM are recommended for its further verification, in addition to further simplification and decoupling of the non-standard DCM code. Many routines still exist within the non-standard version of the DCM that exist within the standard version of the DCM, however with slight modification. It is recommended to further study these routines and simplify the overall code architecture of GSM where possible. Profiling was performed on some GSM simulations to determine which physics models required the most computation time. Some discrepancies within the non-standard DCM version were discovered regarding the use of a few specific routines and are currently under investigation. Few conclusions regarding the discrepancies can be made at this time.

Continued verification of GSM is recommended. It is clear that GSM is fairly well verified at this time apart from some very specific areas of interest within the GSM code. Comparisons to the results of CEM, LAQGSM, and experimental data, when available, are made in the proceeding section for the validation of GSM.

4 VALIDATION OF GSM

The validation of GSM presented here is primarily focused on unit testing via a black-box methodology, *i.e.* without modification of any internal GSM variables or consideration of the internal workings of GSM. The amount and diversity of simulated interactions is assumed to reach all relevant physics models available to GSM. Note that GSM's predecessors, CEM and LAQGSM, have been extensively validated, most recently in Ref. [39–42]. GSM, as stated in previous sections, uses the same underlying physics models and codes that are used in both CEM and LAQGSM, using that of CEM in most cases of repeated models. GSM is tested against results produced by both CEM and LAQGSM when available for this reason. GSM is primarily validated against experimental data here.

Known deficiencies of GSM, and potential unstable areas of GSM, are listed in Appendix A. Software crash protection has been added to many parts of the non-standard DCM code, as was done to a large portion of GSM's underlying CEM code base in Ref. [42]. Said crash protection involves preventing two types of mathematical errors, namely divide-by-zero and square-root protection, where a warning is printed to the user and corrected for in-simulation. It is recommended to streamline the invoked protection within the non-standard DCM code further to reduce the computation time of the simulation. Data obtained from profiling both GSM and LAQGSM has also shown that GSM replicates the physics used in LAQGSM, a thoroughly validated code [39–41], for most physics models. Observed differences in these simulations are currently under investigation to better understand these differences, namely the use of the *repij* routine.

GSM has been shown to produce consistent results across a few machines. It is recommended to transfer GSM's makefile to *cmake* to aid in GSM's portability so it can be run on any system. GSM currently has been seen to operate well on both Linux and macOS systems. GSM uses the *gfortran* Fortran compiler at this time, with no interdependencies on the machine's operating system.

4.1 Unit and Regression Testing of GSM

Much unit and regression testing was completed with GSM. The unit and regression testing presented here primarily focuses on results produced by GSM regarding differential fragment production cross sections.

4.1.1 Proton Induced Reactions

Fig. 3 demonstrates that the predicted production cross sections made by GSM are in good agreement with that of experimental data, and duplicate the predictions made by CEM. LAQGSM predictions were produced for the simulation shown in Fig. 3, and are shown to be an order of magnitude smaller than experiment. LAQGSM data was observed to have better agreement with that of experiment and the other event generators for ${}^6\text{Li}$ near angles representative of backscatter, however this figure is not shown here. It was observed that all of the event generators were within an order of magnitude at all angles, being the least representative of experiment near glancing angles. The GSM and CEM event generators appear to over estimate experiment for low energy ${}^6\text{Li}$ fragments, however have an overall good agreement with the experiment. Fig. 3 demonstrates that neither GSM or CEM well model the affect the coulomb barrier has on the emittance probability of various fragments.

Fig. 3. GSM, CEM, and LAQGSM predictions for the double differential production cross section of ${}^6\text{Li}$ fragments emitted at 20° to a 480 MeV proton beam incident on a ${}^{107}\text{Ag}$ target. Experimental data was obtained from Ref. [43].

GSM, in perfect agreement with the CEM predictions, appears to well predict experiment for the

simulation shown in Fig. 4. GSM and CEM well predict the experiment of Fig. 4 at other angles near perfectly, however have the worst predictions at glancing angles, as is shown in Fig. 4. Note also that Fig. 4 suggests both GSM and CEM over estimate transport of the incident proton through the nucleus, meaning the event generators do not correctly model physics within this energy regime, or that the experiment was not approximately representative of a proton incident upon a single layer of ^{232}Th . The thickness of the target used for the experiment represented in Fig. 4 was 3 cm thick, violating this assumption and suppressing the transport of the incident proton through the ^{232}Th medium. The event generators do agree well with experiment for most other fragment energies. LAQGSM data was not produced for neutron fragments, however was within an order of magnitude for other fragments observed (not shown here).

Fig. 4. GSM and CEM predictions for the double differential production cross section of neutron fragments emitted at 10° to a 1.2 GeV proton beam incident on a ^{232}Th target. Experimental data was obtained from Ref. [44].

Fig. 5 demonstrates predictions from both GSM, CEM, and LAQGSM for the $^{232}\text{Th} (1.2 \text{ GeV } p, X)$ reaction. Both GSM and CEM simulations over-predict experimental data for fragments having kinetic energies between ~ 20 to 60 MeV, while LAQGSM under-predicts the data everywhere but within the same energy region. It is concluded then that improvements made to the CEM coalescence and equilibration models, from Ref. [1, 21, 22, 25, 42], have improved the predictions of the GSM and CEM event generators for most all fragment kinetic energies, particularly for the high energy fragments. It is suggested that more events be simulated using the LAQGSM event generator to better determine its accuracy and precision relative to the experimental data shown in Fig. 5.

Fig. 6 demonstrates the general agreement of data produced by the event generators and LAQGSM.

Fig. 5. GSM, CEM, and LAQGSM predictions for the double differential production cross section of ${}^6\text{Li}$ fragments emitted at 100° to a 1.9 GeV proton beam incident on a ${}^{197}\text{Au}$ target. Experimental data was obtained from Ref. [45].

Note that the predictions made by LAQGSM do not predict the data of the experiment in Fig. 6 as well as the other event generators, that it tends to diverge from experimental results for higher energy ${}^7\text{Li}$ fragments. This affect was not as prevalent for ejected ${}^{10}\text{B}$ fragments, not shown here, at varying angles. Fig. 6 also demonstrates that GSM and CEM well predict the maximum production cross sections found during experiment.

Fig. 7 demonstrates that GSM, like in other figures, produces exactly the results of CEM for reactions involving incident nucleons below ~ 4.5 GeV. It is apparent in Fig. 7 that both event generators underestimate the experimental data observed by roughly half for most fragment energies. Observance of other fragments yielded that LAQGSM was in agreement with the predictions by both GSM and CEM, giving the conclusion that the LAQGSM data would have similar results to those shown in Fig. 7. The underestimation observed questions if the INC and Fermi break-up models used within GSM need further examination, since all fragments and residual nuclei simulated are sufficiently small that the physics modeled in simulation precludes the preequilibrium and evaporation/fission of the residual compound nucleus. More comparisons of this reaction type are recommended to fully determine the necessity of such an investigation considering the fair agreement of the event generator predictions to the data.

Fig. 8 demonstrates the predictions produced by GSM and CEM compared to experimental results. It is seen in Fig. 8 that GSM and CEM do both produce results in good agreement with the experimental data. The results of CEM appear to better predict data at this incident energy than GSM does, mainly for high energy ${}^4\text{He}$ fragments. Note that GSM is using the non-standard DCM for its INC simulation. GSM does

Fig. 6. GSM, CEM, and LAQGSM predictions for the double differential production cross section of ${}^7\text{Li}$ fragments emitted at 35° to a 2.5 GeV proton beam incident on a ${}^{27}\text{Al}$ target. Experimental data was obtained from Ref. [46].

Fig. 7. GSM and CEM predictions for the double differential production cross section of proton fragments emitted at 32° to a 3 GeV proton beam incident on a ${}^9\text{Be}$ target. Experimental data was obtained from Ref. [47].

so for incident nucleons, photons, and pions with kinetic energies above ~ 4.5 GeV, and also for all light- and heavy-ion induced reactions. It is recommended to perform a best-fit analysis to determine the event generator that best predicts experimental data for the reaction shown in Fig. 8. Note however that GSM can use the standard DCM for its INC simulation with a different cutoff energy.

Fig. 8. GSM and CEM predictions for the double differential production cross section of ^4He fragments emitted at 90° to a 5.5 GeV proton beam incident on a ^{238}U target. Experimental data was obtained from Ref. [48].

Fig. 9 shows the angular dependence of the cross section, where 0 degrees represents a forward peaked scatter, and 180 degrees backscatter of the fragment. The predictions shown in Fig. 9 seem to yield the conclusion that GSM better predicts experiment for this reaction, contrary to the conclusion that can be drawn from Fig. 8. Note also that LAQGSM seriously underestimates this experiment for this, and later observed, energy integrated spectrum.

Table II shows the required computation times for each proton-induced reaction. GSM required, on average¹⁰, 101.9% of the time required by CEM when using CEM physics. It is suspected the slight increase in computation times is due to the modified handling of errors in GSM, for which refactoring is recommended. GSM required 50.0%, on average¹¹, and 94.3% of the time required by LAQGSM when using CEM and LAQGSM physics, respectively. A larger sample of experimental data is sought after for proton-induced reactions above ~ 4.5 GeV to provide statistical information on GSM computation

¹⁰The standard deviation in GSM-CEM computation time ratios was observed to be 1.2% for these reactions when using CEM physics.

¹¹The standard deviation in GSM-LAQGSM computation time ratios was observed to be 16.7% (16.6% for CEM-LAQGSM ratios) for these reactions when using CEM physics.

Fig. 9. GSM, CEM, and LAQGSM predictions for the energy integrated production cross section of ^{10}B fragments from a 5.5 GeV proton beam incident on a ^{238}U target. Experimental data was obtained from Ref. [48].

times when LAQGSM physics models are used. Note each simulation using CEM, GSM, and LAQGSM simulated the same number of events, 10 million, to provide comparable computation times.

4.1.2 Neutron Induced Reactions

Fig. 10 shows the predictions made by GSM and CEM for the reaction shown. LAQGSM was used to simulate the reaction, however did not produce any predictions for ^{12}C fragments. It seems that both GSM, in exact agreement with CEM, predicts the reaction well compared to approximate experimental data. The experimental data shown in Fig. 10 is for ^{12}C fragments in an excited state of 4.44 MeV. The comparison from this is at best approximate, however it seems that GSM data is in fair agreement with this experiment. The excited state of the nucleus likely leads to larger cross sections, combined with the low incident energy of the particle, seem to negate the anticipated overestimation of ^{12}C fragment production, as was seen in other reactions with incident particles having kinetic energies below $\sim 4.5 \text{ GeV}$.

Fig. 11 demonstrates a good agreement between experimental data and that of the GSM and CEM event generators. Inference of the data shown in Fig. 11 provides this conclusion, however the event generator data produced does not as well match the slight variations in the data. Not shown in Fig. 11 are large relative uncertainties within the experimental data¹². The general agreement by the experimental data and that of the event generators is brought into question given the large uncertainties within the experimentally

¹²Examples of the uncertainties quoted by Ref. [50–55] include 0.49366 mb/sr/MeV at 17 MeV to $7.52 \cdot 10^{-4}$ mb/sr/MeV at 114 MeV, equating to relative uncertainties up to $\sim 1000\%$.

TABLE II. Computation Times for Proton Induced Reactions (in hours)

Reaction	CEM	GSM	LAQGSM
^{15}N (35.05 MeV p , X)	0.05	0.05	0.08
^{19}F (96 MeV p , X)	0.57	0.58	1.03
^{107}Ag (480 MeV p , X)	1.65	1.67	3.09
^{197}Ni (1.2 GeV p , X)	0.57	0.58	0.98
^{232}Th (1.2 GeV p , X)	0.63	0.64	1.17
^{63}Cu (1.732 GeV p , X)	0.28	0.28	0.46
^{197}Au (1.9 GeV p , X)	0.86	0.87	1.41
^{27}Al (2.5 GeV p , X)	0.97	0.99	2.80
^9Be (3 GeV p , X)	0.31	0.32	1.71
^{208}Pb (3.17 GeV p , X)	1.28	1.30	2.16
^{12}C (3.17 GeV p , X)	0.04	0.04	0.20
^{238}U (5.5 GeV p , X)	1.88	3.56	3.78

Fig. 10. GSM, CEM, and LAQGSM predictions for the energy integrated production cross section of ^{12}C fragments from a 28.15 MeV neutron beam incident on a ^{12}C target. Experimental data was obtained from Ref. [49].

available results. A simulation by LAQGSM for the same number of events produced no recognizable results for any of its fragments, and the results produced were well below those of GSM and CEM.

Fig. 11. GSM and CEM predictions for the double differential production cross section of ${}^4\text{He}$ fragments emitted at 80° to a 175 MeV neutron beam incident on a ${}^{209}\text{Bi}$ target. Experimental data was obtained from Ref. [50–55].

Predictions for ${}^3\text{He}$ fragment production cross sections are compared to experimental data in Fig. 12. Good general agreement is found between GSM and experimental data at low ${}^3\text{He}$ energies, however GSM tends to underestimate the data for higher fragment kinetic energies. LAQGSM predictions for other fragments appear to be in general agreement with that of GSM, and CEM is in perfect agreement with GSM. Error within the experimental data is roughly represented by the size of the markers, being around $\sim 20\%$ for most of the data, relative to the respective datum point. The small error within the experimental data infers that the event generators may need further improvement, however they do provide a fairly accurate first-order estimate of the data of Fig. 12.

Predictions by GSM and CEM for the fragment production of tritium are shown in Fig. 13. Fig. 13 shows general overall agreement between data of the event generators and of experiment. LAQGSM predictions for heavier fragments, such as ${}^7\text{Li}$, were observed to be in fair agreement with the GSM and CEM predictions. Fair agreement of data was observed at all angles observed for the given reaction.

Backscatter predictions made by GSM and CEM are compared to experimentally obtained data in Fig. 14. Fig. 14 demonstrates general agreement with experimentally obtained data, however with a slight overestimation of the measured results. Uncertainties in the data are on the order of $\sim 6\%$ for the lower energy fragments, and up to $\sim 40\%$, relative to the respective data, for the experimental data shown. Also

Fig. 12. GSM and CEM predictions for the double differential production cross section of ^3He fragments emitted at 40° to a 175.4 MeV neutron beam incident on a ^{28}Si target. Experimental data was obtained from Ref. [55–57].

Fig. 13. GSM and CEM predictions for the double differential production cross section of tritium fragments emitted at 90° to a 383 MeV neutron beam incident on a ^{63}Cu target. Experimental data was obtained from Ref. [58].

note the equivalence of the GSM and CEM predictions in Fig. 14.

Fig. 14. GSM and CEM predictions for the double differential production cross section of deuterium fragments emitted at 164° to a 542 MeV neutron beam incident on a ^{209}Bi target. Experimental data was obtained from Ref. [58].

Table III shows the required computation times for each neutron-induced reaction. GSM required, on average¹³, 102.3% of the time required by CEM when using CEM physics. It is suspected the slight increase in computation times is due to the modified handling of errors in GSM. GSM required 44.8%, on average¹⁴, of the time required by LAQGSM when using CEM physics, respectively. Experimental data is sought after for neutron-induced reactions above $\sim 4.5 \text{ GeV}$ to provide statistical information on GSM computation times when LAQGSM physics models are used. Note each simulation using CEM, GSM, and LAQGSM simulated the same number of events to provide comparable computation times. Each reaction shown in Table III simulated 10 million events.

4.1.3 Light-Ion Induced Reactions

As stated near the start of Sec. 4, GSM was observed to have slight discrepancies in the physics models used from that of LAQGSM when profiling various light-ion induced reactions, namely with the use of the *repij* routine. The *repij* routine requires near 4% of the simulation time for most interactions with the non-standard DCM of LAQGSM, and is nearly never used within the non-standard DCM of GSM for

¹³The standard deviation in GSM-CEM computation time ratios was observed to be 2.3% for these reactions when using CEM physics.

¹⁴The standard deviation in GSM-LAQGSM computation time ratios was observed to be 8.5% (8.7% for CEM-LAQGSM ratios) for these reactions when using CEM physics.

TABLE III. Computation Times for Neutron Induced Reactions (in hours)

Reaction	CEM	GSM	LAQGSM
^{12}C (28.15 MeV n , X)	0.56	0.58	0.94
^9Be (60 MeV n , X)	0.35	0.36	0.81
^6Li (118 MeV n , X)	0.27	0.28	0.76
^{209}Bi (175 MeV n , X)	1.41	1.42	3.07
^{28}Si (175.4 MeV n , X)	0.56	0.56	1.17
^{12}C (225 MeV n , X)	0.31	0.33	1.03
^{63}Cu (383 MeV n , X)	1.03	1.02	2.02
^{209}Bi (542 MeV n , X)	2.47	2.50	5.67
^{27}Al (800.0 MeV n , X)	0.73	0.74	1.89

the observed light-ion interactions. The profiling was done using *gprof*, revealing that GSM may deviate from the appropriate physics, or that the produced fragments have different properties than those of GSM normally. It is suspected this is occurring due to missing or modified physics parameters used within the QGSM portion of GSM's INC, and in addition is thought to skew the results produced by GSM. Minimal results are shown regarding light-ion data due to the known deficiencies within GSM, and it is highly recommended to further develop GSM for light- and heavy-ion induced reactions.

Scattering differential cross sections are plotted in Fig. 15. GSM is seen to better predict the angular dependence of the production cross sections than LAQGSM in Fig. 15. The results produced by the event generators however are in poor agreement with the available experimental data. Fig. 15 also shows that LAQGSM was able to produce more predictions for the interaction than GSM, the opposite of that seen in previous figures. The event generators do however produce a spectrum that appears to match that of experimental results, but at two orders of magnitude smaller. The poor data agreement between the event generators and experimental data could also be due to the fact that the incident ^{10}B particles are well below the desired threshold energy of $\sim 4.5 \text{ GeV/A}$. Additionally, the scattering models used in GSM and LAQGSM during the INC simulation may need to be further evaluated and modified to better fit the produced data.

Fig. 16 demonstrates that GSM well predicts experimental data for the shown reaction. GSM is observed to underestimate the experimentally obtained data marginally for low-energy fragments, however underestimates experiment by a factor of ~ 3 for fragments with kinetic energies $\sim 40 \text{ MeV}$. Note however that relative uncertainties were as high as $\sim 70\%$ for fragments near $\sim 40 \text{ MeV}$, and thus the GSM data lies within these deviations. LAQGSM data was compared to predictions made by GSM for ^6Li fragments, and was in near-perfect agreement with GSM for fragment energies up to $\sim 80 \text{ MeV}$. Production cross sections for higher fragment energies were predicted to be less than that of GSM. Observed angular dependence of the experimentally determined cross sections, not shown here, did not agree as well with GSM. GSM had over predicted this data by roughly a factor of 2 near backscattering angles, but was in general agreement

Fig. 15. GSM and LAQGSM predictions for the energy integrated production cross section of ${}^7\text{Li}$ fragments from a 51 MeV ${}^{10}\text{B}$ beam incident on a ${}^7\text{Li}$ target. Experimental data was obtained from Ref. [59].

with experiment for forward peaked angles.

Table IV shows the required computation times for each of the observed light-ion induced reactions. GSM required 76.7%, on average¹⁵, of the time required by LAQGSM when using the non-standard DCM for its INC physics. The increased speed by which GSM computes these reactions is thought to be considerable given how often the models will be used when calculating high-energy spallation physics within a particle transport code, such as MCNP. Note each reaction shown in Table IV simulated 1 million events.

4.2 Continued Validation Efforts of GSM

GSM appears to replicate experimental data well for most of reactions simulated. It is highly recommended that further validation of GSM occur with the inclusion of more tests. The tests should require, in total, the use of all calculation options available to GSM. Analysis tools should be created in addition to aid in this endeavor. This process includes creating tools to analyze particle multiplicities, yields, and other output calculations GSM can perform. For details on these calculation options may be found in Ref. [6]. It is also recommended to perform a best fit analysis for all simulations performed to quantitatively determine how well GSM simulates energetic spallation reactions and their properties during experimentation, in addition to providing a numerical basis for the deprecation of LAQGSM.

¹⁵The standard deviation in GSM-LAQGSM computation time ratios was observed to be 27.6% for these reactions when using the non-standard DCM for its INC physics.

Fig. 16. GSM predictions for the double differential production cross section of ${}^4\text{He}$ fragments emitted at 90° to a 6.7 GeV deuterium beam incident on a ${}^{58}\text{Ni}$ target. Experimental data was obtained from Ref. [60].

TABLE IV. Computation Times for Light-Ion Induced Reactions (in hours)

Reaction	CEM	GSM	LAQGSM
${}^7\text{Li}$ (51 MeV ${}^{10}\text{B}$, X)	N/A	6.64	6.69
${}^{232}\text{Th}$ (220 MeV ${}^{11}\text{B}$, X)	N/A	23.08	20.71
${}^{197}\text{Au}$ (319 MeV ${}^{11}\text{Li}$, X)	N/A	68.86	67.26
${}^1\text{H}$ (490.4 MeV ${}^8\text{He}$, X)	N/A	0.21	0.90
${}^{27}\text{Al}$ (1.14 GeV ${}^{12}\text{C}$, X)	N/A	3.01	4.14
${}^{16}\text{O}$ (1.14 GeV ${}^{12}\text{C}$, X)	N/A	1.71	2.89
${}^{48}\text{Ti}$ (1.14 GeV ${}^{12}\text{C}$, X)	N/A	5.66	6.75
${}^{238}\text{U}$ (4.2 GeV d, X)	N/A	33.45	35.39
${}^{12}\text{C}$ (4.64 GeV ${}^{16}\text{O}$, X)	N/A	1.41	3.04
${}^{58}\text{Ni}$ (6.7 GeV d, X)	N/A	5.69	7.67

Continued validation efforts will focus primarily on expanding the number of reactions GSM is compared against, particularly within its suggested energy regime of $\sim 100 \text{ MeV}$ to $\sim 1 \text{ TeV/A}$. The tests should collectively require the use of all GSM features. Daily regression testing on many interactions is also suggested. This would be done via automated testing, where all differences in results are stored within a central file for analysis later. The regression testing suite is recommended to utilize all of GSM's calculation options for all reaction types within several energy regimes each. The regression testing suite is recommended to contain around 100 simulations or more to be complete.

Continued validation efforts can be further improved and expanded to include the use of white box methods, meaning tested simulations focus on using specific areas of the physics models internal to GSM, taking into account the code architecture of GSM. Recommendations stated above are also strongly encouraged for the continuing validation efforts of GSM. In short, the inclusion of more simulations of various types should be done to further validate the physics simulated by GSM. The portability of GSM should also be studied in more detail, particularly with the use of *cmake* on several differing systems for many reactions.

Further validation of GSM is recommended, however it has been seen that GSM simulates high-energy events well for incident nucleons. More extensive validation of GSM using its other available features, such as fragment multiplicity, is highly recommended in addition to the previously stated recommendations. Further development of GSM, in particular for light- and heavy-ion reactions, is recommended prior to placement of GSM into MCNP.

5 SUMMARY

The purpose of this document was to verify and validate the GSM event generator. It was seen from Sec. 4, in particular Sec. 4.1, that GSM could still be improved upon further. It is highly recommended that GSM be compared against more experimental results, particular those measuring multiplicities, yields, and other characteristics that GSM can compare to. Appendix A lists several known deficiencies in GSM, in addition to several suggested investigations to further improve the integrity and stability of GSM and calculations made by it. Validation of GSM revealed several problem areas of GSM, and in addition showed its strengths. Based on experimental data obtained for production cross sections from light-ion induced reactions, GSM is not recommended to replace LAQGSM in its current state, however shows promise.

The discussion on the verification of GSM, in Sec. 3, concluded that the creation of GSM has many benefits and provides many simplifications to the event generators, and in addition could provide great simplification to other codes intending to use the event generators. It is recommended that further simplification of duplicate physics models internal to GSM be further simplified, and in addition that external code reviews are conducted. Validation of GSM showed that it exactly replicates the results of CEM for incident nucleons with kinetic energies below $\sim 4.5 \text{ GeV}$. It is recommended that several simulations be conducted

on incident pions and photons to reinforce this conclusion. Additionally, light-ion induced reactions yielded many differences from the GSM and LAQGSM event generators. Neither event generator consistently matched experimental data, indicating that the physics being measured for each experiment may not have been purely that of high-energy spallation models, *e.g.* scattering cross sections (see Sec. 4.1.3). Use of the non-standard DCM, being transferred from LAQGSM, is recommended for further investigation to ensure the physics being utilized within the DCM model is similar to that of its use within LAQGSM. It is recommended to investigate the declaration of physics parameters prior to the INC simulation to ensure correct setup of the various physical parameters is done, verifying that the physics and its underlying assumptions being modeled match between GSM and LAQGSM, and that produced secondaries during the cascade have similar properties. A best fit analysis was not completed on the available data, however is highly recommended to quantitatively define the event generator that best matches the experimental data for a given reaction.

It is concluded from the above that GSM is beneficial, however further study ought to be completed based on the results observed in Sec. 4.1.3. The benefits of GSM, namely the reduced length, increased maintainability, and reduced computation times, are thought to be highly beneficial over the LAQGSM event generator. Further investigation as to the cause of the poor results in Sec. 4.1.3 is recommended, and that GSM fully deprecate LAQGSM upon its continued validation of the results in Sec. 4.1.3 and the other features available to GSM.

6 FURTHER RECOMMENDATIONS

It is recommended that the use of the non-standard DCM within GSM be further verified and validated. It is recommended that the physics parameters used to establish the assumptions used within the models be investigated, and from there that the physics GSM models is found to be similar to that of LAQGSM by use of code profiling techniques. It is also recommended that a brief study be done to ensure all necessary parameters are transferred from the non-standard DCM to the remainder of GSM physics, ensuring that no data is omitted from the calculation.

Further simplification of duplicate GSM physics models is also recommended. This simplification would involve detecting all duplicate physics models employed within GSM and verifying the existence of differences in the models. The differences can be incorporated into one model to make it more compact, allowing the overall code to become more maintainable and economical. It is also recommended that code reviews take place when appropriate. It is suggested that the assumption of poorly interacting emitted cascade nucleons be further verified to have little to no bearing on the results of the simulation. Recommendations are also made, however not as strongly as the previous ones, that all common blocks used within the non-standard DCM be eliminated in favor of modules to further update the code and to increase GSM's stability when using the code, and to ensure no parameters are incorrectly declared within

each routine.

Continued validation of GSM is highly recommended. It is suggested that, upon resolving the errors involved with the discrepancies observed in Sec. 4.1.3, GSM be validated again for all appropriate light- and heavy-ion collisions included here, and in addition that GSM be validated against experimental data obtained regarding particle multiplicities and yields, possibly cross sections of reaction “channels”, mass and charge distributions, and possibly double differential cross sections for fission only.

It is also recommended that a regression testing directory be created. This directory is meant to simulate many reactions, and then compare against previously ran interactions to verify that unintended changes within GSM do not occur. This testing directory has yet to be established, but is highly recommended. Additional, but not necessary, improvements to GSM are listed in Appendix A.

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We ask readers of this report to contact the authors of the report using the e-mail addresses¹⁶ provided in case of questions, comments, or discovered “bugs.” We thank them in advance for comments and information about possible problems in using this code and for any information given on bugs that may be discovered.

¹⁶Please *cc* all authors of this document when inquiring about GSM or providing feedback to ensure it is received.

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A KNOWN DEFICIENCIES AND RECOMMENDATIONS IN GSM

GSM has several known deficiencies, most of which are listed here. The purpose of this section is to provide documentation for some of GSM's shortcomings and proposed solutions, providing a basis for future V&V work, or general improvements, on GSM. Note that not all deficiencies within GSM are listed, however most all of those observed are.

1. Anti-lab system use for low energy particles incident on light targets:

- (a) Description: GSM forces the use of the time-dependent cascade model when using the anti-lab system. The anti-lab system is used when the incident particle is heavier than the target nucleus ($A_p > A_t$). This becomes an issue when the incident particle is low in energy, where GSM would typically assume time-independence within the INC model for this reaction.
- (b) Recommendation: Add anti-lab correction terms to the time-independent INC model, and validate its inclusion accordingly.

2. Coulomb barrier corrections

- (a) Description: Historically, fragments produced at energies below the coulomb barrier had to be manually removed because they could not have enough energy to overcome the energy well created by the coulomb barrier. This removal of fragments at low energies could be automatically estimated and removed.
- (b) Recommendation: Creation of a filter that ensures all produced fragments have sufficient kinetic energies to overcome the coulomb barrier is recommended and thought to be sufficient.

3. Fragment reset during INC simulation

- (a) Description: The data variables that GSM uses for its secondary particle storage (its secondary particle "bank") may contain information for up to 150 secondary particles, while those used in the non-standard DCM-QGSM model can contain information for up to 5 999 secondary particles. Secondary particles that no longer interact are stored into GSM's variable arrays immediately prior to what would be the storage of the secondaries within the non-standard DCM-QGSM hybrid INC model. These arrays are emptied at a point near their maximum capacity (150 secondaries) by first simulating the coalescence of the stored secondaries, then by tallying the remaining fragments, and those produced via coalescence, into the *dadz* and *dadz4* arrays, as is done for all fragments and secondaries in GSM. Once the arrays are emptied, information on the remaining secondary particles is stored into the emptied arrays, and the process repeats until the arrays are no longer nearly filled. This method assumes that the secondaries produced in the different secondary particle "batches" will not interact with secondaries from other "batches",

potentially producing less light and heavy fragments, *e.g.* fragments from d, t, ^3He , etc., up to ^{28}Mg .

- (b) Recommendation: The assumption of non-interaction between secondaries of different “batches” can be eliminated by increasing the size of the internal GSM arrays. It is recommended to perhaps create a central parameter within the routines using these GSM arrays, and then dynamically allocate memory for those arrays up to 110% of the number of produced secondaries. This method would ensure the size of the arrays is sufficient for storage of produced secondary particle information from the INC, equilibration, evaporation/fission, and Fermi break-up models. It is also recommended to reduce the size of the arrays internal to the non-standard DCM-QGSM code for memory management purposes.

4. Perturbation of energy dependence regarding the F_j model

- (a) Description: The F_j model is an improvement to the γ_j model used in the simulation of the emitted cascade nucleon coalescence probability [21]. The F_j model is energy dependent, where the parameterization relies on the kinetic energy of the incident particle. The calculation of F_j was not properly established for perturbative calculations, but only for a single simulation, and the calculation of the F_j values was not corrected for when the incident particle’s kinetic energy was incrementally increased for that simulation, resulting in incorrect F_j values used within perturbative calculations.
- (b) Recommendation: Placement of the initialization of the F_j values within GSM should be moved later during the initialization of GSM. This recommendation has been completed, however the results of the discrepancy have not yet been validated for perturbative calculations.

A short list of recommended improvements to GSM are included below. These recommendations are not necessary, however will aid in the code simplification of GSM and will help make GSM more robust to errors and may help improve its memory management.

1. Cleanup of post-INC physics in main routine

- (a) Description: The main routine in GSM sets up initial parameters and makes calls to the INC, equilibration, and evaporation models. The equilibration and evaporation of excited and compound nuclei is considered for both the target and incident particle. As a result, the main routine is difficult to navigate and very long, not complying well with standard coding practices.
- (b) Recommendation: It is recommended to branch the main routine into more routines. The branching of the main routine would be split into the declaration of parameters with calls to the INC, an expanded equilibration, expanded evaporation, and expanded Fermi break-up routines.

The “expansion” can act as a step to further simplify the main routine so it’s structure is, in essence, similar to the following:

```
subroutine gsm03()  
  .  
  .  
  .  
  call declareParameters()  
  
  do i = 1, numEvents  
  
30    continue  
  
    ! Reset storage of fragment data  
    call resetArrays()  
  
    call INCModel()  
    if ( checksFail ) go to 30    ! Re-run particle event  
  
    call coalescenceModel()  
    if ( checksFail ) go to 30    ! Re-run particle event  
  
    call equilibrationModel()  
    if ( checksFail ) go to 30    ! Re-run particle event  
  
    ! For compound target nucleus  
    if ( aResTarg <= 12 ) then  
      call fermiBreakUp()  
    else  
      call evaporationModel()  
    end if  
    if ( checksFail ) go to 30    ! Re-run particle event  
  
    ! For compound projectile nucleus  
    if ( aResProj <= 12 ) then  
      call fermiBreakUp()  
    else
```

```

        call evaporationModel()
    end if
    if ( checksFail ) go to 30    ! Re-run particle event

    call storeFragments()
end do

call createOutput()
return

end subroutine gsm03

```

2. General code modernization

- (a) Description: Many portions of GSM are written using Fortran77 standards, with much Fortran90 and Fortran2003 spread out over various routines in GSM. The non-standard DCM-QGSM hybrid INC model within GSM uses significant amounts of Fortran66 and Fortran77, with very little Fortran90 spread throughout its code.
- (b) Recommendation: It is recommended that much of the Fortran66 code be modernized to current standards, using languages such as Fortran2003 and Fortran2008. Additionally, the inclusion of comments within these portions of code are highly recommended, and the linguistic unification of GSM's code is recommended¹⁷.

3. Upgrade of most, or all, common blocks

- (a) Description: GSM relies heavily on the use of *common blocks* for its simulations. Common blocks are a feature of the Fortran77 programming language that allow for routines to access data from other programmatic routines easily without passing numerous variables between each other. The common blocks used within GSM oftentimes do not include all the variables available to that common block, resulting in differing sizes of the named common block throughout the program. This is not of concern in terms of memory management, however is a poor programming practice. Additionally, inclusion of common blocks allows one routine the change some, or all, of the variables within the common block, allowing for unintended changes to variables within GSM. This again gives rise to another poor programming practice, compared to modern standards, making GSM susceptible to potential errors.

¹⁷Variables within GSM are mostly four to eight letter acronyms, whose acronyms are representative of the physical parameter (or theoretical variable), in either English, French, German, or Russian. Simplifying these variables to use a single language, namely English, will help reduce the technical debt in the program.

- (b) Recommendation: It is recommended to replace all common blocks with modules, or similar, for this method of data storage. Modules are suggested as an alternative because they can act similar to common blocks, however are safer to use. Use of modules will allow for the simplification of the routines themselves and the safety of unused variables. As a simple example, common blocks can be used as follows:

```

subroutine setTargetA(tempA)

    implicit real*8 (A-H), (O-Z)
    integer*4 projectileA , projectileZ

    ! /input/ block also contains ‘‘targetZ’’, ‘‘cm0’’,
    !    and ‘‘t0mev’’ variables.
    common / input / projectileA , projectileZ , targetA

    targetA = tempA

    return
end subroutine setTargetA

```

Use of a module within the same subroutine as above would yield the following:

```

subroutine setTargetA(tempA)

    ! inputParams module has same variables as /input/ common
    !    block above, however only ‘‘targetA’’ is accesible
    !    within this subroutine
    use inputParams , only : targetA

    implicit none
    real(kind=8), intent(in) :: tempA

    targetA = tempA

    return
end subroutine setTargetA

```

The above example demonstrates several improvements that modules provide over common blocks. One such improvement is that the variables within the common block do not need to

be declared within the subroutine. This is because they are all centrally declared within the module. This allows for the variables to all be the same size throughout the program, something GSM fails at currently. The above examples also demonstrate how the declaration and use of variables within GSM can be easily updated when transferring data to modules. The use of modules also allows for all data variables to be easily modified if necessary. Changing the size of an array within a common block, for example, would require changing the size of it within *all* uses of the common block within the entire program. Use of a module would instead require only modifying the array within the module, and in addition would allow opportunities to make GSM significantly more robust. The robustness could come about by adding a variable that sets, or is representative of, the size of the array within the module or some physical limitation. The routines using this array throughout GSM could then use this as a check to ensure that the array's limits are never exceeded when the array is being filled, or the array could instead be dynamically allocated, and subsequently deallocated, throughout the simulation. Variables used in such a manner could help ensure that limitations within subroutines are never exceeded. Clearly, the use of modules in place of common blocks will allow for a significantly more robust code.

4. Simplification of Fermi break-up uses

- (a) Description: GSM applies Fermi break-up physics (see Sec. 2.6) at all stages of the simulation where appropriate. GSM simulates the Fermi break-up in consistent ways, however must transform variables prior to the routines use, and is done several times within GSM and its routines.
- (b) Recommendation: It is recommended to create a “layer” around the Fermi break-up model within GSM. The “layer” will act as a method of unifying the use of Fermi break-up within GSM, further simplifying its organization, readability, and data storage.

5. Code reduction

- (a) Description: Many parts of the CEM and LAQGSM event generator code are similar, exactly matching each other in some areas of code. Although the primary physics routines used within these event generators have been reduced for use inside GSM, there are still several areas with minor and negligible differences.
- (b) Recommendation: The removal of these near-duplicate routines is recommended, and the differences between the subroutines and functions implemented within that of CEM and its use determined by a flagged variable. The reduction in code will allow for further simplification and maintainability of GSM for future developers, in addition to a potential reduction in GSM's required computation time.