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CEM03.03 and LAQGSM03.03 Event Generators for MCNP6, MCNPX and MARS15 Transport Codes.

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## CEM03.03 and LAQGSM03.03 Event Generators for MCNP6, MCNPX, and MARS15 Transport Codes

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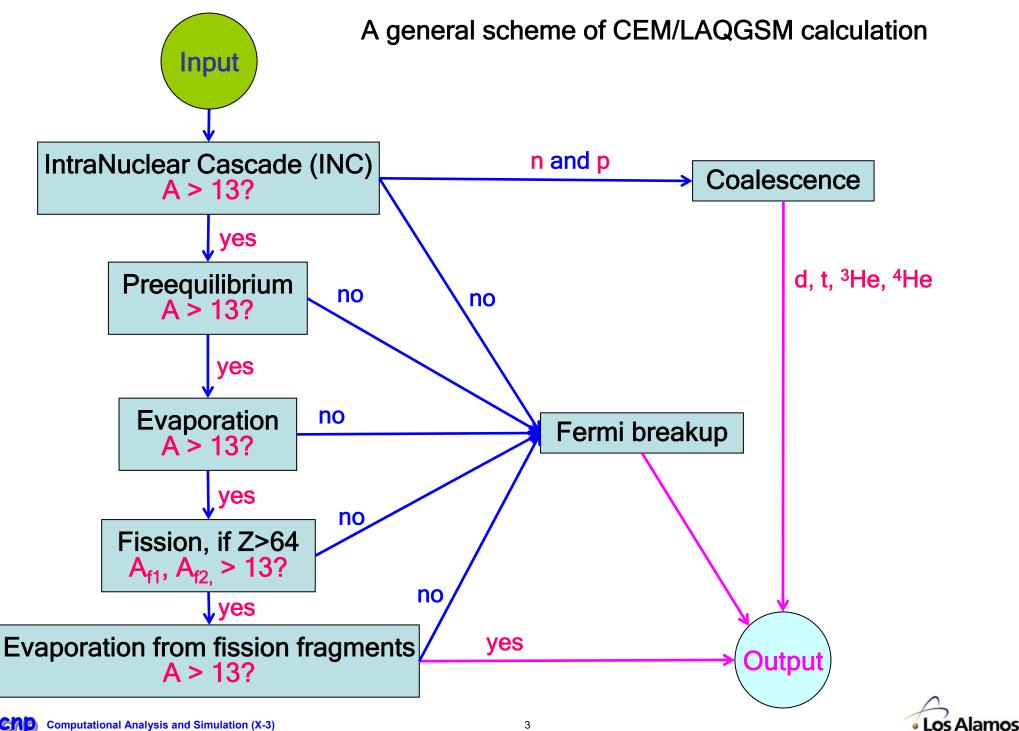


### • Introduction

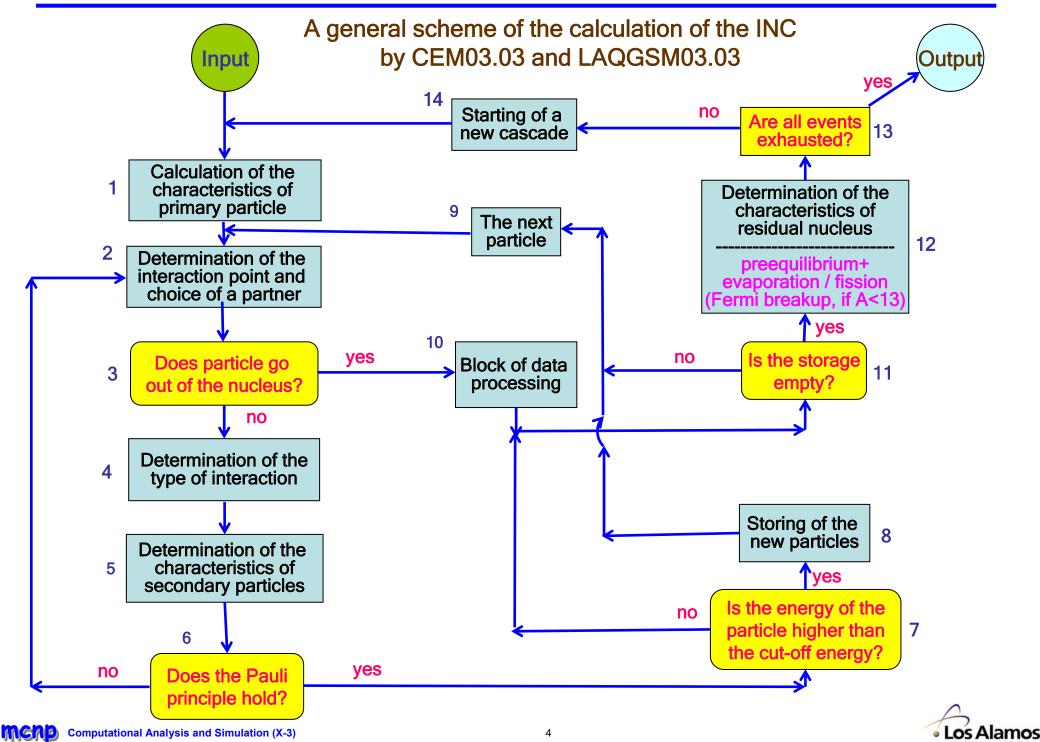
- INC of CEM03.03 and LAQGSM03.03
- The coalescence model
- Preequilibrium [the Modified Exciton Model (MEM)]
- Evaporation
- Fission
- Fermi break-up of light nuclei (A<13)
- Fission-like binary-decay by GEMINI and multifragmentation by the Statistical Multifragmentation Model (SMM) in the "G" and "S" versions of CEM03.01 and LAQGSM03.01
- Summary













The INC of CEM03.03 is based on the "standard" (non-timedependent) version of the Dubna cascade model [1,2], improved and developed further at LANL during recent years [3-6]:

**1)** V. S. Barashenkov, K. K. Gudima, and V. D. Toneev, JINR Communications P2-4065 and P2-4066, Dubna (1968); P2-4661, Dubna (1969); Acta Physica Polinica <u>36</u> (1969) 415.

2) V. S. Barashenkov and V. D. Toneev, *Interaction of High Energy Particle and Nuclei with Atomic Nuclei*, Atomizdat, Moscow (1972); V. S. Barashenkov, *et al.*, Sov. Phys. Usp. <u>16</u> (1973) 31.

3) S. G. Mashnik and A. J. Sierk, Proc. SARE-4, Knoxville, TN, Sep. 13-16, 1998, pp. 29-51 (nucl-th/9812069).

4) S. G. Mashnik and A. J. Sierk, Proc. AccApp00, Washington, DC, USA, Nov. 12-16, 2000, pp. 328-341 (nucl-th/0011064).

5) S. G. Mashnik, K. K. Gudima, A. J. Sierk, R. E. Prael, Proc. ND2004, Sep. 26 — Oct. 1, 2004, Santa Fe, NM, AIP Conf. Proc. <u>769</u>, pp. 1188-1192 (nucl-th/0502019)

6) S. G. Mashnik, M. I. Baznat, K. K. Gudima, A. J. Sierk, R. E. Prael, J. Nucl. and Radiochem. Sci. <u>6</u>, (2005) pp. A1-A19 (nucl-th/0503061).

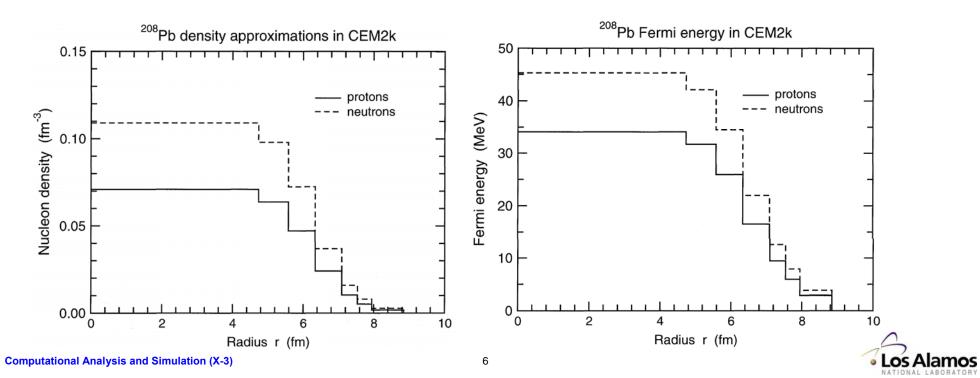




The nuclear matter density  $\rho(r)$  is described by a Fermi distribution

$$\rho(r) = \rho_p(r) + \rho_n(r) = \rho_0 \{1 + exp[(r-c)/a]\}$$
where  $c = 1.07A^{1/3}$  fm and  $a = 0.545$  fm

the target nucleus is divided by concentric spheres into seven zones The energy spectrum of the target nucleons is estimated with the local Fermi energy  $T_F(r) = \hbar^2 [3\pi^2 \rho(r)]^{2/3}/(2m_N)$ 





$$\begin{split} NN &\to NN, \qquad NN \to \pi NN, \qquad NN \to \pi_1, \cdots, \pi_i NN \\ \pi N \to \pi N, \qquad \pi N \to \pi_1, \cdots, \pi_i N \qquad (i \geq 2) \\ \pi NN \to NN \\ \sigma_{\gamma A} &= L \frac{Z(A-Z)}{A} \sigma_{\gamma d} \\ \gamma + p \quad \to \quad p + \pi^0 , \\ \quad \to \quad n + \pi^+ , \\ \quad \to \quad p + \pi^0 + \pi^0 , \\ \quad \to \quad n + \pi^+ + \pi^0 . \end{split}$$

 $V \equiv V_N(r) = T_F(r) + \epsilon, \quad V_\pi \simeq 25 \text{ MeV},$ 

Pauli principle forbids a number of intranuclear collisions





The integral cross sections for the free NN,  $\gamma$ N, and  $\pi$ N interactions are approximated using a special algorithm of interpolation/extrapolation through a number of picked points, mapping as well as possible available experimental data.

For CEM97, we have developed an improved, as compared with the standard Dubna INC, algorithm for approximation of cross sections and developed simple and fast approximations for elementary cross sections which fit very well presently available experimental data not only to 5 GeV, the upper recommended energy for the present version of the CEM, but up to 50-100 GeV and higher, depending on availability of data (see details in: S. G. Mashnik and A. J. Sierk, LA-UR-98-5999; E-print: nucl-th/9812069.)

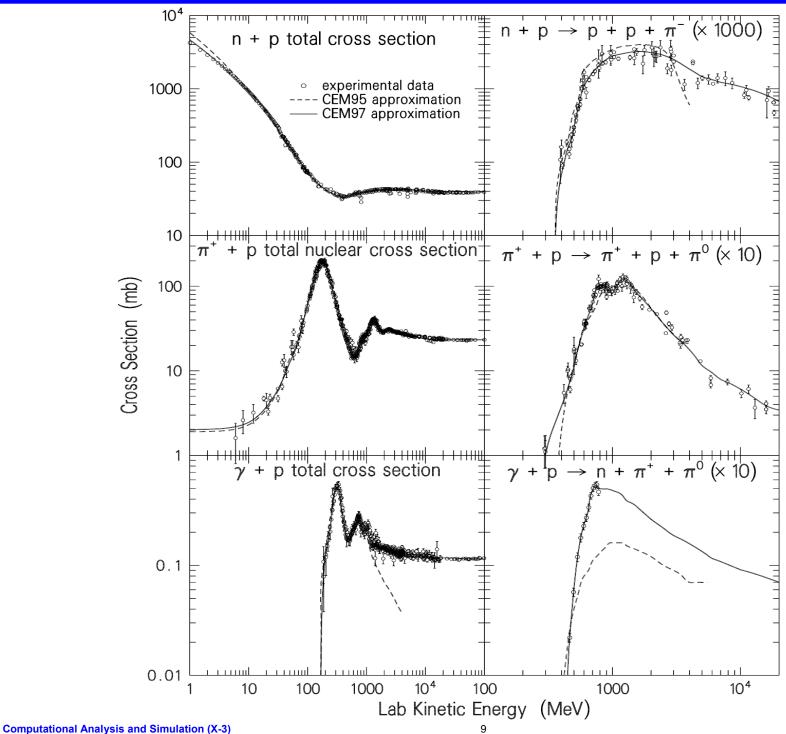
We have developed new approximations for 34 different types of elementary cross sections induced by nucleons, pions, and gammas. Integral cross sections for other types of interactions taken into account in CEM03.01 are calculated from isospin considerations using the former as input.



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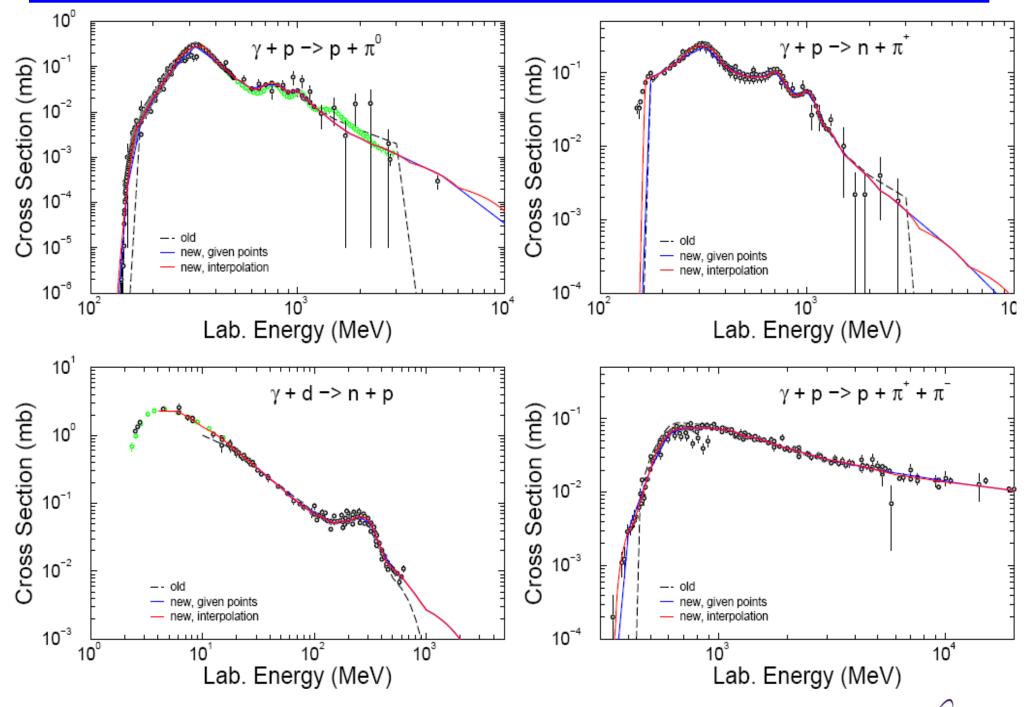
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Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions, ICTP, 4 - 8 February 2008, S.G. Mashnik et al., LA-UR-08-0867



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Computational Analysis and Simulation (X-3)



The cosine of the angle of emission of secondary particles in the c.m. system is calculated by the Dubna INC as a function of a random number  $\xi$ , distributed uniformly in the interval [0,1] as

$$\cos \theta = 2\xi^{1/2} \left[ \sum_{n=0}^{N} a_n \xi^n + (1 - \sum_{n=0}^{N} a_n) \xi^{N+1} \right] - 1 ,$$

where N= M= 3, 
$$a_n = \sum_{k=0}^M a_{nk} T_\gamma^k \ ,$$

where the coefficients  $a_{nk}$  were fitted to the then available experimental data at a number of incident kinetic energies  $T_i$ , then interpolated and extrapolated to other energies.

The distribution of secondary particles over the azimuthal angle  $\varphi$  is assumed isotropic.

For elementary interactions with more than two particles in the final state, the Dubna INC uses the statistical model to simulate the angles and energies of products.







For the improved version of the INC in CEM03.01, we use currently available experimental data and recently published systematics proposed by other authors and have developed new approximations for angular and energy distributions of particles produced in nucleon-nucleon and photon-proton interactions.

So, for pp, np, and nn interactions at energies up to 2 GeV, we did not have to develop our own new approximations analogous to the ones described above, since reliable systematics have been developed recently by Joseph Cugnon et al. for the Liege INC, then improved still further by Helder Duarte for the BRIC code; we simply incorporate into CEM03.01 the systematics by Duarte.

J. Cugnon, C. Volant, and S. Vuillier, Nucl. Phys. A620 (1997) 475; A. Boudar, J. Cugnon, S. Leray, and C. Volant, Phys. Rev. C 66 (2002) 044615; Th. Aoust and J. Cugnon, Eur. Phys. J. A21 (2004) 79;

Helder Duarte, Proc ADTT'99, Praha, Czech Republic, June 7--11, 1999, web page <u>http://fjfi.cvut.cz/con\\_adtt99;</u> Proc. 10th Int. Conf. on Nuclear Reaction Mechanisms, Varenna, Italy, June 9-13, 2003; http://lxmi.mi.infn.it/~gadioli/registered.htm; Phys. Rev. C 75 (2007) 024611.





Similarly, for  $\gamma p$  and  $\gamma n$  interactions, we take advantage of the event from the Moscow INC kindly sent us by its coauthor, Dr. Igor Pshenichnov.

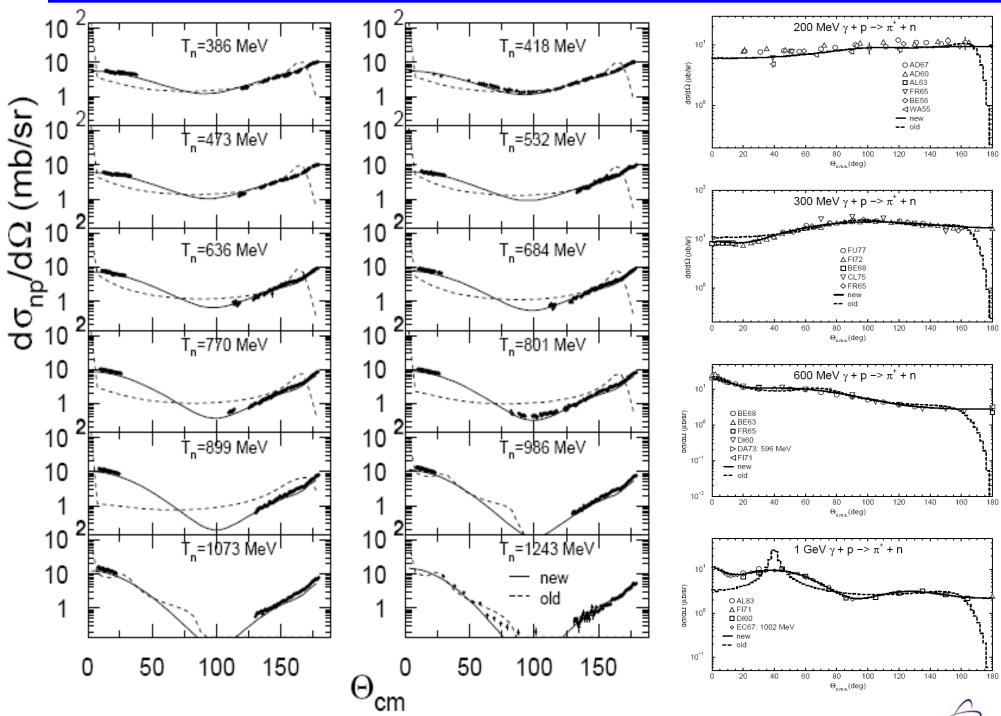
In CEM03.01, we use part of a data file with smooth approximations through presently available experimental data, developed for the Moscow INC and have ourselves developed a simple and fast algorithm to simulate unambiguously  $d\sigma/d\Omega$  and to choose the corresponding value of  $\Theta$  for any  $E_{\gamma}$ , using a single random number  $\zeta$ uniformly distributed in the interval [0,1].

A. S. Iljinov, I. A. Pshenichnov, N. Bianchi, E. De Sanctis,
B. V. Muccifora, M. Mirazita, and P. Rossi,
Nucl. Phys. A616 (1997) 575.





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**MCND** Computational Analysis and Simulation (X-3)



The condition for transition from the INC stage of a reaction to preequilibrium is considered by CEM03.03 differently for cascade particles with energies below and above 150 MeV:

1) An effective local optical absorptive potential is defined from the local interaction cross section of the particle, including Pauli-blocking effects. This imaginary potential is compared to one defined by a phenomenological global optical model. We characterize the degree of similarity or difference of these imaginary potentials by the parameter

$$\mathcal{P} = |(W_{opt.\,mod.} - W_{opt.\,exp.})/W_{opt.\,exp.}|.$$

When this parameter increases above an empirically chosen value, the particle leaves the cascade, and is then considered to be an exciton. At incident energies below 100 MeV, CEM03.01 uses a fixed value of 0.3 for this parameter, just as all its predecessors did. With this value, we find that the cascade stage of the CEM is generally shorter than that in other cascade models. This leads to an overestimation of preequilibrium particle emission at incident energies above about 150 MeV, and correspondingly to an underestimation of neutron production from such reactions. This is why:

2) At higher incident energies, the "sharp cut-off" method with a cutoff energy  $T_{cut} = 1 \text{ MeV}$  for the cascade particles was proposed in CEM2k. This "ad hoc" rough criterion solved the problem of underestimating neutron production at high energies, but provided an unphysical discontinuity in some observables calculated by MCNPX using CEM2k.

3) In CEM03.01, this problem is solved by using a smooth transition from the first criterion to the second one in the energy interval from 75 to 225 MeV, so that no discontinuities are produced in results from CEM03.01.



The initial versions of CEM, just like LAQGSM and other INC-type models, calculate the total reaction cross section, using the geometrical cross section, and the number of inelastic, and elastic, simulated events, namely:

$$\sigma_{in} = \sigma_{geom} N_{in} / (N_{in} + N_{el}).$$

This approach provides a reasonable good agreement with available data at incident energies above about 100 MeV, but is not reliable at lower bombarding energies and for some photonuclear reactions. To address this problem, we have incorporated into CEM2k the NASA systematics by Tripathi et al. for all incident protons and neutrons with energies above the maximum in the NASA reaction cross sections, the Kalbach systematics for neutrons of lower energy, and, in CEM03.01, the Kossov systematics for all photonuclear reactions:

R. K. Tripathi, F. A. Cucinotta, and J. W. Wilson, NIM B117 (1996) 347;

C. Kalbach, J. Phys. G: Nucl. Part. Phys. 24 (1998) 847:

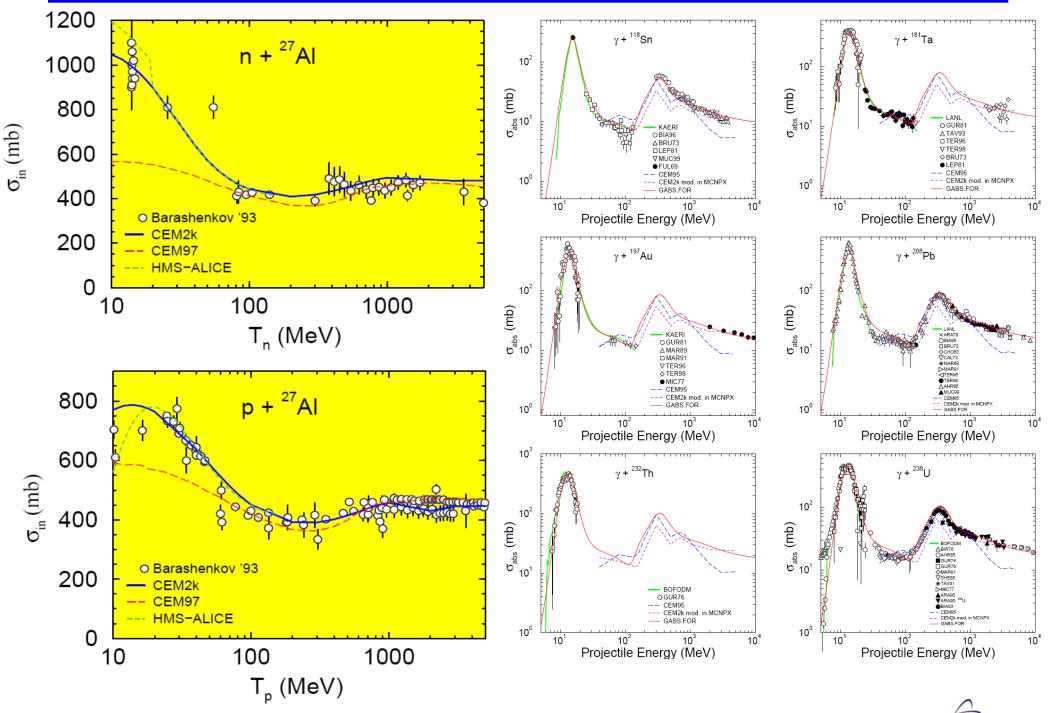
M. V. Kossov, Eur. Phys. J. A 14 (2002) 377.

Computational Analysis and Simulation (X-3)





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**MCND** Computational Analysis and Simulation (X-3)



#### The INC of CEM03.03 does not take into account the so-called "trawling" effect:

Than is, in the beginning of the simulation of each event, the nuclear density distributions for the protons and neutrons of the target are calculated and stored in the memory and a subsequent decrease of the nuclear density with the emission of cascade particles is not taken into account.

Our analysis of different characteristics of nucleon- and pion-induced reactions for targets from C to Am has shown that this effect may be neglected at incident energies below about 5 GeV in the case of heavy targets like actinides and below about 1 GeV for light targets like carbon.

At higher incident energies the progressive decrease of nuclear density with the development of the intranuclear cascade has a strong influence on the calculated characteristics and this effect has to be taken into account.

This is why, in transport codes that use as event generators both CEM03.01 and our high-energy code LAQGSM03.01, we recommend simulating nuclear reactions with CEM03.01 at incident energies up to about 1 GeV for light nuclei like C and up to about 5 GeV for actinide nuclei, and to switch to simulations using LAQGSM03.01, which considers the "trawling" effect and provide better results, at higher energies of transported particles, and this is why we present here and use in MCNPX/6 and MARS both our CEM and LAQGSM event generators.



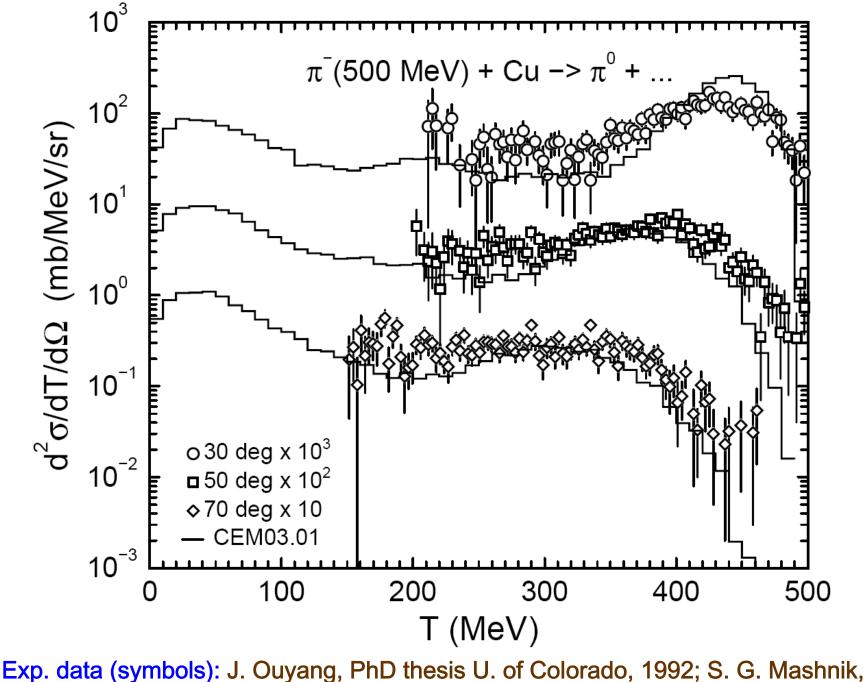


# In comparison with the initial version [1,2] of INC, in CEM03.03 we have:

- 1) Developed better approximations for the total elementary cross sections;
- 2) Developed new approximations to describe more accurately experimental elementary energy and angular distributions of secondary particles from hadron-hadron and photon-hadron interactions;
- 3) Normalized photonuclear reactions to detailed systematics developed by
   M. Kossov and nucleon-induced reactions, to NASA and Kalbach systematics;
- 4) The condition for transition from the INC stage of a reaction to preequilibrium was changed; on the whole, the INC stage in CEM03.03 is longer while the preequilibrium stage is shorter in comparison with previous versions;
- 5) Incorporation of real binding energies for nucleons in the cascade instead of the approximation of a constant separation energy of 7 MeV used in the initial versions of the CEM; imposing momentum-energy conservation for each simulated even (provided only "on the average" by the initial versions);
- 6) The algorithms of many INC routines were changed and almost all INC routines were rewritten, which speeded up the code significantly;
- 7) Some preexisting bugs in the INC were fixed.







R. J. Peterson, A. J. Sierk, M. R. Braunstein, Phys. Rev. <u>C61</u> (2000) 034601





The INC stage of reactions is described by LAQGSM03.03 with a recently improved version [1] of the time-depending intranuclear cascade model developed initially in Dubna, often referred in the literature simply as the Dubna intranuclear Cascade Model, DCM [2], using the Quark-Gluon String Model (QGSM) [3] to describe elementary interactions at energies above 4.5 GeV.

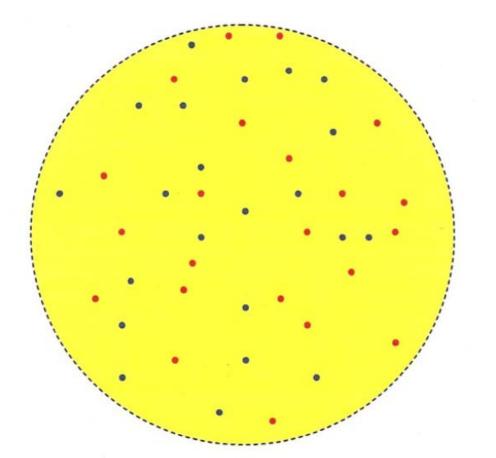
[1] S.G. Mashnik, K.K. Gudima, M.I. Baznat, A.J. Sierk, R.A. Prael, N.V. Mokhov, LANL Report, LA-UR-06-1764, Los-Alamos (2006).
[2] V.D. Toneev, K.K. Gudima, Nucl. Phys. A400 (1983) 173c.
[3] N.S. Amelin, K.K. Gudima, V.D. Toneev, Sov. J. Nucl. Phys. 51 (1990) 327; ibid. 51 (1990) 1730; ibid. 52 (1990) 172; N. S. Amelin, CERN/IT/ASD Report CERN/IT/99/6, Geneva, Switzerland (1999).





#### LAQGSM uses a continuous nuclear distribution (no "zones")

$$\rho(r) = \rho_p(r) + \rho_n(r) = \rho_0 \{1 + exp[(r-c)/a]\}$$
where  $c = 1.07A^{1/3}$  fm, and  $a = 0.545$  fm

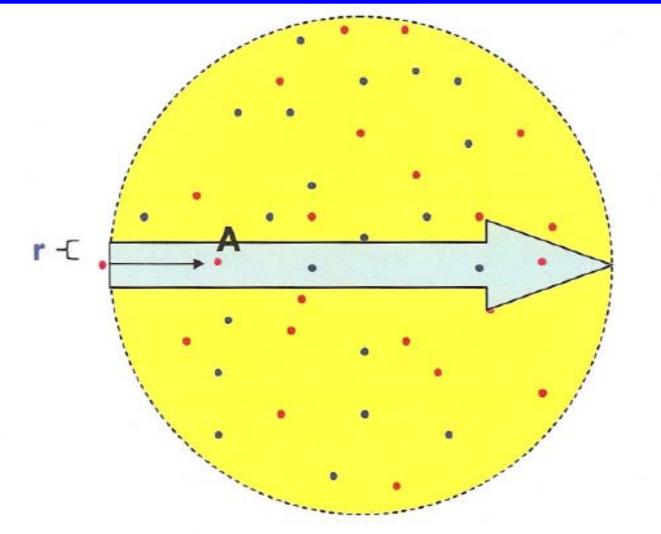


Before starting to simulate an INC event, position of all IntraNuclear nucleons are simulated and "frozen"







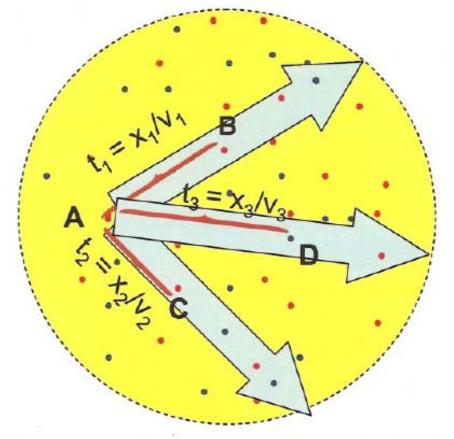


The projectile interacts (in point **A**) with the nearest target nucleon met inside the cylinder with the radius **r** 

 $r = r_{int} + \lambda/2\pi$ , where  $r_{int} = 1.3$  fm;  $\lambda/2\pi$  is the de Broglie wavelength







 $t_{1(2,3,...)}^{f}$  is the formation time of the cascade particle #1(2,3,...) If  $t_2 < t_1$ ,  $t_2 < t_3$ ,..., and  $t_2 > t_2^{f}$ , particle #2 interacts first in point C IntraNuclear nucleons involved in interactions become "cascade" particles and are removed from the status of "frozen" target nucleons (trailing effect)

The formation time:  $t^{f} = (E/m)t_{f}^{0}$ ;  $t_{f}^{0} = C_{t} \hbar/m_{\pi}$ ;  $C_{t} = 1.0$  for mesons and ~0.0 for baryons





				• • •	
	$\gamma p$ -interactions	$\gamma n$ -interactions		$\gamma p$ -interactions	$\gamma n$ -interactions
1	$\gamma p \to \pi^+ n$	$\gamma n \rightarrow \pi^- p$	33		$\gamma n \to \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 n$
2	$\gamma p \rightarrow \pi^0 n$	$\gamma n \rightarrow \pi^0 n$	34		$\gamma n \to \pi^+ \pi^- \pi^0 \pi^0 \pi^0 \pi^0 n$
3	$\gamma p \to \Delta^{++} \pi^-$	$\gamma n \to \Delta^+ \pi^-$	35	$\gamma p \to \pi^+ \pi^+ \pi^- \pi^- \pi^0 \pi^0 p$	$\gamma n \to \pi^+ \pi^+ \pi^- \pi^- \pi^0 \pi^0 n$
4	$\gamma p \rightarrow \Delta^+ \pi^0$	$\gamma n \to \Delta^0 \pi^0$	36	$\gamma p \to \pi^+ \pi^+ \pi^+ \pi^- \pi^- \pi^- p$	$\gamma n \to \pi^+ \pi^+ \pi^+ \pi^- \pi^- \pi^- n$
5	$\gamma p \to \Delta^0 \pi^+$	$\gamma n \to \Delta^- \pi^+$	37	$\gamma p  ightarrow \pi^+ \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 n$	$\gamma n \rightarrow \pi^- \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 p$
6	$\gamma p  ightarrow  ho^0 p$	$\gamma n \to  ho^0 n$	38	$\gamma p  ightarrow \pi^+ \pi^+ \pi^- \pi^0 \pi^0 \pi^0 n$	$\gamma n \rightarrow \pi^+ \pi^- \pi^- \pi^0 \pi^0 \pi^0 p$
7	$\gamma p  ightarrow  ho^+ n$	$\gamma n  ightarrow  ho^- p$	39	$\gamma p \rightarrow \pi^+ \pi^+ \pi^+ \pi^- \pi^- \pi^0 n$	$\gamma n \rightarrow \pi^+ \pi^+ \pi^- \pi^- \pi^- \pi^0 p$
8	$\gamma p \to \eta p$	$\gamma n \to \eta n$			
9		$\gamma n  ightarrow \omega n$	40	$\gamma p  ightarrow \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 p$	$\gamma n \rightarrow \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 n^0$
10	/1	$\gamma n \to \Lambda K^0$	41	$\gamma p \rightarrow \pi^+ \pi^- \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 p$	$\gamma n \rightarrow \pi^+ \pi^- \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 n$
11	$\gamma p \to \Sigma^0 K^+$	$\gamma n \to \Sigma^0 K^0$	42	$\gamma p \rightarrow \pi^+ \pi^+ \pi^- \pi^- \pi^0 \pi^0 \pi^0 p$	$\gamma n \rightarrow \pi^+ \pi^+ \pi^- \pi^- \pi^0 \pi^0 \pi^0 n$
12	$\gamma p \rightarrow \Sigma^+ K^0$	$\gamma n \to \Sigma^- K^+$	43	$\gamma p \rightarrow \pi^+ \pi^+ \pi^+ \pi^- \pi^- \pi^- \pi^0 p$	$\gamma n \rightarrow \pi^+ \pi^+ \pi^+ \pi^- \pi^- \pi^- \pi^0 n$
13	$\gamma p \rightarrow \eta' p$	$\gamma n \to \eta' n$	44	$\gamma p \to \pi^+ \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 n$	$\gamma n \rightarrow \pi^- \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 p$
14		$\gamma n \to \phi n$	45	$\gamma p \rightarrow \pi^+ \pi^+ \pi^- \pi^0 \pi^0 \pi^0 \pi^0 n$	$\gamma n \rightarrow \pi^+ \pi^- \pi^- \pi^0 \pi^0 \pi^0 \pi^0 p$
15	/1 1	$\gamma n \rightarrow \pi^+ \pi^- n$	46	$\gamma p \to \pi^+ \pi^+ \pi^+ \pi^- \pi^- \pi^0 \pi^0 n$	$\gamma n \rightarrow \pi^+ \pi^+ \pi^- \pi^- \pi^- \pi^0 \pi^0 p$
	$\gamma p \to \pi^0 \pi^+ n$	$\gamma n \to \pi^0 \pi^- p$	47	$\gamma p \to \pi^+ \pi^+ \pi^+ \pi^+ \pi^- \pi^- \pi^- n$	$\gamma n \rightarrow \pi^+ \pi^+ \pi^- \pi^- \pi^- \pi^- \pi^- p$
17		$\gamma n  ightarrow \pi^0 \pi^0 n$			
18	$\gamma p \to \pi^0 \pi^0 \pi^0 p$	$\gamma n \to \pi^0 \pi^0 \pi^0 n$	48	$\gamma p  ightarrow \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 p$	$\gamma n  ightarrow \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 n$
19	$\gamma p \rightarrow \pi^+ \pi^- \pi^0 p$	$\gamma n \to \pi^+ \pi^- \pi^0 n$	49	$\gamma p \to \pi^+ \pi^- \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 p$	$\gamma n \to \pi^+ \pi^- \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 n$
20	$\gamma p  ightarrow \pi^+ \pi^0 \pi^0 n$	$\gamma n  ightarrow \pi^- \pi^0 \pi^0 p$	50	$\gamma p \to \pi^+ \pi^+ \pi^- \pi^- \pi^0 \pi^0 \pi^0 \pi^0 p$	$\gamma n \to \pi^+ \pi^+ \pi^- \pi^- \pi^0 \pi^0 \pi^0 \pi^0 n$
21	$\gamma p \rightarrow \pi^+ \pi^+ \pi^- n$	$\gamma n \rightarrow \pi^+ \pi^- \pi^- p$	51	$\gamma p \to \pi^+ \pi^+ \pi^- \pi^- \pi^- \pi^0 \pi^0 p$	$\gamma n \to \pi^+ \pi^+ \pi^- \pi^- \pi^- \pi^0 \pi^0 n$
22	$\gamma p \to \pi^0 \pi^0 \pi^0 \pi^0 p$	$\gamma n \to \pi^0 \pi^0 \pi^0 \pi^0 n$	52	$\gamma p \rightarrow \pi^+ \pi^+ \pi^+ \pi^+ \pi^- \pi^- \pi^- \pi^- p$	$\gamma n \to \pi^+ \pi^+ \pi^+ \pi^+ \pi^- \pi^- \pi^- \pi^- n$
23		$\gamma n  ightarrow \pi^+ \pi^- \pi^0 \pi^0 n$	53	$\gamma p \to \pi^+ \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 n$	$\gamma n \to \pi^- \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 p$
24		$\gamma n  ightarrow \pi^+ \pi^+ \pi^- \pi^- n$	54	$\gamma p \to \pi^+ \pi^+ \pi^- \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 n$	$\gamma n \to \pi^+ \pi^- \pi^- \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 p$
25	$\gamma p \to \pi^+ \pi^0 \pi^0 \pi^0 n$	$\gamma n \to \pi^- \pi^0 \pi^0 \pi^0 p$	55	$\gamma p \rightarrow \pi^+ \pi^+ \pi^+ \pi^- \pi^- \pi^0 \pi^0 \pi^0 n$	$ \gamma n \to \pi^+ \pi^+ \pi^- \pi^- \pi^- \pi^0 \pi^0 \pi^0 p $
26	$\gamma p  ightarrow \pi^+ \pi^+ \pi^- \pi^0 n$	$\gamma n  ightarrow \pi^+ \pi^- \pi^- \pi^0 p$	56		$ \begin{array}{c} \gamma n \rightarrow \pi & p \\ \gamma n \rightarrow \pi^{+} \pi^{+} \pi^{+} \pi^{-} \pi^{-} \pi^{-} \pi^{-} \pi^{0} p \end{array} $
			- 50		
27	$\gamma p \to \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 p$	$\gamma n \to \pi^0 \pi^0 \pi^0 \pi^0 \pi^0 n$	Neuro	annovinational for a se	
28	$\gamma p  ightarrow \pi^+ \pi^- \pi^0 \pi^0 \pi^0 p$	$\gamma n  ightarrow \pi^+ \pi^- \pi^0 \pi^0 \pi^0 n$	-		nd γn cross sections from
29	$\gamma p \to \pi^+ \pi^+ \pi^- \pi^- \pi^0 p$	$\gamma n \to \pi^+ \pi^+ \pi^- \pi^- \pi^0 n$	A. S. II	jinov et al.,Nucl. Phys. /	A616 (1997) 575,
30	$\gamma p \to \pi^+ \pi^0 \pi^0 \pi^0 \pi^0 n$	$\gamma n \to \pi^- \pi^0 \pi^0 \pi^0 \pi^0 p$	kindly i	provided us by Dr. laor	Pshenichnov, have been

A. S. Iljinov et al., Nucl. Phys. A616 (1997) 575, kindly provided us by Dr. Igor Pshenichnov, have been incorporated into LAQGSM03.01



Gnd	Computational Analysis and Simulation (X-3)

 $\gamma p \rightarrow \pi^+ \pi^+ \pi^+ \pi^- \pi^- n$ 

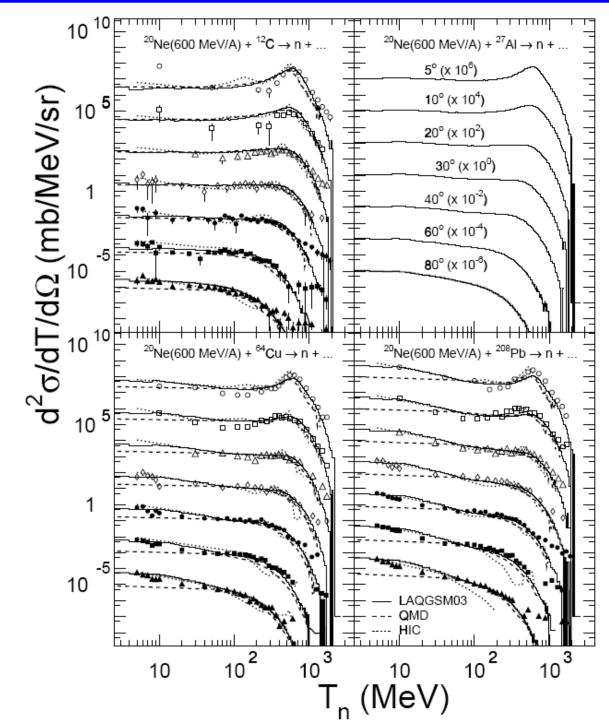
31

32

 $| \gamma p \to \pi^+ \pi^+ \pi^- \pi^0 \pi^0 n | \gamma n \to \pi^+ \pi^- \pi^- \pi^0 \pi^0 p$ 

 $\gamma n \rightarrow \pi^+ \pi^+ \pi^- \pi^- \pi^- p$ 



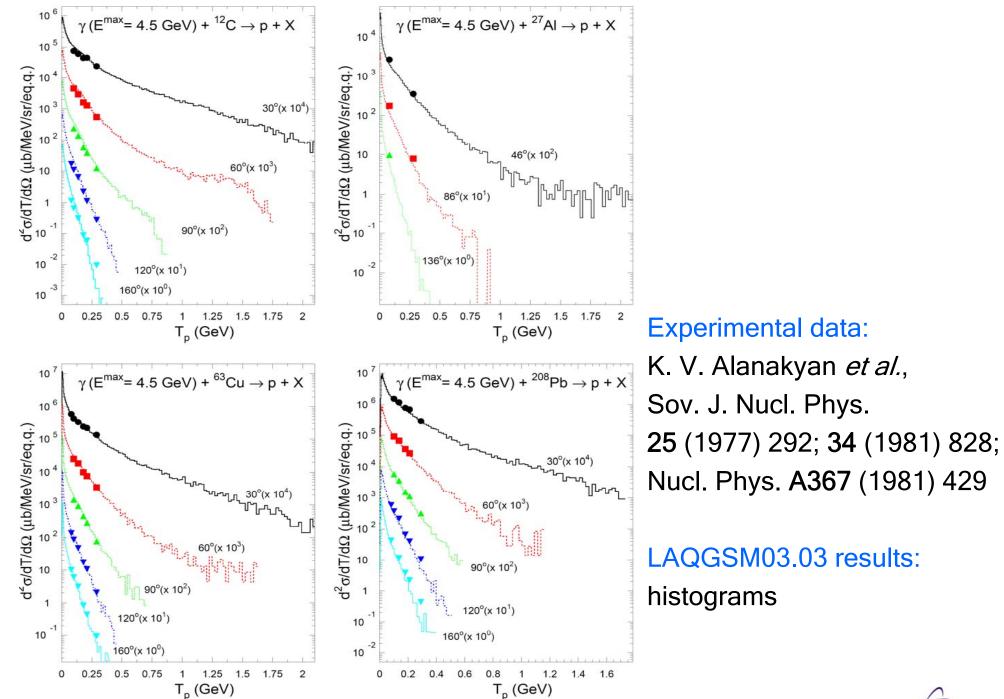


Proc. ND2004: Hiroshi Iwase, Yoshiyuki Iwata, Takashi Nakamura, Konstantin Gudima, Stepan Mashnik, Arnold Sierk, Richard Prael, AIP Conf. Proc. 769 (2005) 1066-1069 (nucl-th/0501066)





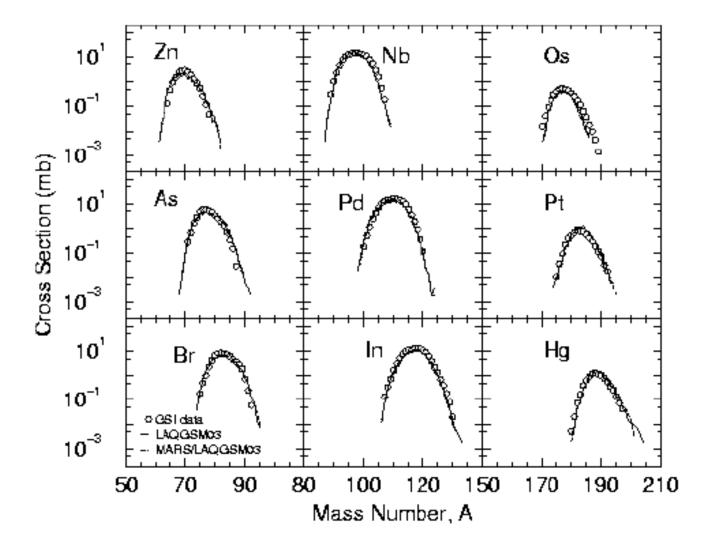






Computational Analysis and Simulation (X-3)





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,
Radiation Protection
Dosimetry, Vol. 116,
No. 1-4 (2005) 99-103

N. V. Mokhov,

Figure 2. Nuclide mass yield in p + U interaction at 1 GeV as calculated with original LAQGSM03 and that implemented into MARS 15, and measured in Ref. (9–10).





The coalescence model implemented in LAQGSM/CEM is described in [1]; We have changed the coalescence momentum radii p<sub>0</sub> for the various light composite particles up to <sup>4</sup>He by fitting them to measured data on various reactions and have fixed several bugs observed in the original version [1].

[1] V. D. Toneev and K. K. Gudima, Nucl. Phys. A400 (1983) 173c.

$$W_d(\vec{p}, b) = \int \int d\vec{p}_p d\vec{p}_n \rho^C(\vec{p}_p, b) \rho^C(\vec{p}_n, b) \delta(\vec{p}_p + \vec{p}_n - \vec{p}) \Theta(p_c - |\vec{p}_p - \vec{p}_n|)$$

#### LAQGSM:

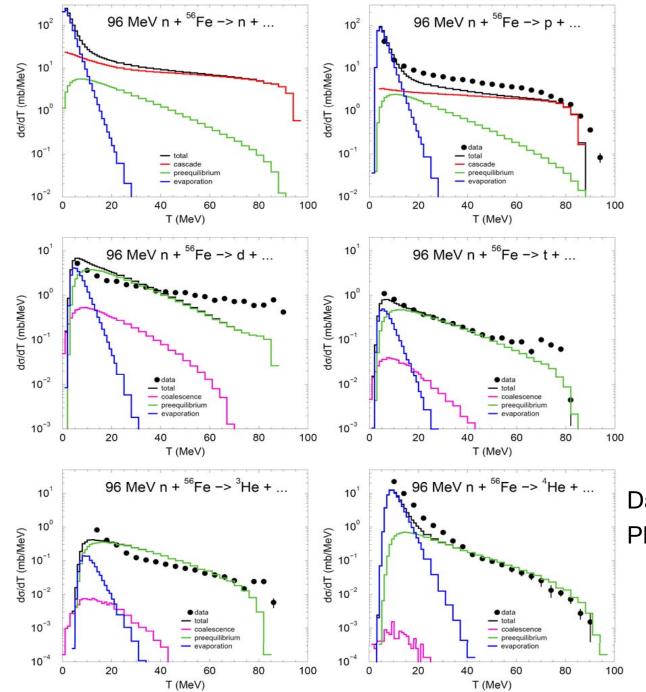
 $p_c(d) = 90 \text{ MeV/c}; P_c(t) = p_c(^{3}\text{He}) = 108 \text{ MeV/c}; p_c(^{4}\text{He}) = 115 \text{ MeV/c}$ 

#### CEM:

 $p_c(d) = 150 \text{ MeV/c}; p_c(t) = P_c(^{3}\text{He}) = 175 \text{ MeV/c}; p_c(^{4}\text{He}) = 175 \text{ MeV/c}$ 





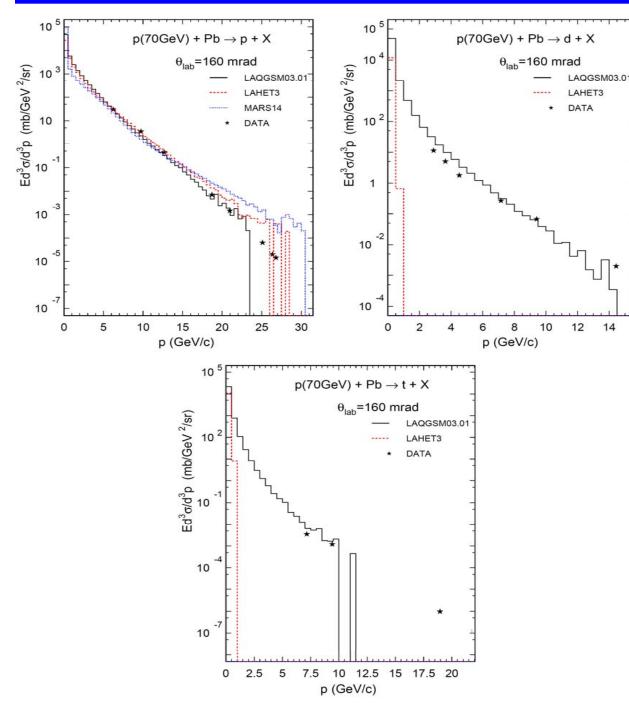


#### Data: V. Blideanu *et al*., Phys. Rev. C **70** (2004) 014607



Computational Analysis and Simulation (X-3)





Data: L. M. Barkov *et al.,* Sov. J. Nucl. Phys. **35** (1982) 694; **37** (1983) 732; **41** (1985) 227





The preequilibrium part of reactions is described with the latest version [1] of the Modified Exciton Model (MEM) [2,3] from the improved Cascade-Exciton Model (CEM) [4] released in the Code CEM03.01 [1]:

- [1] S.G. Mashnik, K.K. Gudima, A.J. Sierk, M.I. Baznat, N.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/psr-532.html (2006).
- [2] K. K. Gudima, G. A. Ososkov, and V. D. Toneev, "Model for Pre-Equilibrium Decay of Excited Nuclei," Sov. J. Nucl. Phys. 21 (1975) 138.
- [3] S. G. Mashnik and V. D. Toneev, "MODEX the Program for Calculation of the Energy Spectra of Particles Emitted in the Reactions of Pre-Equilibrium and Equilibrium Statistical Decays," JINR Communication P4-8417, Dubna (1974).
- [4] K. K. Gudima, S. G. Mashnik, and V. D. Toneev, "Cascade-Exciton Model of Nuclear Reactions: Model Formulation," Nucl. Phys. A401 (1983) 329.





We take into account all possible nuclear transitions changing the number of excitons *n* with  $\Delta n = +2$ , -2, and 0, as well as all possible multiple subsequent emissions of n, p, d, t, <sup>3</sup>He, and <sup>4</sup>He.

For a preequilibrium nucleus with excitation energy *E* and number of excitons n=p+h, the partial transition probabilities changing the exciton number by  $\Delta n$  are

$$\lambda_{\Delta n}(p,h,E) = \frac{2\pi}{\hbar} |M_{\Delta n}|^2 \omega_{\Delta n}(p,h,E) \; .$$

The emission rate of a nucleon of the type *j* into the continuum is estimated according to the detailed balance principle

$$\Gamma_j(p,h,E) = \int_{V_j^c}^{E-B_j} \lambda_c^j(p,h,E,T) dT ,$$
  
$$\lambda_c^j(p,h,E,T) = \frac{2s_j+1}{\pi^2\hbar^3} \mu_j \Re_j(p,h) \frac{\omega(p-1,h,E-B_j-T)}{\omega(p,h,E)} T\sigma_{inv}(T)$$





CEM considers the possibility of fast d, t, <sup>3</sup>He, and <sup>4</sup>He emission at the preequilibrium stage of a reaction in addition to the emission of nucleons. (We plan to include preequilibrium emission of clusters heavier than <sup>4</sup>He in the following versions of our codes.)

We assume that in the course of a reaction  $p_j$  excited nucleons (excitons) are able to condense with probability  $\gamma_j$  forming a complex particle which can be emitted during the preequilibrium state. The "condensation" probability  $\gamma_j$  is estimated in those references as the overlap integral of the wave function of independent nucleons with that of the complex particle (cluster)

$$\gamma_j \simeq p_j^3 (V_j/V)^{p_j-1} = p_j^3 (p_j/A)^{p_j-1}$$

This is a rather crude estimate. In the usual way the values  $\gamma_j$  are taken from fitting the theoretical preequilibrium spectra to the experimental ones. In CEM03.01, we fitted  $\gamma_j$  to nucleon-induced reactions experimental spectra.





The CEM predicts forward peaked (in the laboratory system) angular distributions for preequilibrium particles. CEM03.01 assumes that a nuclear state with a given excitation energy E\* should be specified not only by the exciton number *n* but also by the momentum direction  $\Omega$ .

The scattering cross section is assumed to be isotropic in the reference frame of the interacting excitons, thus resulting in an asymmetry in both the nucleus center-of-mass and laboratory frames. The angular distributions of preequilibrium complex particles are assumed to be similar to those for the nucleons in each nuclear state. This approach provides reasonably results, but the Kalbach systematics agrees better with experimental data, especially at low incident energies.

For application needs, in CEM03.01, we have incorporated the Kalbach systematics for angular distribution of complex particles and nucleons at energies below 210 MeV to replace the original CEM approach .

C. Kalbach, "Systematics of Continuum Angular Distributions: Extensions to Higher Energies," Phys. Rev. 37 (1988) 2350.





By "preequilibrium particles" we mean particles which are emitted after the cascade stage of a reaction but before achieving statistical equilibrium at a time  $t_{eq}$ , which is fixed by the condition

$$\lambda_{+}(n_{eq}, E) = \lambda_{-}(n_{eq}, E)$$
$$n_{eq} \simeq \sqrt{2gE}$$

The original version of CEM provides an overestimation of preequilibrium particle emission from different p+A and A+A reactions we have analyzed lately.

A way to solve this problem suggested by Veselsky and adopted in CEM03.01 assumes that the ratio of the number of excitons *n* at each preequilibrium reaction stage to the number of excitons in the equilibrium configuration  $n_{eq}$ , corresponding to the same excitation energy, to be a crucial parameter for determining the probability of preequilibrium emission  $P_{pre^*}$ . This probability for a given preequilibrium reaction stage is evaluated using the formula

$$P_{pre}(n/n_{eq}) = 1 - \exp\left(-\frac{(n/n_{eq}-1)}{2\sigma_{pre}^2}\right)$$

for  $n_{eq} \ge n$  and equal to zero for  $n \ge n_{eq}$ ; in CEM03.01, we use  $\sigma_{pre} = 0.4$ .

M. Veselsky, Nucl. Phys. A705 (2002) 193

Computational Analysis and Simulation (X-3)





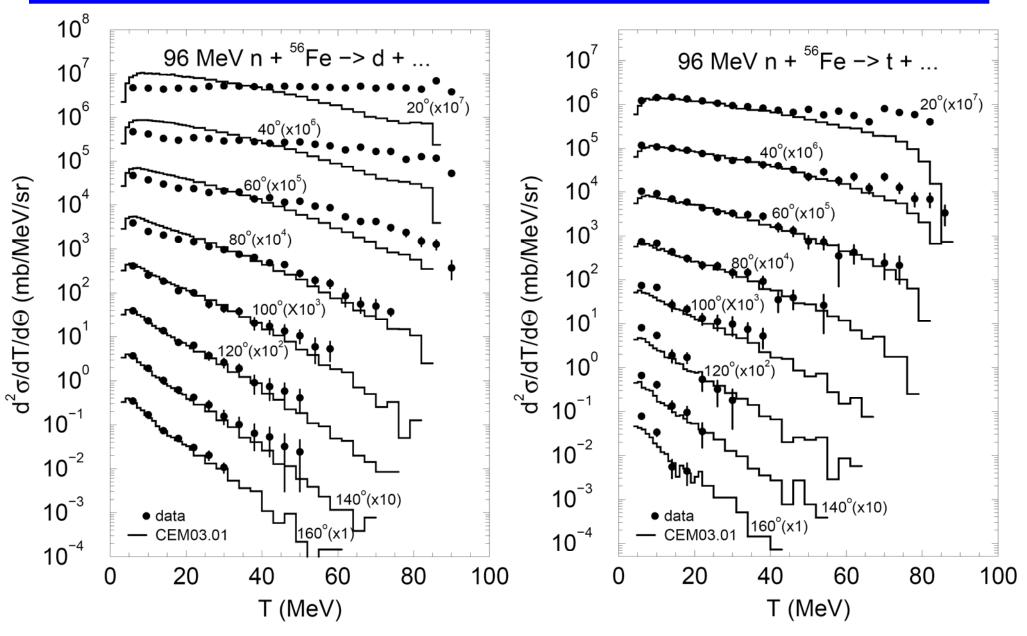
In comparison with the initial version [2] of CEM, the preequilibrium (PREC) part of CEM03.01 have been changed:

- the condition for transition from the preequilibrium stage of a reaction to evaporation/fission was changed; on the whole, the preequilibrium stage in CEM03.01 is shorter while the evaporation stage is longer in comparison with previous versions;
- the widths for complex-particle emission were changed by fitting the probability of several excitons to "coalesce" into a complex particle that may be emitted during the preequilibrium stage to available experimental data on reactions induced by protons and neutrons;
- 3) Kalbach systematics for angular distribution of complex particles and nucleons with T < 210 MeV was incorporated into CEM/LAQGSM;
- 4) algorithms of many PREC routines were changed and almost all PREC routines were rewritten, which speeded up the code significantly;
- 5) some old bugs were discovered and fixed.







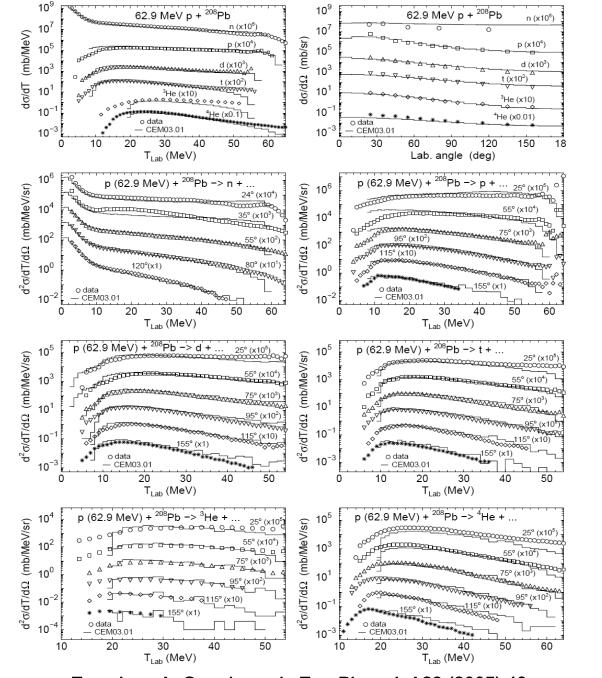


Experimental data: V. Blideanu et al., Phys. Rev. C 70 (2004) 014607

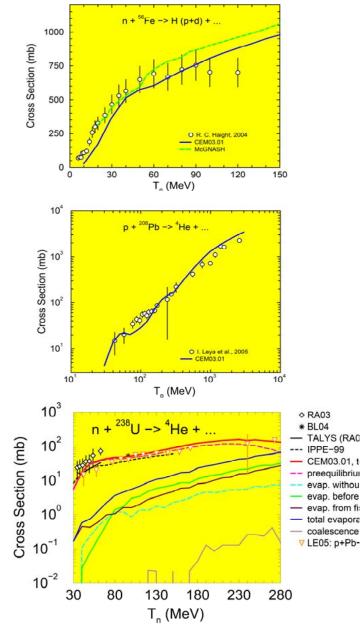




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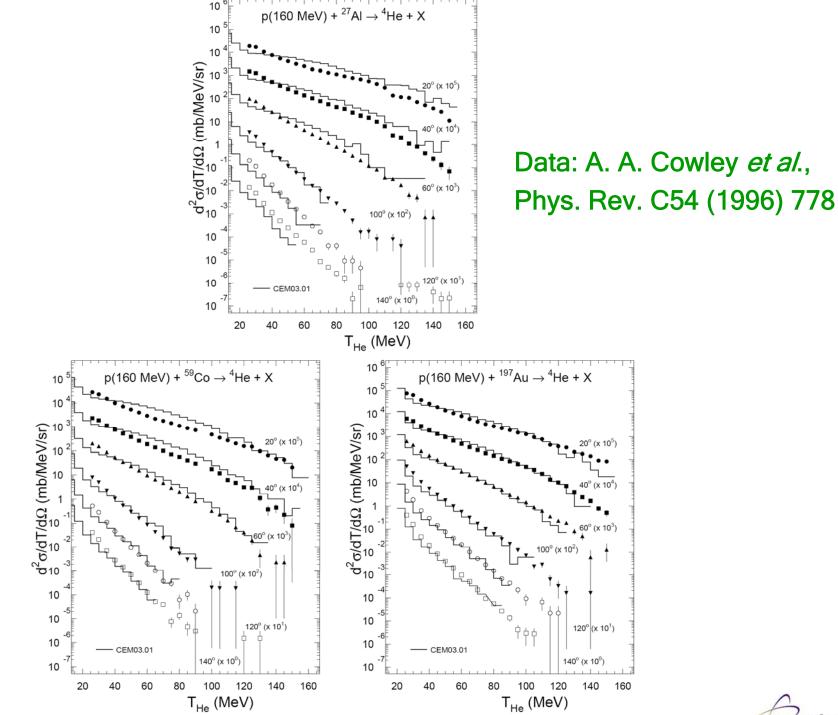


Exp. data: A. Guertin et al., Eur. Phys. J. A23 (2005) 49



Data: R. C. Haight, LA-UR-04-4010, Los Alamos (2004); McGNASH results are from: P. Talou et al., Proc. AccApp05, NIM A, 2006; Data: RA03: E. Raeymackers et al., Phys. Rev. C68 (2003) 024604; BL04: V. Blideanu et al., Phys. Rev. C70 (2004) 014607; LE05: I. Leya et al., NIM B229 (2005) 1

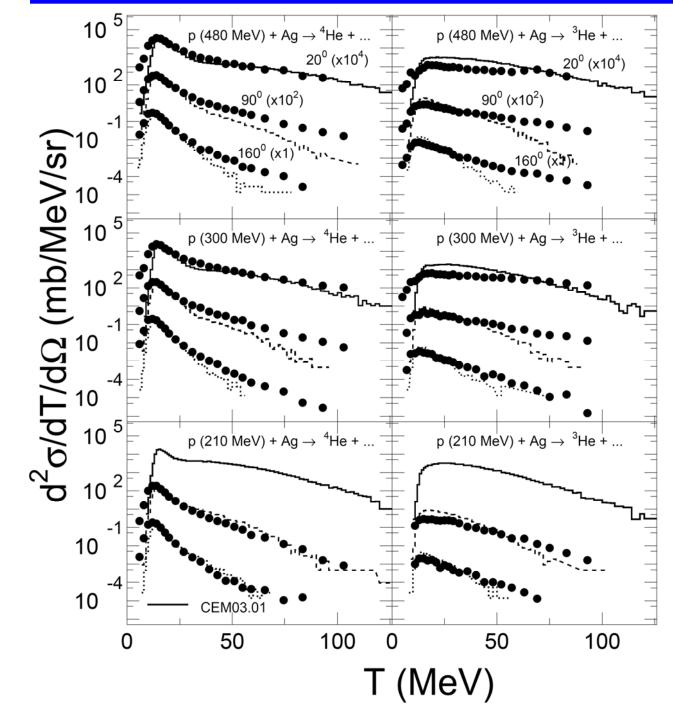








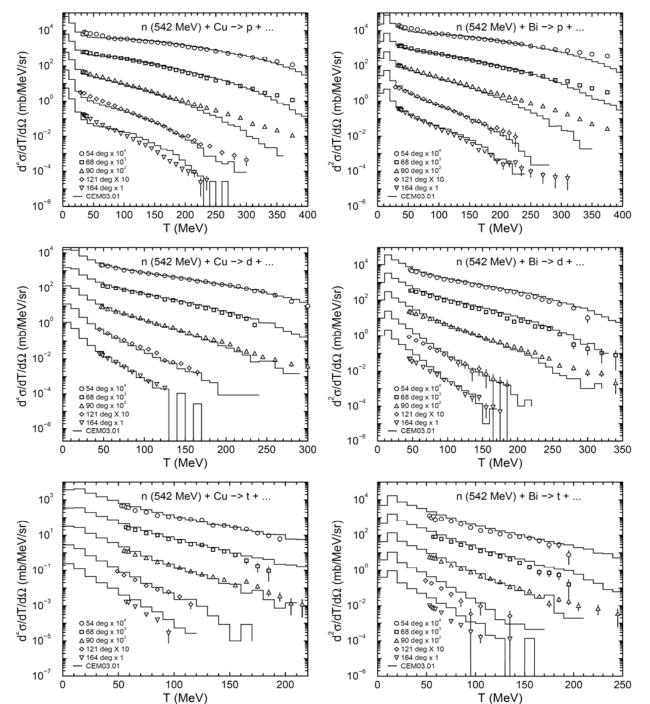




Data: R. E. L. Green, R.G. Korteling, Phys. Rev. C18 (1978) 311







Data: J. Franz *et al.*, Nucl. Phys. **A510** (1990) 774





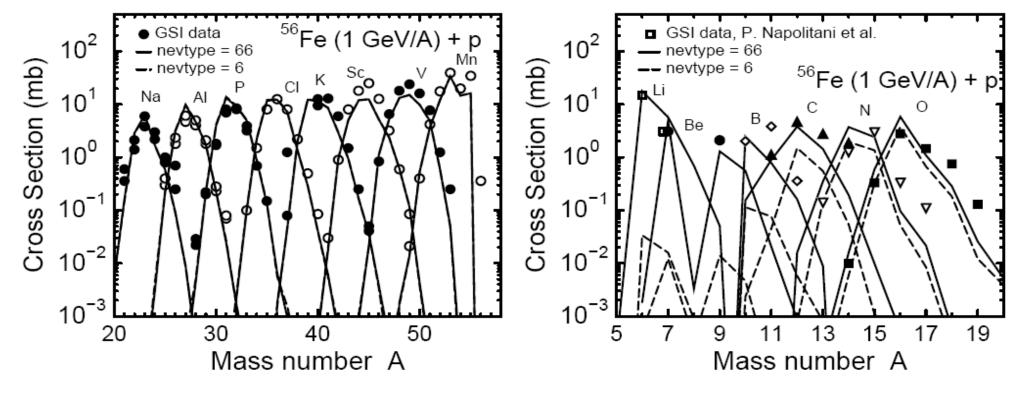
The evaporation stages of reactions is calculated with an improved version of the Generalized Evaporation Model (GEM2) by Furihata (several routines by Furihata from GEM2 were slightly modified in CEM03.01/LAQGSM03.01; some bugs found in GEM2 were fixed).

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

$Z_j$	Ejectil	es					
0	n						
1	р	d	$\mathbf{t}$				
2	<sup>3</sup> He	$^{4}\mathrm{He}$	<sup>6</sup> He	<sup>8</sup> He			
3	<sup>6</sup> Li	$^{7}\mathrm{Li}$	<sup>8</sup> Li	<sup>9</sup> Li			
4	$^{7}\mathrm{Be}$	<sup>9</sup> Be	$^{10}\mathrm{Be}$	$^{11}\mathrm{Be}$	$^{12}\mathrm{Be}$		
5	$^{8}\mathrm{B}$	$^{10}\mathrm{B}$	$^{11}\mathrm{B}$	$^{12}\mathrm{B}$	$^{13}\mathrm{B}$		
6	$^{10}\mathrm{C}$	$^{11}\mathrm{C}$	$^{12}\mathrm{C}$	$^{13}\mathrm{C}$	$^{14}\mathrm{C}$	$^{15}\mathrm{C}$	$^{16}\mathrm{C}$
7	$^{12}\mathrm{N}$	$^{13}\mathrm{N}$	$^{14}\mathrm{N}$	$^{15}\mathrm{N}$	$^{16}N$	$^{17}\mathrm{N}$	
8	$^{14}\mathrm{O}$	$^{15}\mathrm{O}$	$^{16}\mathrm{O}$	$^{17}\mathrm{O}$	$^{18}\mathrm{O}$	$^{19}\mathrm{O}$	$^{20}O$
9	$^{17}\mathrm{F}$	$^{18}\mathrm{F}$	$^{19}\mathrm{F}$	$^{20}$ F	$^{21}\mathrm{F}$		
10	$^{18}\mathrm{Ne}$	$^{19}\mathrm{Ne}$	$^{20}\mathrm{Ne}$	$^{21}\mathrm{Ne}$	$^{22}\mathrm{Ne}$	$^{23}\mathrm{Ne}$	$^{24}\mathrm{Ne}$
11	$^{21}$ Na	$^{22}$ Na	$^{23}$ Na	$^{24}$ Na	$^{25}$ Na		
12	$^{22}Mg$	$^{23}\mathrm{Mg}$	$^{24}\mathrm{Mg}$	$^{25}\mathrm{Mg}$	$^{26}Mg$	$^{27}\mathrm{Mg}$	$^{28}\mathrm{Mg}$







GSI experimental data: C. Villagrasa-Canton et al., Phys. Rev. C 75 (2007) 04460;

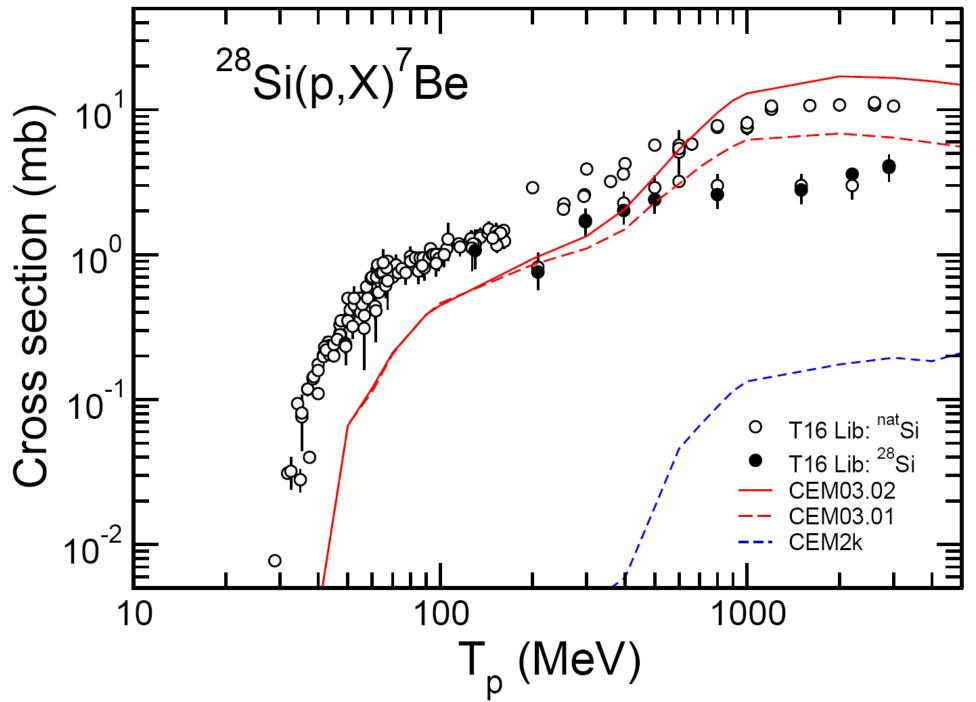
P. Napolitani et al., Phys. Rev. C 70 (2004) 054607



**Computational Analysis and Simulation (X-3)** 

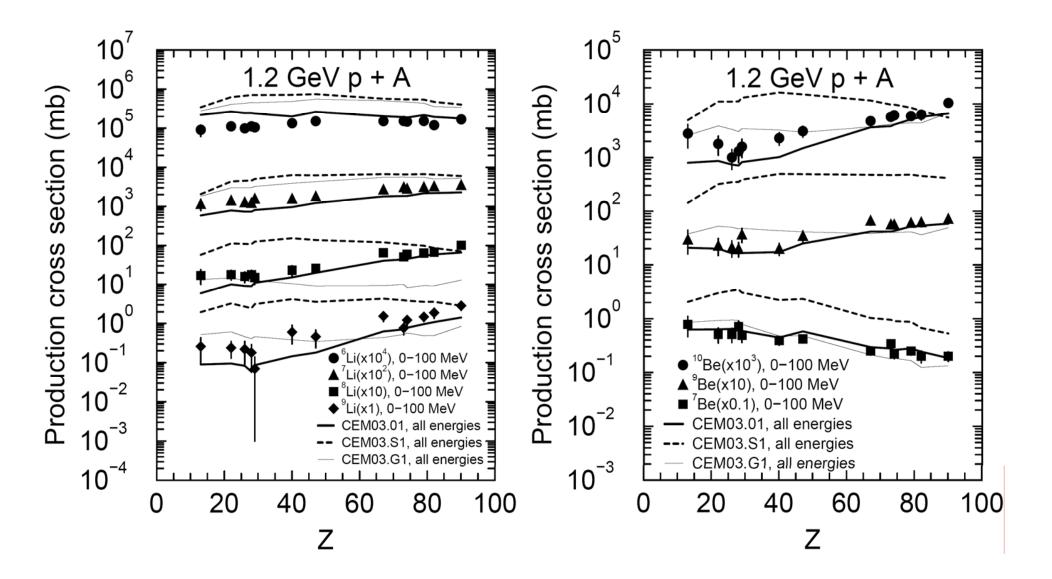
Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions, ICTP, 4 - 8 February 2008, S.G. Mashnik et al., LA-UR-08-0867







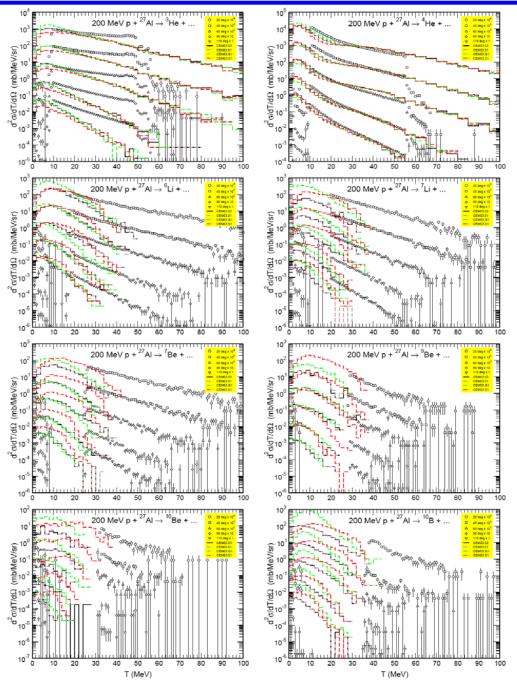




NESSI data: C.-M. Herbach et al., Nucl. Phys. A765 (2006) 426-463







iThemba data: H. Machner et al., Phys. Rev. C73 (2006) 044606







Fission is calculated with an improved version of GEM2 that is an extension by Shiori Furihata of the RAL fission model of Francis Atchison.

We have changed the calculation of the fission cross sections; several routines by Furihata from GEM2 were slightly modified in CEM03.03/LAQGSM03.03; some bugs found in GEM2 were fixed.

#### 1) Fission cross section calculation:

1)  $70 \leq Z_j \leq 88$ the Weisskopf and Ewing statistical model

$$P_{f} = \frac{\Gamma_{f}}{\Gamma_{f} + \Gamma_{n}} = \frac{1}{1 + \Gamma_{n}/\Gamma_{f}}$$

$$\Gamma_{n} = 0.352 (1.68J_{0} + 1.93A_{i}^{1/3}J_{1} \qquad J_{0} = \frac{(s_{n} - 1)e^{s_{n}} + 1}{2a_{n}},$$

$$+A_{i}^{2/3}(0.76J_{1} - 0.05J_{0})),$$

$$s_{n} (= 2\sqrt{a_{n}(E - Q_{n} - \delta)}) \quad a_{n} = (A_{i} - 1)/8 \qquad J_{1} = \frac{(2s_{n}^{2} - 6s_{n} + 6)e^{s_{n}} + s_{n}^{2} - 6}{8a_{n}^{2}}$$

$$\Gamma_{f} = \frac{(s_{f} - 1)e^{s_{f}} + 1}{a_{f}}, a_{f} = a_{n} (1.08926 + 0.01098(\chi - 31.08551)^{2}), \text{ and } \chi = Z^{2}/A.$$

$$B_{f} = Q_{n} + 321.2 - 16.7\frac{Z_{i}^{2}}{A} + 0.218\left(\frac{Z_{i}^{2}}{A_{i}}\right)^{2}$$
(b) Computational Analysis and Simulation (X-3)



<b>9</b> )	7		89
$\Delta$	$\Delta_i$	/	-09
	J	_	

$$\log(\Gamma_n/\Gamma_f) = C(Z_i)(A_i - A_0(Z_i)),$$

C(Z) and  $A_0(Z)$  are constants

In CEM03.03 and LAQGSM03.03, we have adjusted the original values of  $a_f/a_n$  and C(Z), namely:

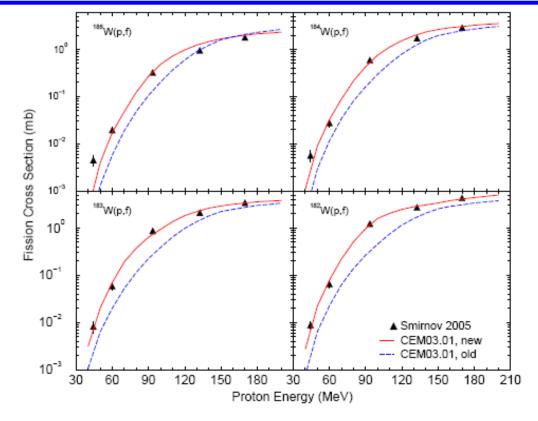
$$a_f \to C_a \times a_f$$

 $C(Z_i) \to C_c \times C(Z_i)$ 

Z	C(Z)	$A_0(Z)$
89	0.23000	219.40
90	0.23300	226.90
91	0.12225	229.75
92	0.14727	234.04
93	0.13559	238.88
94	0.15735	241.34
95	0.16597	243.04
96	0.17589	245.52
97	0.18018	246.84
98	0.19568	250.18
99	0.16313	254.00
100	0.17123	257.80
101	0.17123	261.30
102	0.17123	264.80
103	0.17123	268.30
104	0.17123	271.80
105	0.17123	275.30
106	0.17123	278.80







S. G. Mashnik, A. J. Sierk, K. K. Gudima, M. I. Baznat, Proc. NPDC19, Journal of Physics: Conference Series, <u>41</u> (2006) 340-351 (nucl-th/0510070)

**Figure 3.** Experimental [31] proton-induced fission cross sections of <sup>186</sup>W, <sup>184</sup>W, <sup>183</sup>W, and <sup>182</sup>W compared with improved (red solid lines) and old (blue dashed lines, from [31]) CEM03.01 calculations.



**MGAP** Computational Analysis and Simulation (X-3)



#### 2) Fission fragments distributions calculation:

#### Mass Distribution

For a pre-fission nucleus with  $Z_i^2/A_i \leq 35$ , only symmetric fission is allowed

For nuclei with 
$$Z_i^2/A_i > 35$$
,  $P_{asy} = \frac{4870e^{-0.36E}}{1 + 4870e^{-0.36E}}$ 

**2.5.2.a.** Asymmetric fission. For asymmetric fission, the mass of one of the post-fission fragments  $A_1$  is selected from a Gaussian distribution of mean  $A_f = 140$  and width  $\sigma_M = 6.5$ . The mass of the second fragment is  $A_2 = A_i - A_1$ .

**2.5.2.b. Symmetric fission.** For symmetric fission,  $A_1$  is selected from the Gaussian distribution of mean  $A_f = A_i/2$  and two options for the width  $\sigma_M$  as described below.

$$\sigma_M = C_3 (Z_i^2 / A_i)^2 + C_4 (Z_i^2 / A_i) + C_5 (E - B_f) + C_6.$$
(61)

The constants  $C_3 = 0.122$ ,  $C_4 = -7.77$ ,  $C_5 = 3.32 \times 10^{-2}$ , and  $C_6 = 134.0$  were obtained by fitting with GEM2 the recent Russian collection of experimental fission-fragment mass distributions [102]. In this expression, the fission barriers  $B_f$  by Myers and Swiatecki [103] are used.





**2.5.3. Charge Distribution.** The charge distribution of fission fragments is assumed to be a Gaussian distribution of mean  $Z_f$  and width  $\sigma_Z$ .  $Z_f$  is expressed as

$$Z_f = \frac{Z_i + Z_1' - Z_2'}{2},\tag{62}$$

where

$$Z'_{l} = \frac{65.5A_{l}}{131 + A_{l}^{2/3}}, l = 1 \text{ or } 2.$$
(63)

The original Atchison model uses  $\sigma_Z = 2.0$ . An investigation by Furihata [85] suggests that  $\sigma_Z = 0.75$  provides a better agreement with data; therefore  $\sigma_Z = 0.75$  is used in GEM2 and in our code.

**2.5.4.** Kinetic Energy Distribution. The kinetic energy of fission fragments [MeV] is determined by a Gaussian distribution with mean  $\epsilon_f$  and width  $\sigma_{\epsilon_f}$ .

$$\epsilon_f = \begin{cases} 0.131 Z_i^2 / A_i^{1/3}, \\ 0.104 Z_i^2 / A_i^{1/3} + 24.3, \end{cases}$$
(64)

for  $Z_i^2/A_i^{1/3} \leq 900$  and  $900 < Z_i^2/A_i^{1/3} \leq 1800$ , respectively, according to Rusanov *et al.* [102]. By fitting the experimental data by Itkis *et al.* [104], Furihata found the following expression for  $\sigma_{\epsilon_f}$ 

$$\sigma_{\epsilon_f} = \begin{cases} C_1(Z_i^2/A_i^{1/3} - 1000) + C_2, \\ C_2, \end{cases}$$
(65)

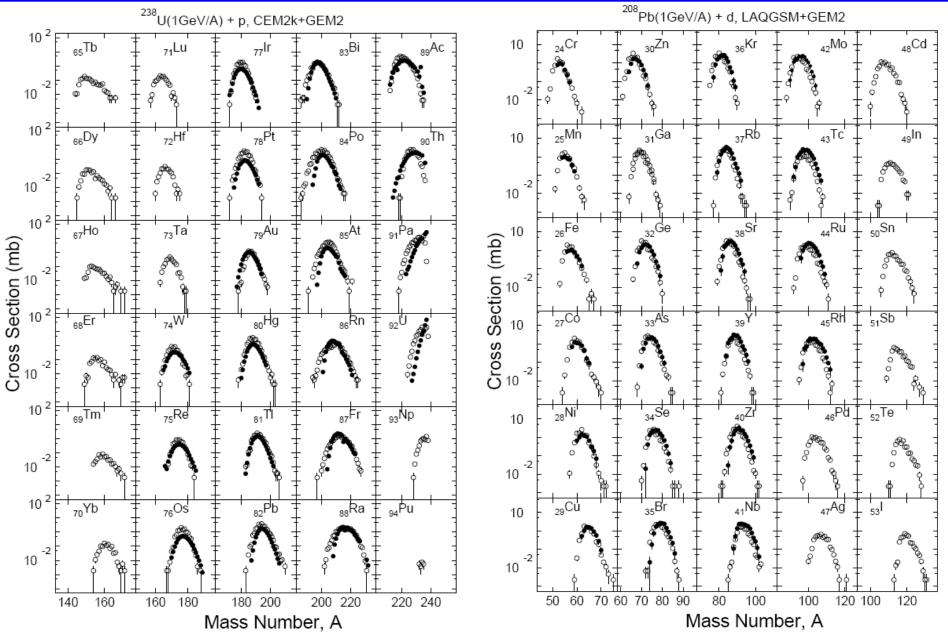
for  $Z_i^2/A_i^{1/3}$  above and below 1000, respectively, and the values of the fitted constants are  $C_1 = 5.70 \times 10^{-4}$  and  $C_2 = 86.5$ . The experimental data used by Furihata for fitting are the values extrapolated to the nuclear temperature 1.5 MeV by Itkis *et al.* [104]. More details may be found in [85].

Computational Analysis and Simulation (X-3)



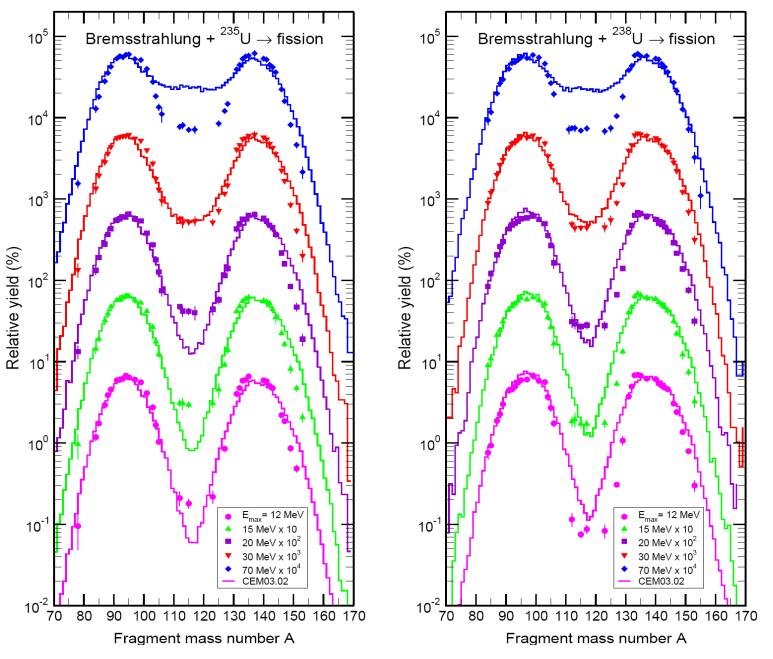


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GSI data (filled circles): M. Bernas *et al.*, Nucl. Phys. <u>A725</u> (2003) 213; T. Enqvist *et al.*, Nucl. Phys. A703 (2003) 435; LAQGSM results: open circles





Data: E. Jacobs et al., Phys. Rev. C: 19 (1979) 422; 21 (1980) 237





# The Fermi breakup model code used in LAQGSM03.03 and in CEM03.03 was developed in the group of Prof. Barashenkov at JINR, Dubna and is described in details in [1].

[1] N. Amelin, "Physics and Algorithms of the Hadronic Monte-Carlo Event Generators. Notes for a Developer," CERN/IT/ASD Report CERN/IT/99/6, Geneva, Switzerland (1999); "GEANT4, Users' Documents, Physics Reference Manual," last update: 08/04/1999; <u>http://wwwinfo.cern.ch/asd/geant4/G4UsersDocuments/UsersGuides/</u> <u>PhysicsReferenceManual/html/PhysicsReferenceManual.html/.</u>

The total probability per unit time of a nucleus (A,Z) with excitation energy U to breakup into n components is:

$$W(E,n) = (V/\Omega)^{n-1} \rho_n(E), \quad E = U + M(A,Z), \quad \Omega = (2\pi\hbar)^3$$
  
 $V = 4\pi R^3/3 = 4\pi r_0^3 A/3,$ 

where  $r_0 = 1.4$  fm, is the only "free" parameter (fixed) of the model.





The density  $\rho_n(E)$  can be defined as  $\rho_n(E) = M_n(E)S_nG_n$ 

the phase space factor

$$M_n(E) = \int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} \delta\left(\sum_{b=1}^n \vec{p_b}\right) \delta\left(E - \sum_{b=1}^n \sqrt{p^2 + m_b^2}\right) \prod_{b=1}^n d^3 p_b$$

the spin factor

$$S_n = \prod_{b=1}^n (2s_b + 1)$$

the permutation factor

$$G_n = \prod_{j=1}^k \frac{1}{n_j!}$$
 and k is defined by  $n = \sum_{j=1}^k n_j$ 

For the non-relativistic case

$$W(E,n) = S_n G_n \left(\frac{V}{\Omega}\right)^{n-1} \left(\frac{1}{\sum_{b=1}^n m_b} \prod_{b=1}^n m_b\right)^{3/2} \frac{(2\pi)^{3(n-1)/2}}{\Gamma(3(n-1)/2)} E^{3n/2-5/2}$$

where  $\Gamma(x)$  is the gamma function

Computational Analysis and Simulation (X-3)



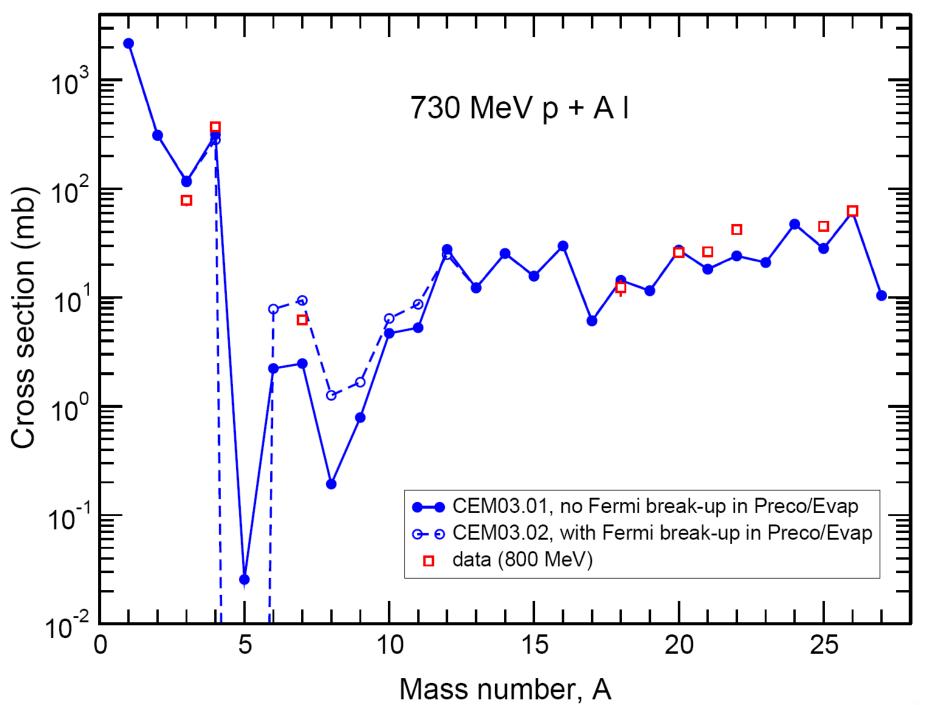


In comparison with its initial version [1] used in QGSM, we have modified the Fermi breakup model in the "03.02" versions of CEM and LAQGSM:

- To decay some unstable light fragments like <sup>5</sup>He, <sup>5</sup>Li, <sup>8</sup>Be, <sup>9</sup>B, *etc.*, that were produced by the original Fermi breakup model;
- Several bugs/uncertainties observed in the original version [1] were fixed; this solved the problem of the production of "nucleon stars" like "nuclides" xn and yp allowed by the original version;
- 3) We have incorporated the Fermi breakup model at the preequilibrium and evaporation stages of reactions (earlier, it was used only after the INC).









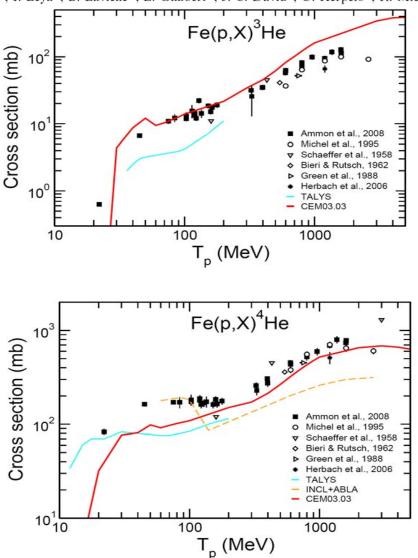




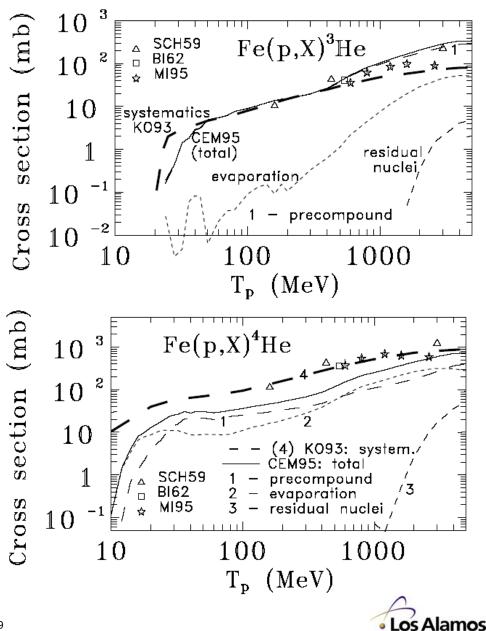
The Ammon et al. data and TALYS and INCL+ABLA results are from:

Nuclear Instruments and Methods in Physics Research B 266 (2008) 2–12 Cross sections for the production of helium, neon and argon isotopes by proton-induced reactions on iron and nickel

K. Ammon<sup>a,\*</sup>, I. Leya<sup>a</sup>, B. Lavielle<sup>b</sup>, E. Gilabert<sup>b</sup>, J.-C. David<sup>c</sup>, U. Herpers<sup>d</sup>, R. Michel<sup>e</sup>



S. G. Mashnik, A. J. Sierk, O. Bersillon, and T. Gabriel, *Cascade-Exciton Model Detailed Analysis of Proton Spallation at Energies from 10 MeV to 5 GeV*, LANL Report LA-UR-97-2905, http://t2.lanl.gov/publications/publications.html



Computational Analysis and Simulation (X-3)



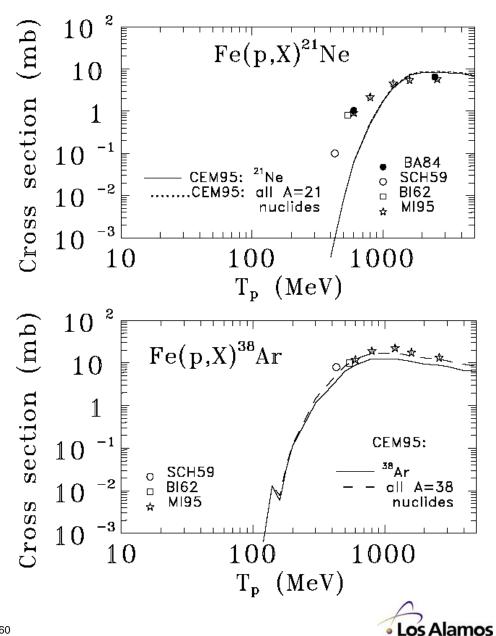
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Fe(p,X)<sup>21</sup>Ne 10 Cross section (mb) 00 10 mmon et al., 2008 Michel et al., 1995 Schaeffer et al., 1958 10<sup>-2</sup> Bieri & Rutsch, 1962 Villagrasa et al., 2007 Baros & Regnier, 1984 INCL+ABLA CEM03.03 10<sup>-3</sup> 100 1000 10 T<sub>p</sub> (MeV)  $10^{2}$ 38 Fe(p,X) Άr Cross section (mb) 10 10<sup>0</sup> Ammon et al., 2008 10 Michel et al., 1995 Schaeffer et al., 1958 Bieri & Rutsch, 1962 10<sup>-2</sup> Villagrasa et al., 2007 TALYS INCL+ABLA CEM03 03 10<sup>-3</sup>. 10 100 1000 T<sub>p</sub> (MeV)

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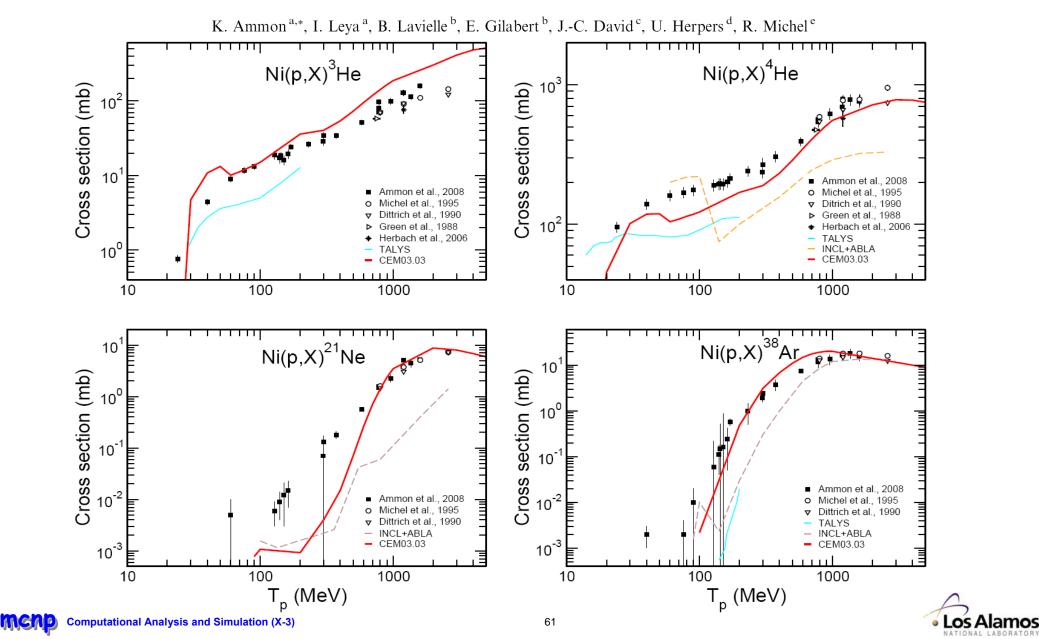


mend **Computational Analysis and Simulation (X-3)** 

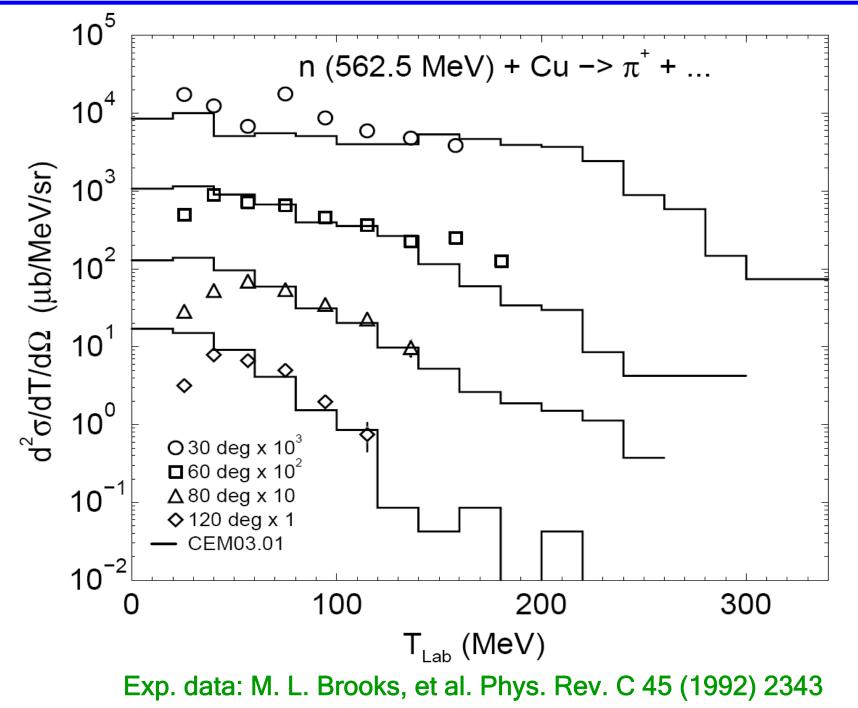


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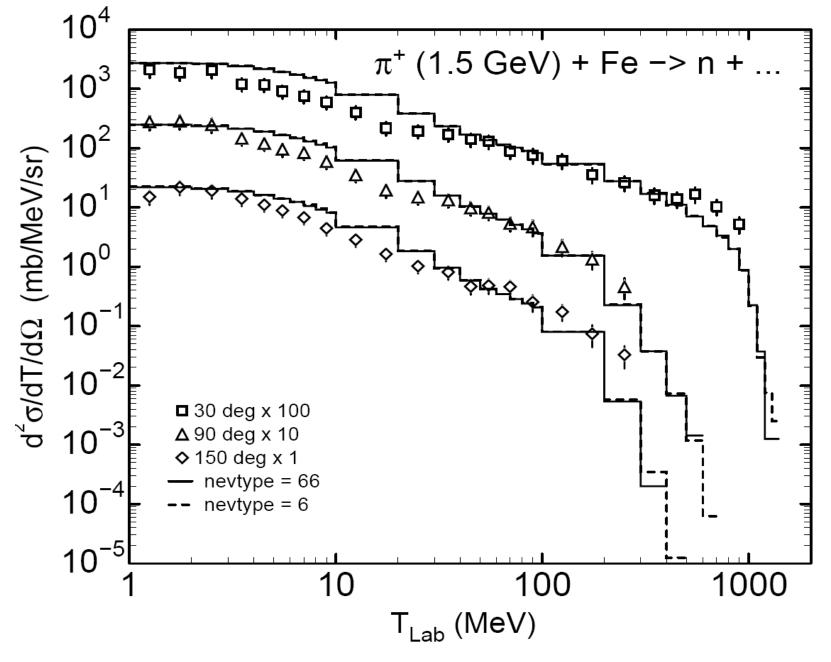










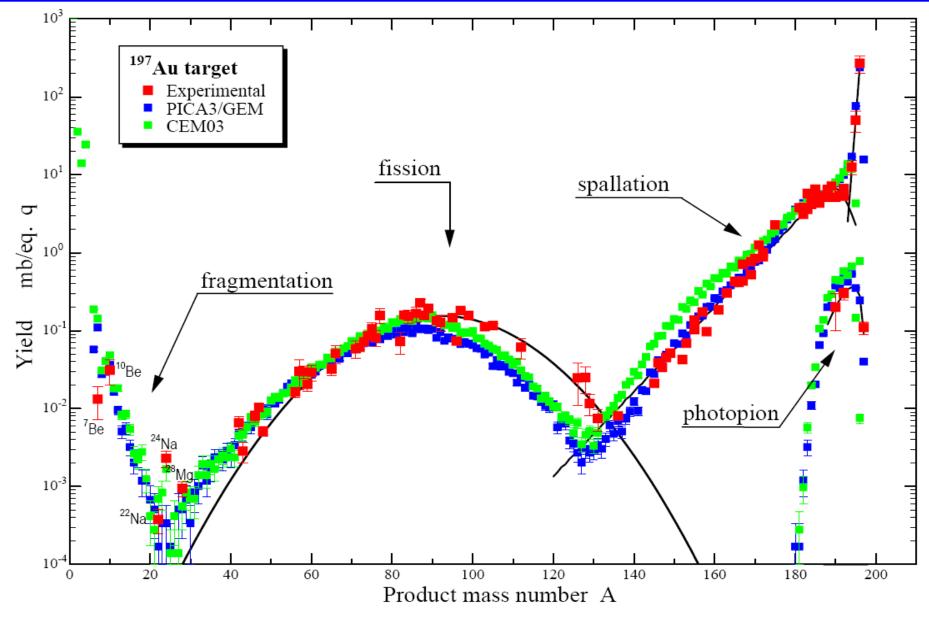


Exp. data: T. Nakamoto et al., J. Nucl. Sci. Techn. 34 (1997) 860



Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions, ICTP, 4 - 8 February 2008, S.G. Mashnik et al., LA-UR-08-0867



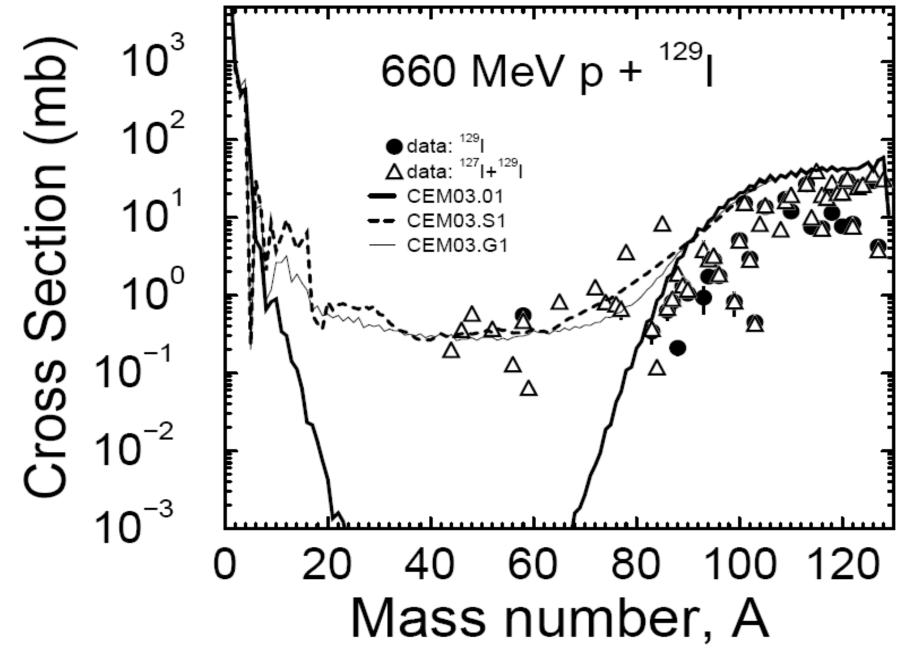


E<sub>0</sub> = 1 GeV bremsstrahlung induced data: Koh Sakamoto, J. Nucl. Radiochem. Sci. 4 (2003) A9



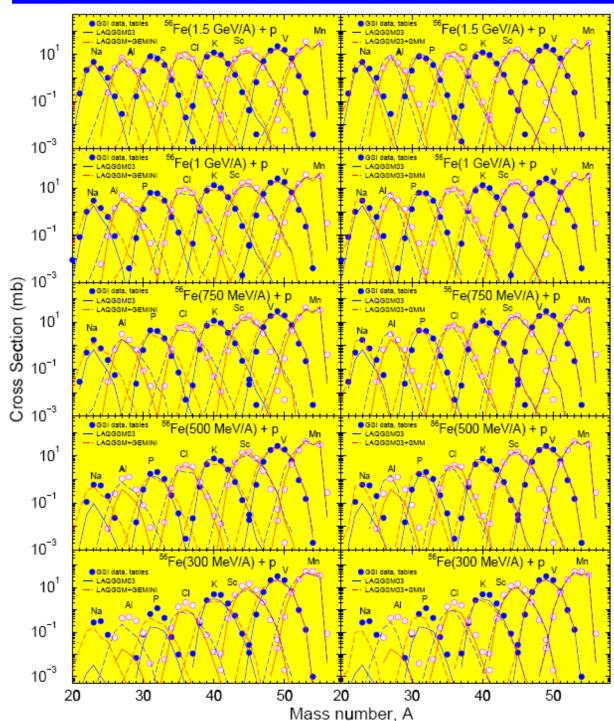


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JINR data: J. Adam et al., Part. Nucl. Lett. 4 (2004) 53 (arXiv:nucl-ex/0403056)





**Computational Analysis and Simulation (X-3)** 

GIS data (circles) : C. Villagrasa et al., AIP Conf. Proc. **769** (2005) 842; PhD thesis, Universite de Paris XI, France, 2003.

To describe production of light fragments, we developed the G and S versions of our codes:

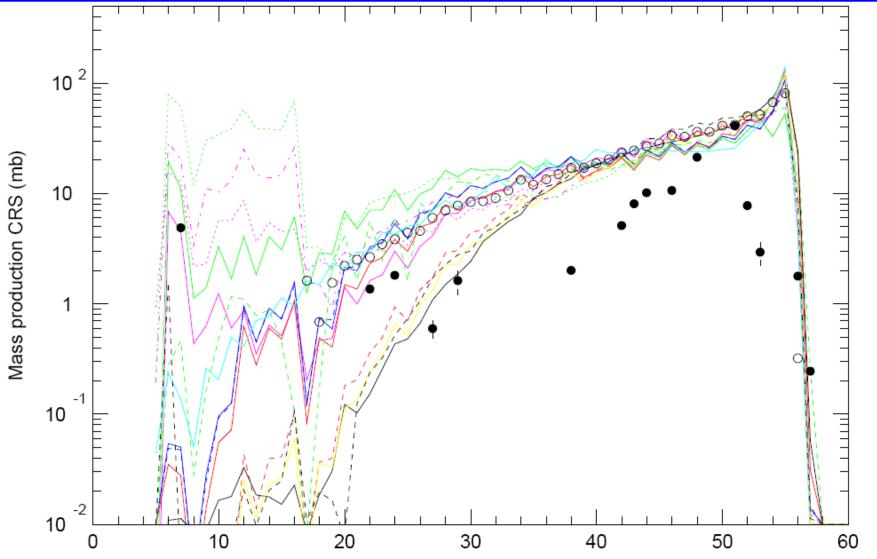
1) Using the fission-like binary-decay model **GEMINI**: R.J. Charity *et al.*, Nucl. Phys. **A476** (1988) 516 ("G" stands for **GEMINI**);

2) Using the Statistical Multifragmentation Model (SMM): J.P. Bondorf, A.S. Botvina, A.S. Iljinov, I.N. Mishustin, and K. Sneppen, Phys. Rep. **257** (1995) 133 ("S" stands for SMM)







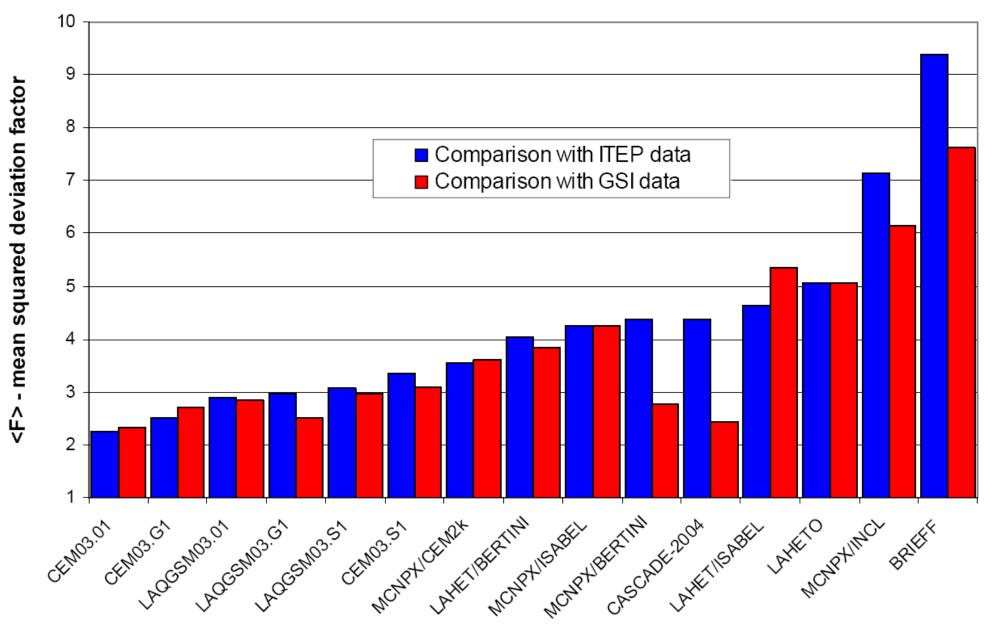


Experimental and calculated 1.5 GeV p + <sup>56</sup>Fe product yields as functions of A: GIS data (open circles) : C. Villagrasa-Canton et al., Phys. Rev. C75 (2007) 044603. ITEP data (filled circles): ISTC Project # 3266, Yu. E. Titarenko et al., LANL Reports LA-UR-06-4098 and LA-UR-07-2659; Proc. ND2007, E-print: arXiv:0705.1020.





Theoretical predictions on 56Fe(p,x) residuals





**Computational Analysis and Simulation (X-3)** 

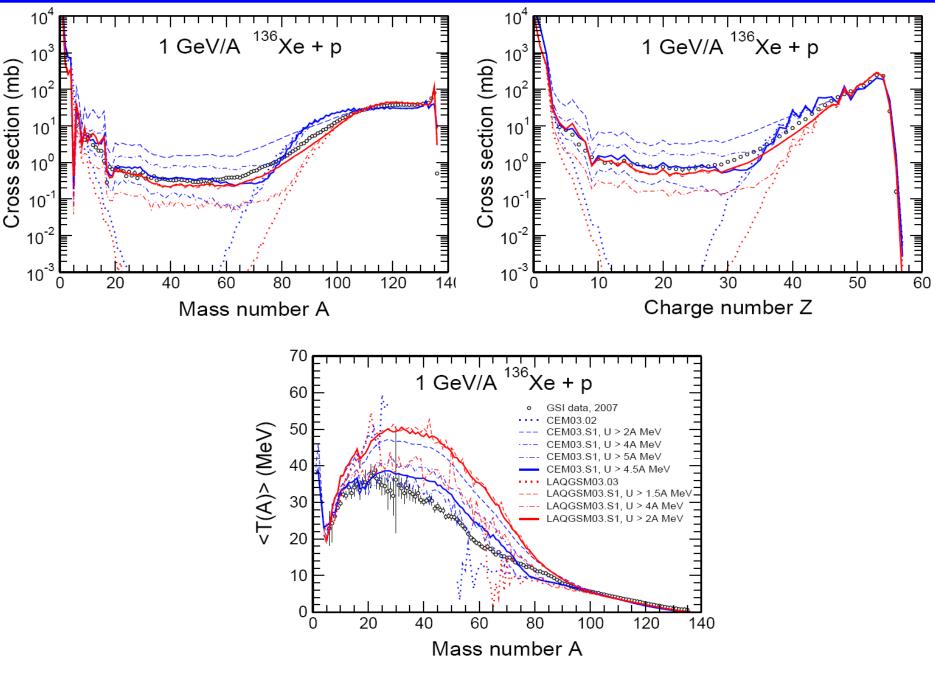


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CEM03.S1 and LAQGSM03.S1 are exactly the same as CEM03.01 and LAQGSM03.01, but consider also multifragmentation of excited nuclei produced after the preequilibrium stage of reactions, when their Excitation energy is above 2A MeV, using the Statistical Multifragmentation Model (SMM) by Botvina et al. (the "S" in the extension of CEM03.S1 and LAQGSM03.S1 stands for SMM).

- J. P. Bondorf, A. S. Botvina, A. S. Iljinov, I. N. Mishustin, and K. Sneppen, Phys. Rep. 257 (1995) 13;
- A. S. Botvina, A. S. Iljinov, I. N. Mishustin, J. P. Bondorf, R. Donangelo, and K. Snappen, Nucl Phys. A475 (1987) 663;
- A. S. Botvina, K. K. Gudima, A. S. Iljinov, and I. N. Mishustin, Phys. At. Nucl. 57 (1994) 628;
- A. S. Botvina, A. S. Iljinov, and I. N. Mishustin, Nucl. Phys. A507 (1990) 649;
- A. S. Botvina, A. S. Iljinov, and I. N. Mishustin, Sov. J. Nucl. Phys. 42 (1985) 712;
- A. S. Botvina, present ICTP-IAEA Advanced Workshop on Model Codes, 2008.

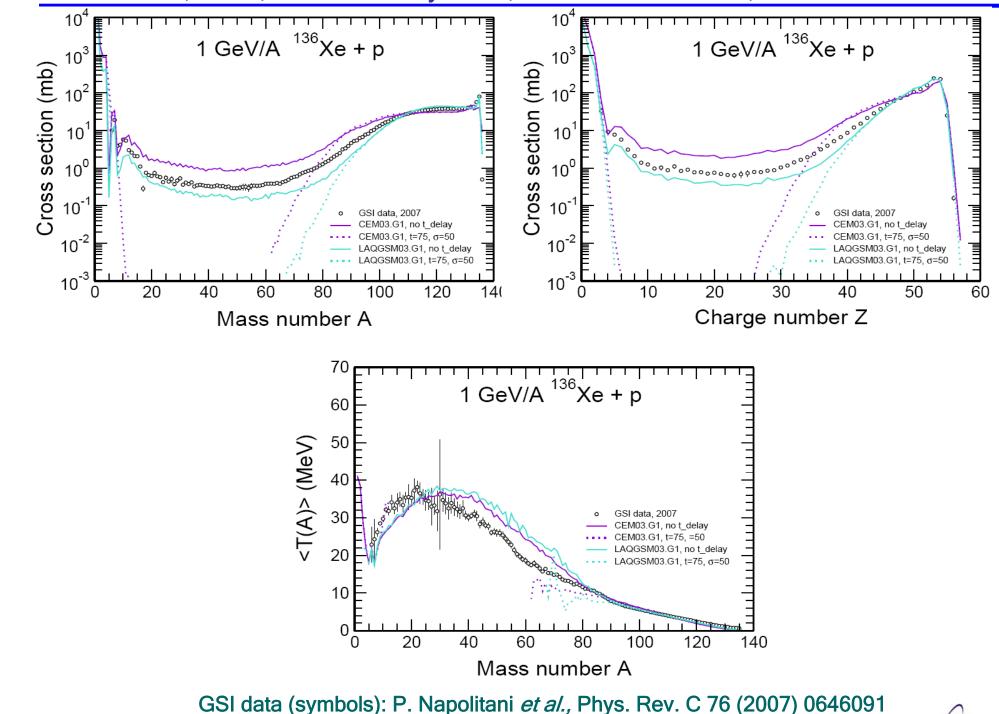
Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions, ICTP, 4 - 8 February 2008, S.G. Mashnik et al., LA-UR-08-0867



GSI data (symbols): P. Napolitani et al., Phys. Rev. C 76 (2007) 0646091









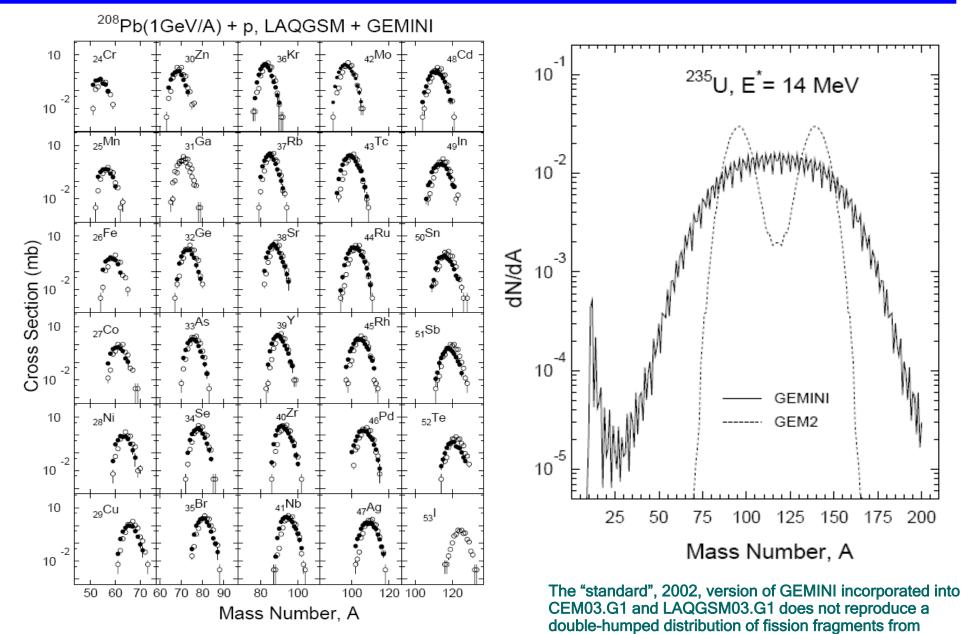


CEM03.G1 and LAQGSM03.G1 are exactly the same as CEM03.01 and LAQGSM03.01, but uses the fission-like binary-decay model GEMINI of Charity et al., which considers evaporation of all possible fragments, instead of using the GEM2 model (the "G" in the extension of CEM03.G1 and LAQGSM03.G1 stands for GEMINI).

- L. G. Sobotka, M. A. McMahan, R. J. McDonald, C. Signarbieux, G. J. Wozniak, M. L. Padgett, J. H. Gu, Z. H. Liu, Z. Q. Yao, and L. G. Moretto, Phys. Rev. Lett. 53 (1984) 200;
- R. J. Charity, M. A. McMahan, G. J. Wozniak, R. J. McDonald, L. G. Moretto, D. G. Sarantites, L. G. Sobotka, G. Guarino, A. Pantaleo, L. Fiore, A. Gobbi, and K. D. Hildenbrand, Nucl. Phys. A483 (1988) 371;
- R. J. Charity, D. R. Bowman, Z. H. Liu, R. J. McDonald, M. A. McMahan, G. L. Wozniak, L. G. Moretto, S. Bardley, W. L. Kenoe, and A. C. Mignerey, Nucl. Phys. A476 (1988) 516;
- R. J. Charity, Phys. Rev. C 58 (1988) 1073;
- R. J. Charity, L. G. Sobotka, J. Cibor, K. Hagel, M. Murray, J. B. Natowitz, R. Wada, Y. El Masri, D. Fabris, G. Nebbia, G. Viesti, M. Cinausero, E. Fioretto, G. Prete, A. Wagner, and H. Xu, Phys. Rev. C 63 (2001) 024611; http://www.chemistry.wustl.edu/~rc/gemini/;
- R. J. Charity, present ICTP-IAEA Advanced Workshop on Model Codes, 2008.







GSI experimental data (filled circles) are from: Enqvist, T. et al., *Nucl. Phys. A* 686, 481-524 (2001). Results by LAQGSM03.G1 (open circles) were calculated using  $t_delay = 75$  and *sig\_delay* = 50 in GEMINI (see details in: E-print: nucl-th/0501075, v2). actinides (see details in: E-print: nucl-th/0501075, v2). The



## Event generators for applications must:

- Be universal and describe arbitrary reactions without any free parameters
- Provide as good as possible agreement with available experimental data and have a good predictive power
- Not require too much computing time





## Comparison MCNPX\_LAQGSM with PHITS

### Itacil C. Gomes

(Courtesy of Itacil C. Gomes)







# 400MeV/u Uranium Beam on 0.2cm Thick Lithium target

- Pencil beam of U-238 zero radius
- MCNPX run 1.e+09 particles in 7:01:50 wall clock hours using 64 processors.
- PHITS run 6.3e+06 particles in 9:18:56 wall clock hours using 64 processors.
- Both runs were in Bassi, last generation IBM parallel machine.
- The ratio is 210.32 times faster for MCNPX.

(Courtesy of Itacil C. Gomes)





#### Summary

- CEM03.03 and LAQGSM03.03 and their "S" and "G" versions describe nuclear reactions of interest to Spallation Applications better than earlier versions
- As a rule, CEM03.03 and LAQGSM03.03 describe such reactions not worse than other codes presently available, and are often much faster, which is very important in complex simulations
- CEM03.01 is available now to users from RSICC and from NEA/OECD as the Code Package PSR-532
- The latest versions of our codes, CEM03.03 and LAQGSM03.03, have been or are being incorporated into MCNP6, MCNPX, and MARS15, to be available to users from RSICC and NEA/OECD
- There are still some problems important for Spallation Applications to be solved, but we understand the physical basis of these shortcomings and are able to improve predictability as we have done previously

Thank the Organizers, and especially, Dr. Sylvie Leray, for inviting me to present this lecture and for financial support of my trip; I am grateful to ICTP for kind hospitality!

Computational Analysis and Simulation (X-3)



