Validation of the statistical multifragmentation model of the Geant4 toolkit

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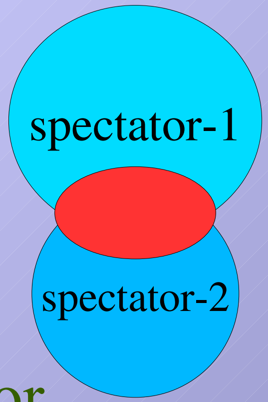
FIAS

Simulating nucleus-nucleus collisions in Geant4:



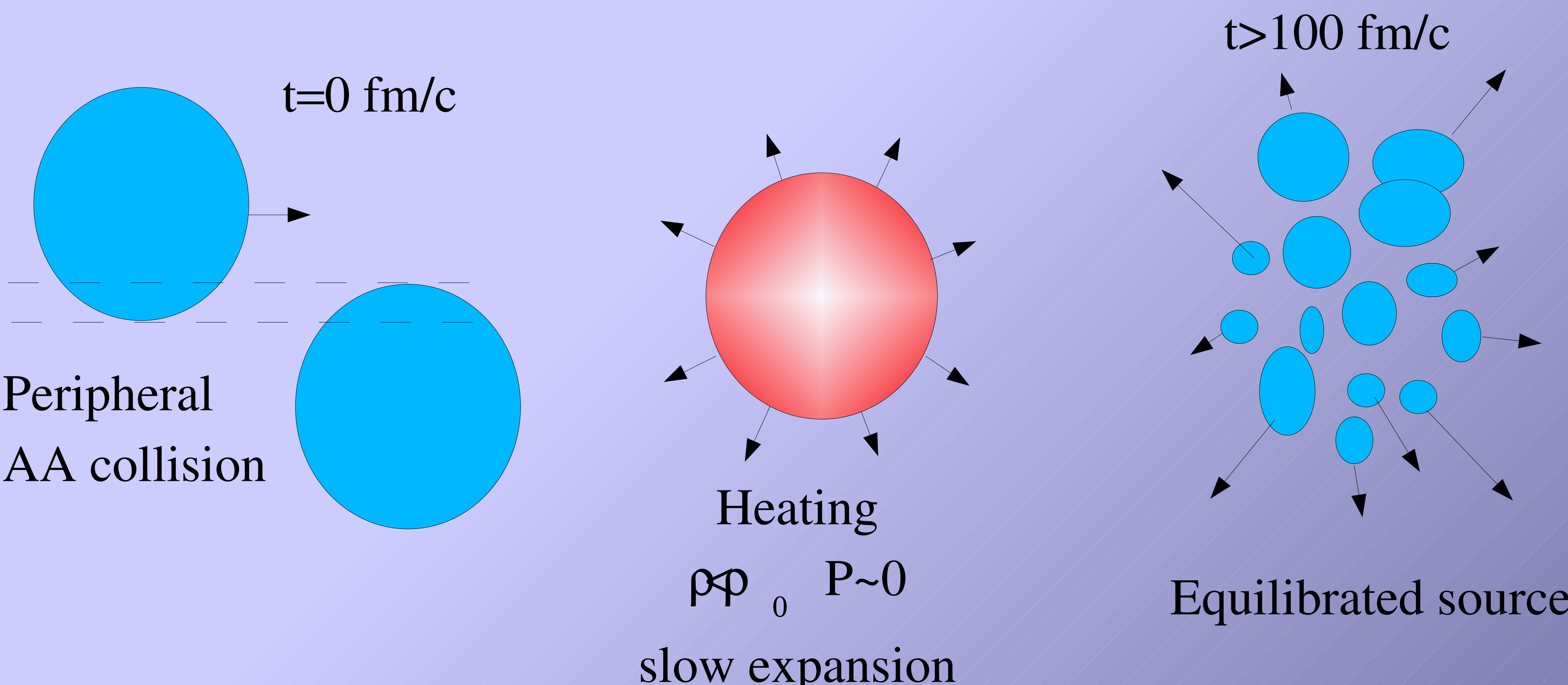
- **(Light) Ion Binary Cascade model** + **Evaporation model** (or statistical multifragmentation model for decay of **highly excited** residual nuclei)

- **Cascade model** describes collision geometry - number of participating nucleons, sizes of spectator fragments and their excitation energy.

- **De-excitation process** is simulated according to the mass, charge and excitation energy of the system. Decay channels are considered statistically. The properties of resulting fragments (their binding energy, excitations) are taken into account.

- Fermi break-up model is used to simulate decays of highly excited light nuclei up to ^{16}O (this model works stable and has been validated before)

Multifragmentation at E>3 MeV/nucleon*

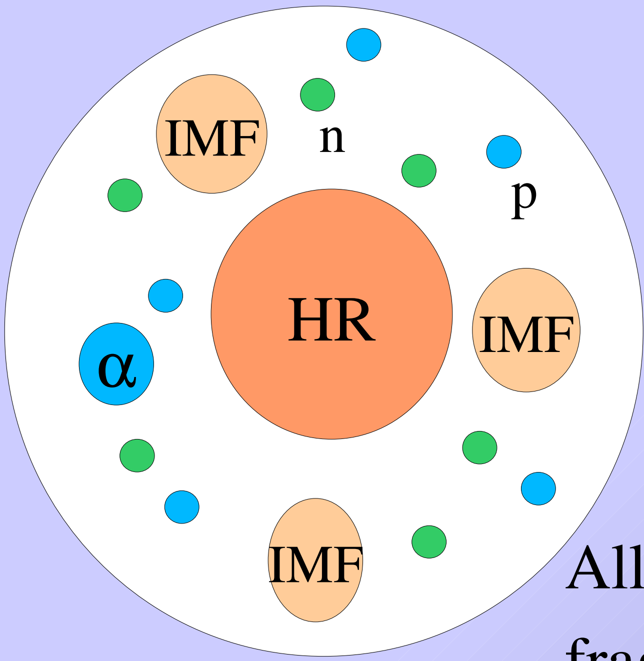


Can be well understood within an equilibrium statistical approach
(Randrup&Koonin, D.H.E. Gross et al, Bondorf-Mishustin-Botvina, Hahn&Stoecker,...)

C++ version of the SMM model is implemented in GEANT4 by Vicente Lara

Statistical description of nuclear break-up

J.P. Bondorf, R. Donangelo, I.N. Mishustin, et al., Nucl. Phys. A443 (1985) 321; A444 (1985) 460;
J.P. Bondorf, A.S. Botvina, A.S. Iljinov, I.N. Mishustin, K. Sneppen, Phys. Rep. 257 (1995) 133



Ensemble of nucleons and fragments in thermal equilibrium characterized by

neutron number N_0

proton number Z_0, $N_0+Z_0=A_0$

excitation energy $E^*=E_0-E_{CN}$

break-up volume $V=(1+\kappa)V_0$

All break-up channels are enumerated by the sets of fragment multiplicities or partitions, $f=\{N_{AZ}\}$, $M_f=\Sigma N_{AZ}$

- Baryon number and charge conservation
- in micro-canonical description: $\Sigma\, A N_{AZ}=A_0$, $\Sigma\, Z N_{AZ}=Z_0$

  or in macro canonical: $\Sigma\, A\langle N_{AZ}\rangle=A_0$, $\Sigma\, Z\langle N_{AZ}\rangle=Z_0$

- Statistical distribution of probabilities: $W_f \sim \exp\{S_f(A_0, Z_0, E^*, V)\}$

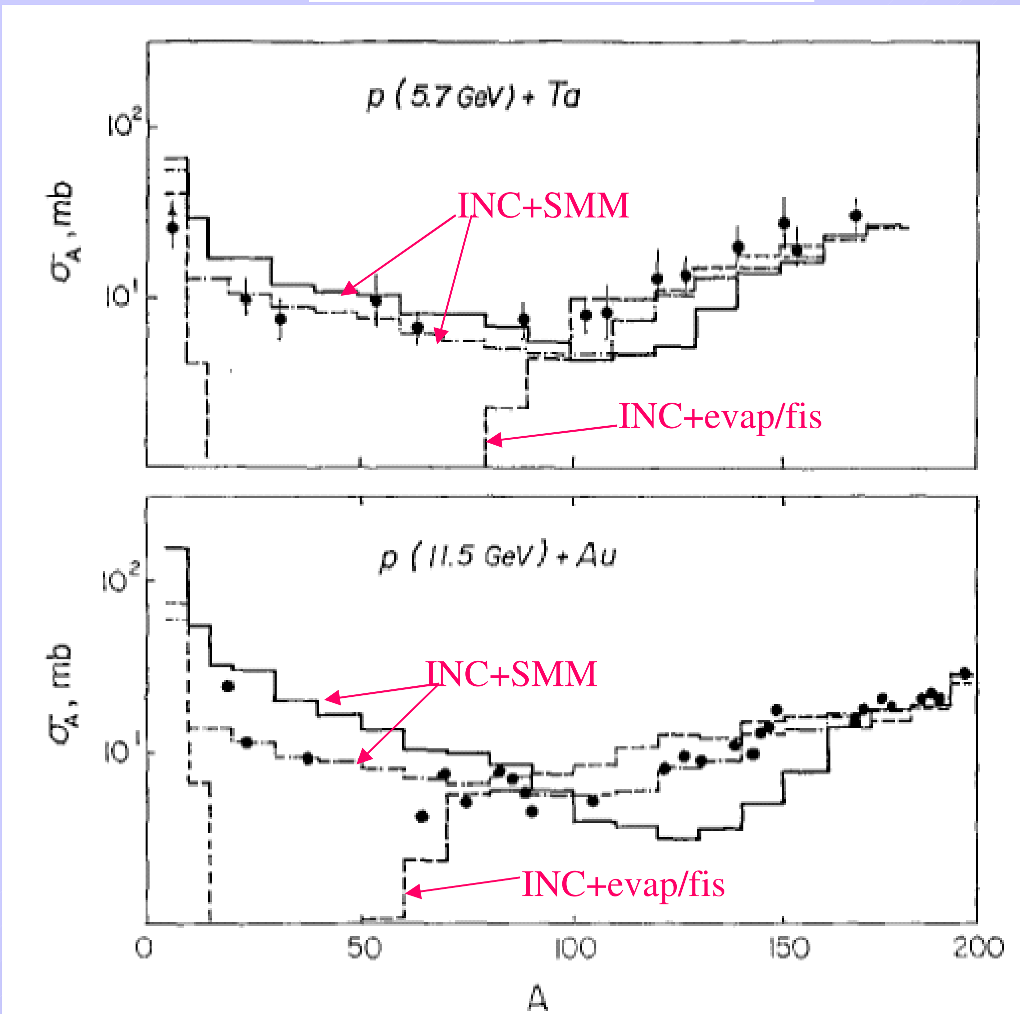
Statistical multifragmenation model (SMM) at work: pA-collsions

experiment: J.R.Grover, Phys.Rev. **126**(1962)1540

S.Kaufman et al., Phys.Rev. **C14**(1976)1121

FRS @ GSI

Nuclear Physics **A507** (1990) 649–674



PHYSICAL REVIEW C **70**, 054607 (2004)

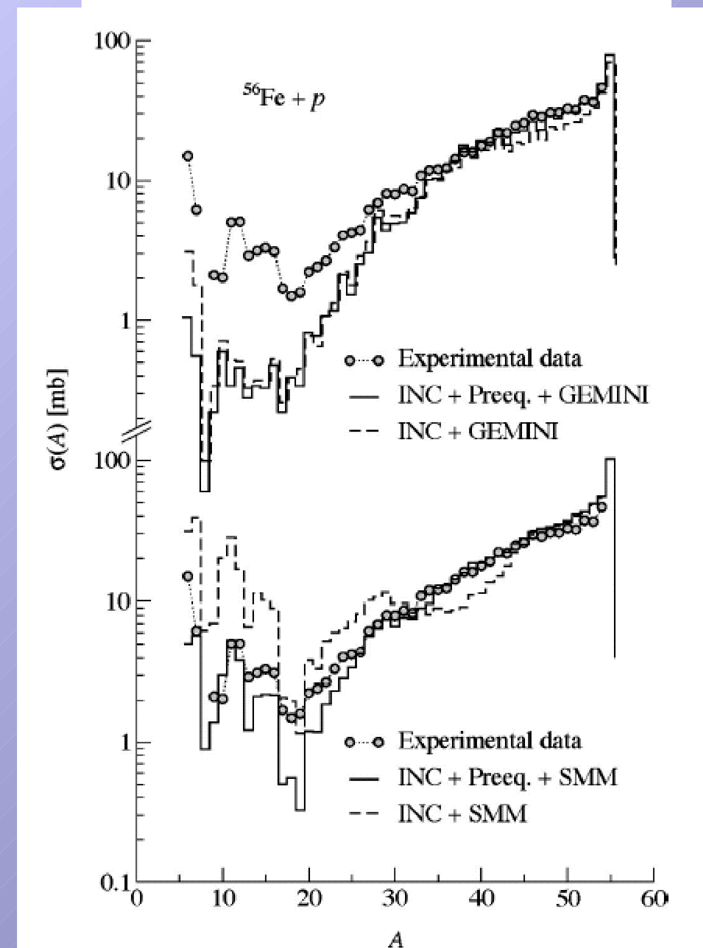


FIG. 15. Comparison of the measured mass distributions as a function of the mass number for the system ^{56}Fe+p with the results of GEMINI (upper part) and SMM (lower part). SMM is more sensitive than GEMINI to the effect of a pre-equilibrium phase.

SMM at work: nucleus-nucleus collisions:

Au(35MeV/N)+Au, peripheral

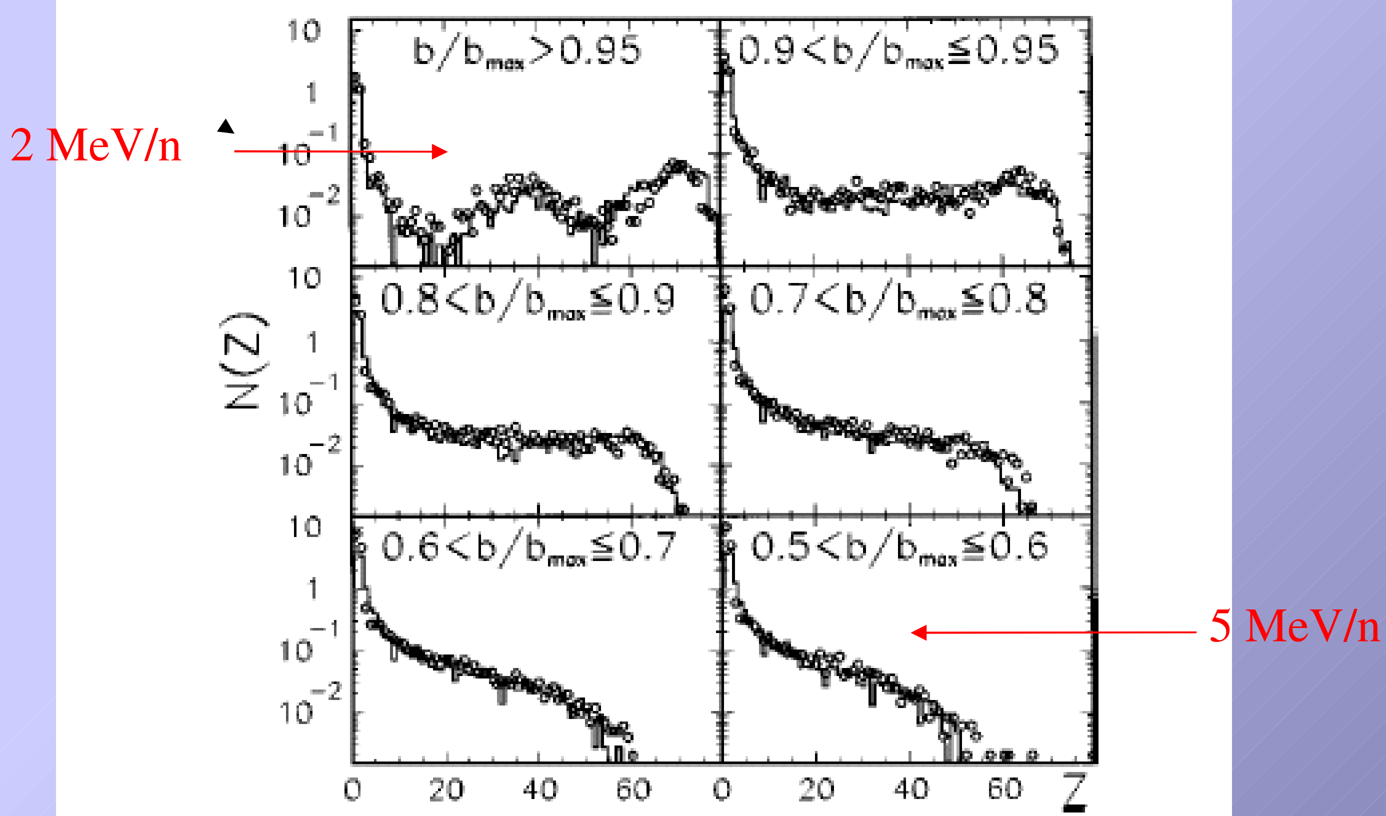


FIG. 8. Charge distributions for peripheral and midperipheral collisions (open point: experimental data; histogram: SMM predictions).

M.D'Agostino et al., Nucl.Phys. A**650** (1999) 329

Problems found while transporting ^{20}Ne or ^{58}Ni in water with G4:

- ---> Begin of Event: 239000
-
- G4Solver::SetIntervalLimits: Interval must be wider than tolerance.
- G4Solver::SetIntervalLimits: Limit1=9.555e-05 Limit2=1.875e-05 tolerance=0.0001
- G4Solver::Brent: The interval must be properly set.
- G4StatMFMacroMultiplicity: ChemPa=9.555e-05 ChemPb=1.875e-05
- G4StatMFMacroMultiplicity: fChemPa=-0.0143467 fChemPb=1
-
- In src/G4StatMFMacroMultiplicity.cc, line 119:
- ===> G4StatMFMacroMultiplicity::CalcChemicalPotentialMu: I couldn't find the root.
- G4HadronicProcess failed in ApplyYourself call for
- \- Particle energy[GeV] = 1.1874322
- \- Material = Water
- \- Particle type = Ne20[0.0]
-
- *** G4Exception : 007
- issued by : G4HadronicProcess
- GeneralPostStepDoIt failed.
- *** Fatal Exception *** core dump ***
-
- *** G4Exception: Aborting execution ***
-

Not very frequent, but still bothering:

- ---> Begin of Event: 81000
-
- G4StatMFMacroTemperature: Ta=1.17188e-07 Tb=78433.6
- G4StatMFMacroTemperature: fTa=-0.291297 fTb=-4.57743e+07
-
- In src/G4StatMFMacroTemperature.cc, line 94:
- ===> G4StatMFMacroTemperature::CalcTemperature: I couldn't bracket the solution.
- G4HadronicProcess failed in ApplyYourself call for
- - Particle energy[GeV] = 5.4732288
- - Material = Water
- - Particle type = Ni58[0.0]
-
-
- *** G4Exception : 007
- issued by : G4HadronicProcess
- GeneralPostStepDoIt failed.
- *** Fatal Exception *** core dump ***
-
- *** G4Exception: Aborting execution ***
-

To find the reason one needs stand-alone (unit) tests.

The statistical multifragmentation is not frequently invoked in calculations – only in some ~10% of events, while hadrons or nuclei are transported through the media.

Benchmarking in stand-alone tests is more instructive:

- Statistical Multifragmentation Model written by Alexander Botvina in FORTRAN, uses REAL*4 floats (single precision)

against

- Geant4 G4StatMF model written in C++, uses double precision floats (G4double)

- Should one expect full agreement despite of differences in floating point calculations?

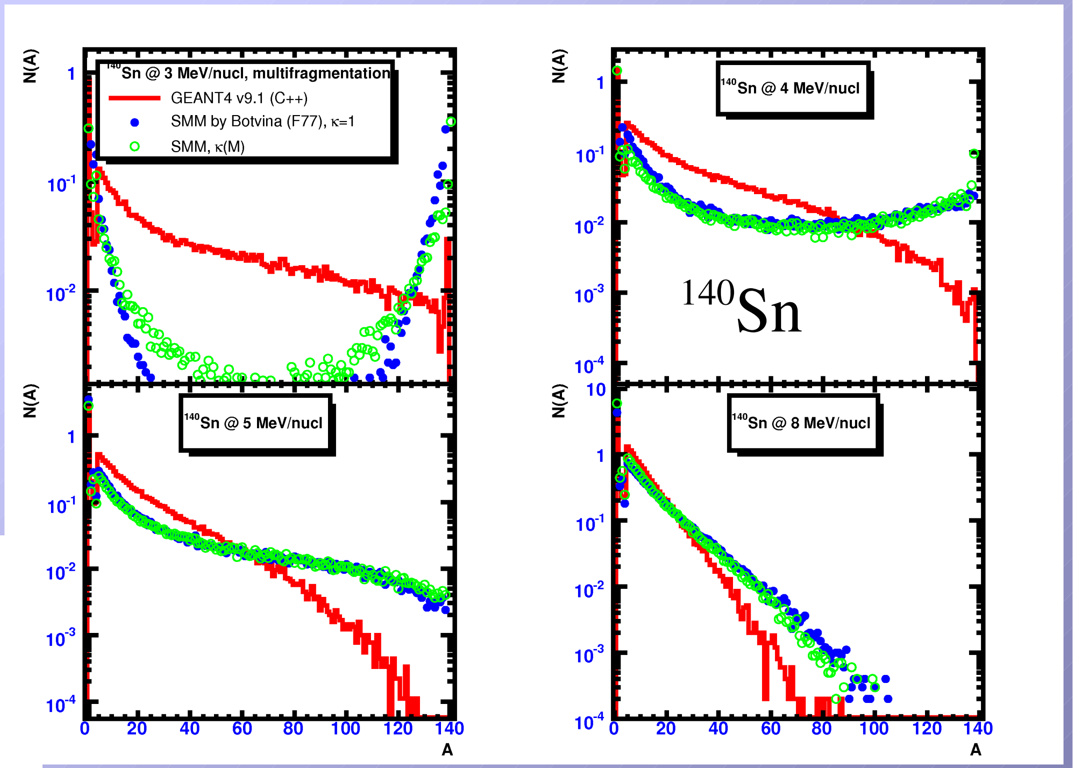
Stand-alone unit tests revealed more problems, in particular for ^{23}O:

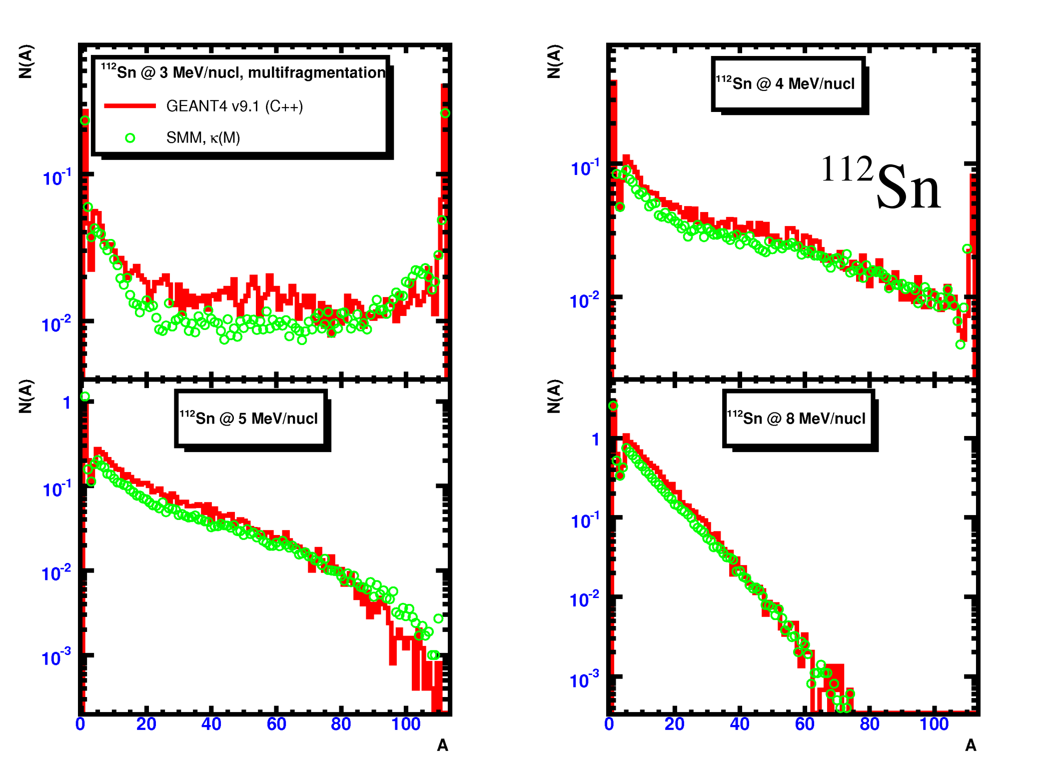
-
- ########## Test the Statistical Multifragmentation model of GEANT4
- Please choose Z from 8 to 100: 8
- Please choose A from 17 to 250: 23
- Please choose the low limit for the range of excitation energy (per nucleon in MeV) : from 0 to 100: 2
- Please choose the upper limit for the range of excitation energy (per nucleon in MeV) : from 0 to 100: 8
- Please choose the number of bins in histograms (10 - 1000): 100
- Please enter the average number of break-up events in each bin (10 - 10000): 1000
- Please enter the file name to write histograms (.root will be supplied): O23
- Histograms will be written to O23.root
- G4Solver::SetIntervalLimits: Interval must be wider than tolerance.
- G4Solver::SetIntervalLimits: Limit1=9.555e-05 Limit2=1.875e-05 tolerance=0.0001
- G4Solver::Brent: The interval must be properly set.
- G4StatMFMacroMultiplicity: ChemPa=9.555e-05 ChemPb=1.875e-05
- G4StatMFMacroMultiplicity: fChemPa=-0.0143467 fChemPb=1
- In src/G4StatMFMacroMultiplicity.cc, line 119:
- ===> G4StatMFMacroMultiplicity::CalcChemicalPotentialMu: I couldn't find the root.
- Aborted
-

The code crashed very frequently for neutron reach nuclei, e.g. ^{50}N and proton reach nuclei, e.g. ^{55}Sn.

Why numerical results do depend on implementation: C++ vs FORTRAN?

The fragment mass distributions agree well for ^{112}Sn but completely disagree for ^{140}Sn !

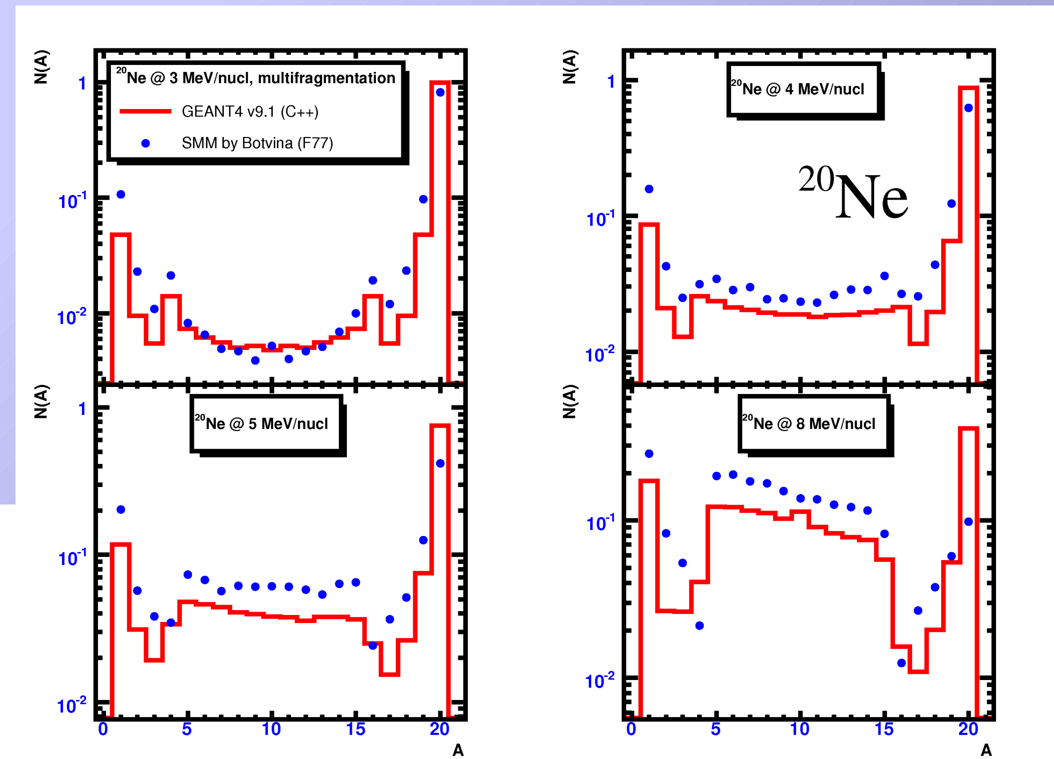


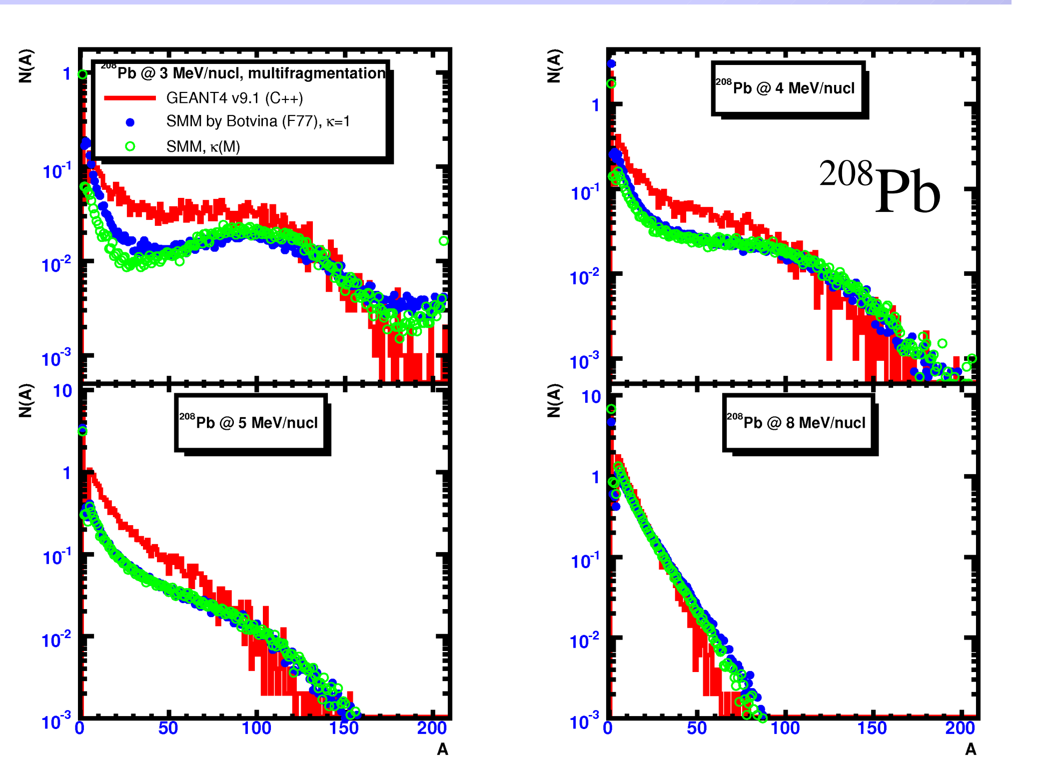


SMM calculations done for κ=1 and κ(M) depending on fragment multiplicity. Both options differ from G4 results obtained with κ(M). What is the reason?

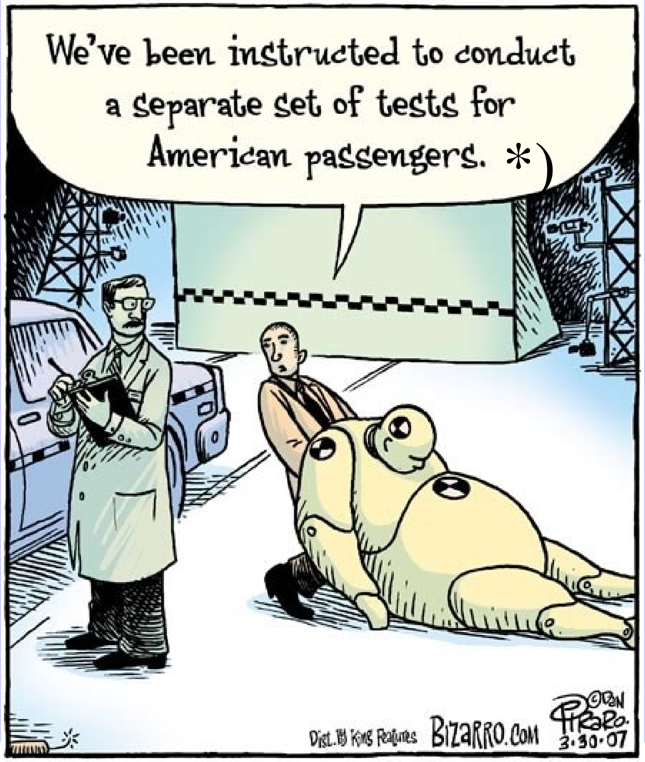
Results depend on implementation? C++ vs FORTAN, more examples on systems close to stability line:

The shapes of mass distributions agree for ^{20}Ne but differ for ^{208}Pb !

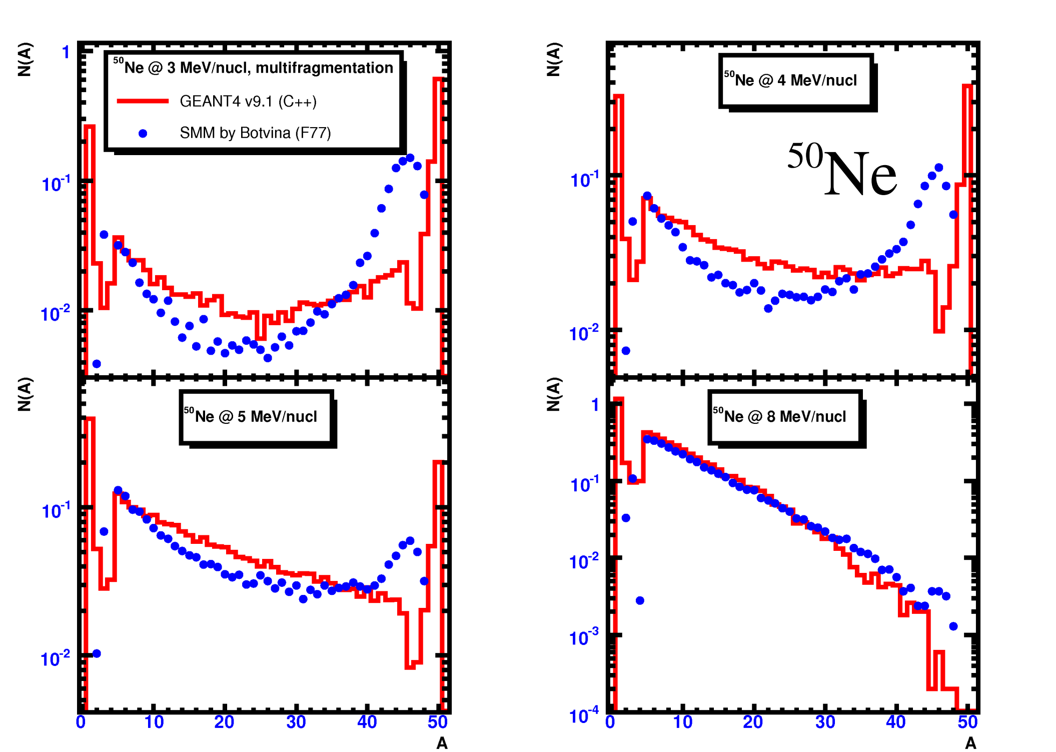


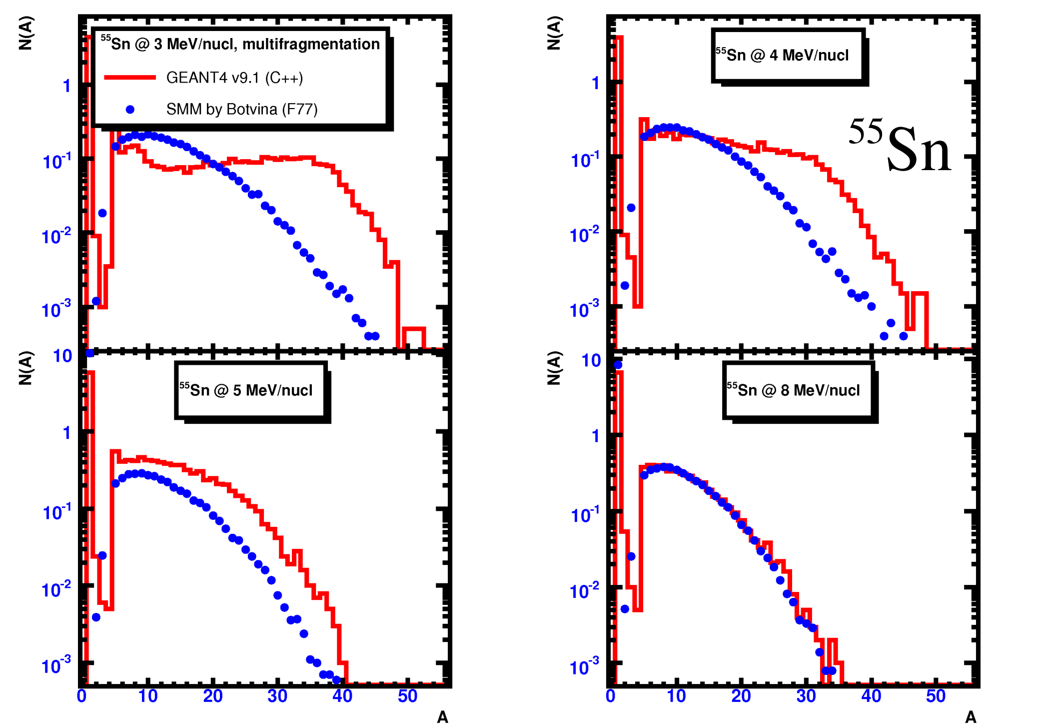


Exotic nuclear systems: crash tests for the both codes



) Also valid for "New Russians" (nouveau riche)





Apparent disagreement for ^{50}Ne and ^{55}Sn at moderate excitations!

Summary of corrections to G4StatMF:

- Additional check in the bracketing procedure of (G4StatMFMacroMultiplicity) to find the chemical potential μ as a root of *F*(μ)=0. This avoids the case when the initial interval is tighter than the requested tolerance.

- Accept Z=A fragments for considering in G4StatMFMacroCanonical. This avoids infinite loops for very proton reach systems.

- Increased number of trials in sampling of decay channels in G4StatMFMacroCanonical. However, since the procedure become very slow for systems with A/Z<1.2, it is advisable do not apply G4StatMF for such systems (use evaporation, changes to G4ExcitationHandler)

- Fixed a memory leak in G4StatMFMacroCanonical::ChooseZ

- Fixed an infinite loop problem in G4StatMFChannel

- The calculation of the fragment symmetry energy for G4StatMFMacroMultiNucleon is corrected – the agreement with the FORTRAN SMM code is achieved.

Calculations of the ensemble's average temperature: G4StatMF (C++) vs SMM (F77)

	Temperature (in MeV) for given excitation energy and nucleus											
	3 MeV/nucleon			4 MeV/nucleon			5 MeV/nucleon			8 MeV/nucleon		
Nucleus	G4	fixed G4	F77 SMM	G4	fixed G4	F77 SMM	G4	fixed G4	F77 SMM	G4	fixed G4	F77 SMM
^{140}Sn	6.91	5.64	5.87	7.14	6.18	6.34	7.16	6.40	6.43	8.	7.20	7.15
^{112}Sn	5.65	5.44	5.52	6.23	6.06	5.83	6.44	6.30	6.15	7.39	7.28	7.06
^{55}Sn	21.61	5.73	7.29	22.1	6.38	8.10	22.5	7.09	8.94	24.	9.52	11.76

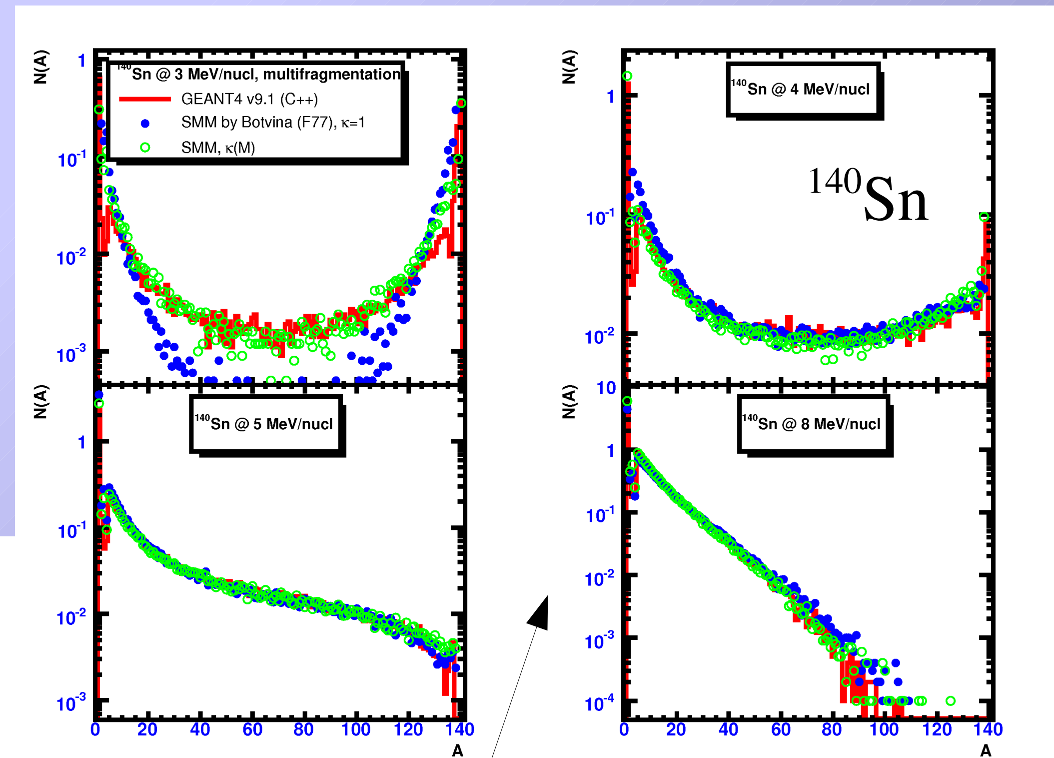
- In the original version (G4 9.1) the ensemble's average temperature $<T>$ calculated for proton-reach system ^{55}Sn was found to be larger than the critical temperature T_C

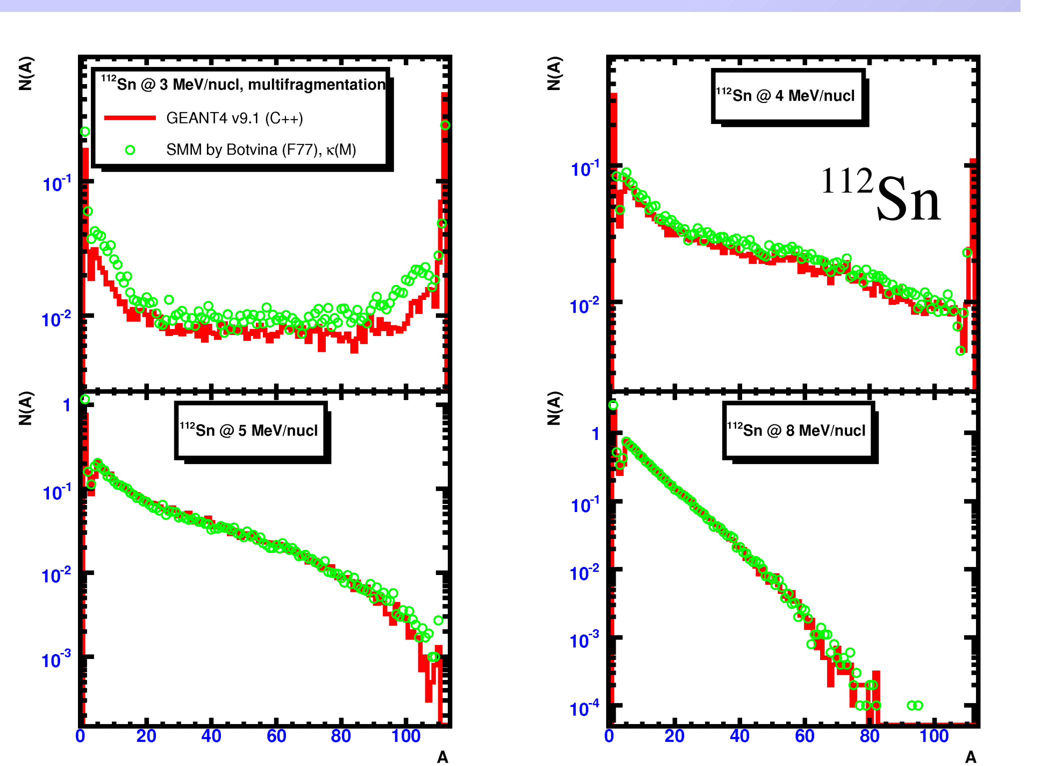
  This was not good!

- Also for ^{140}Sn and ^{112}Sn there were up to 1 MeV differences.
- Fixes in calculations of the fragment's symmetry energy were introduced. New results agree much better with F77 SMM (within 0.2 MeV for ^{140}Sn and ^{112}Sn).

Once fixes were introduced much better agreement is found...

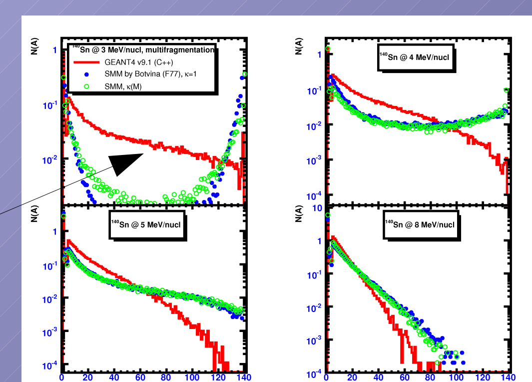
Now the calculations with κ(M) agree well both for ^{112}Sn and ^{140}Sn for all excitation energies!





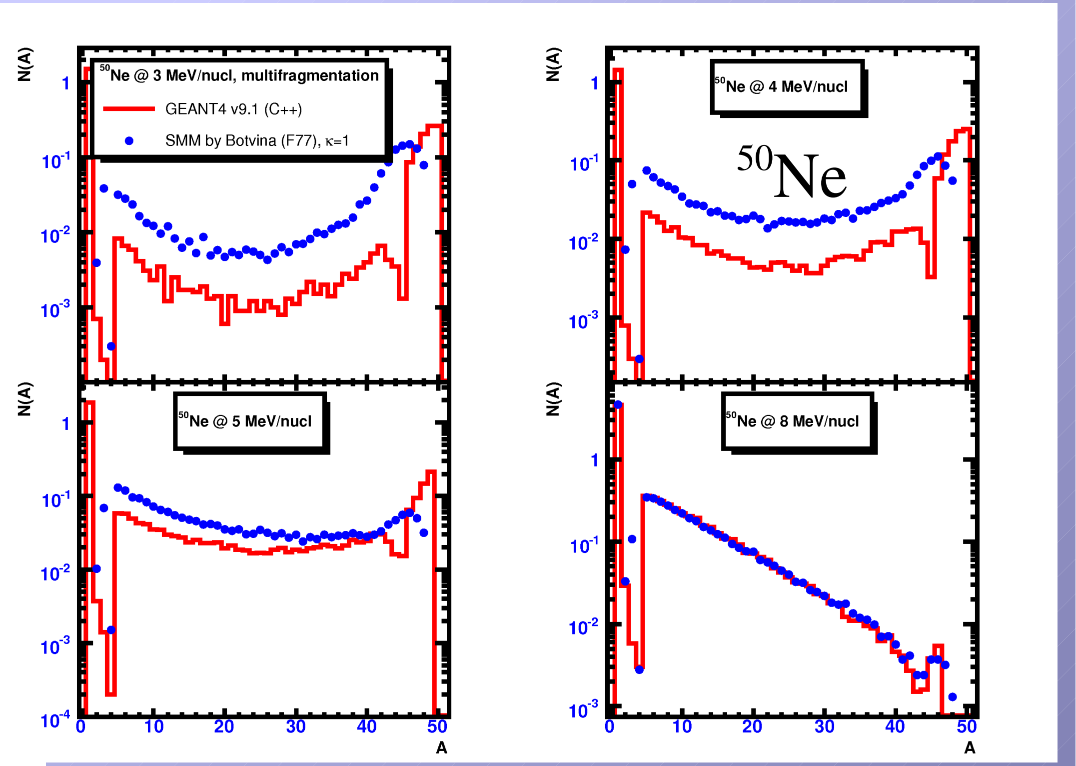
Seems much better now!

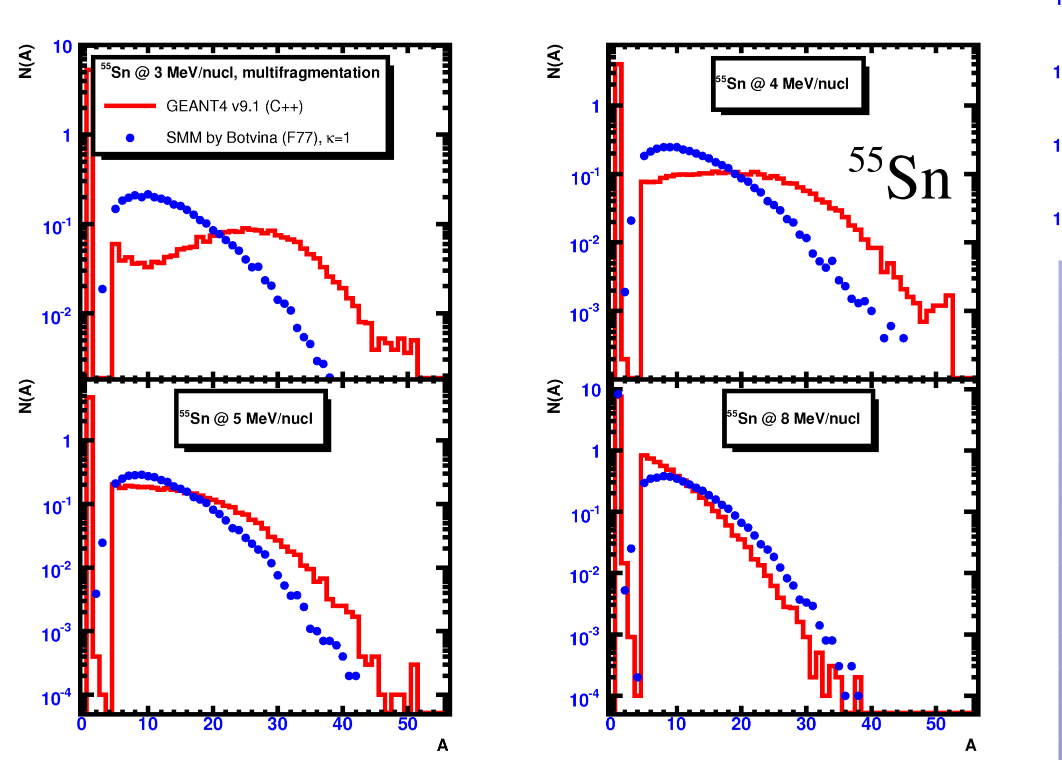
This was before the corrections were introduced.



More crash tests after the fixes were introduced...

Still not in complete agreement for ^{50}Ne and ^{55}Sn, but now G4StatMF works STABLE for such exotic nuclei!



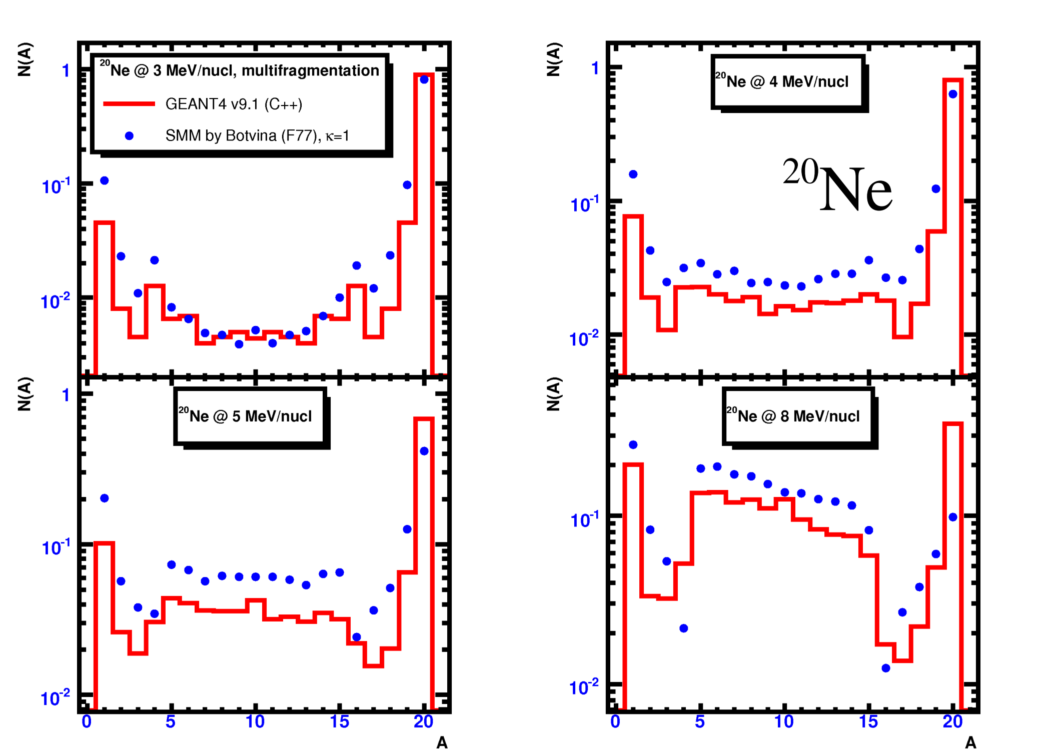


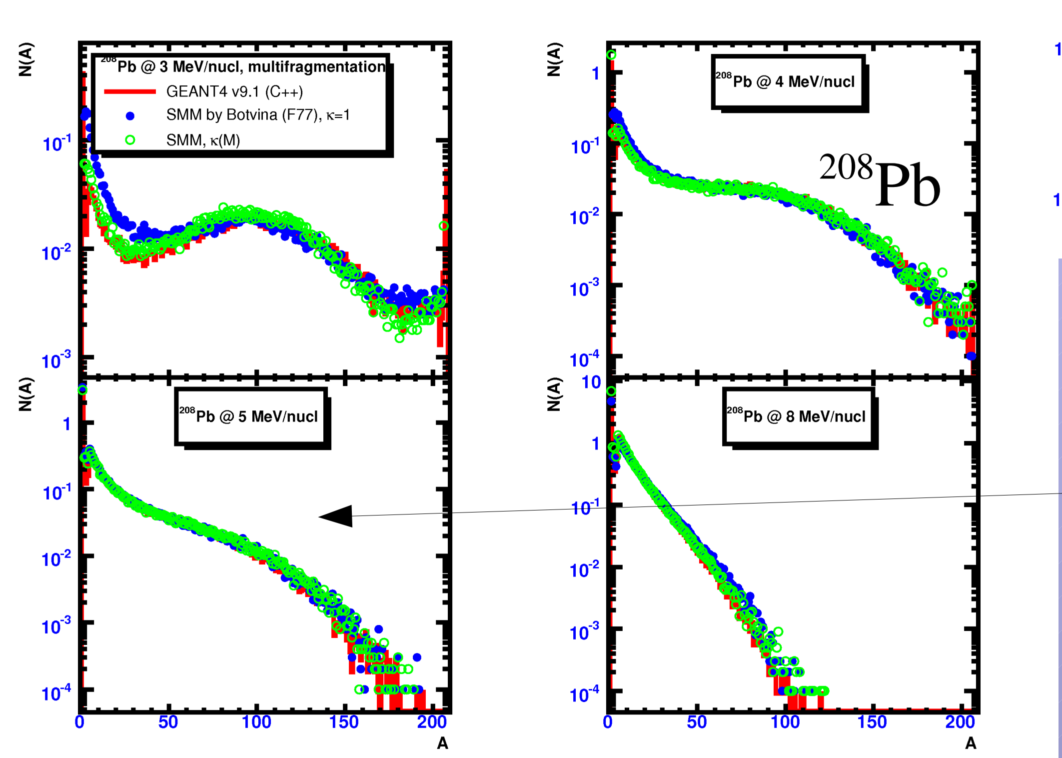
The rates of production of such exotic residual nuclei are quite low, so one can tolerate possible inaccuracy in calculations for such systems.

The results of two SMM implementations (C++ and FORTRAN) are in much better agreement now:

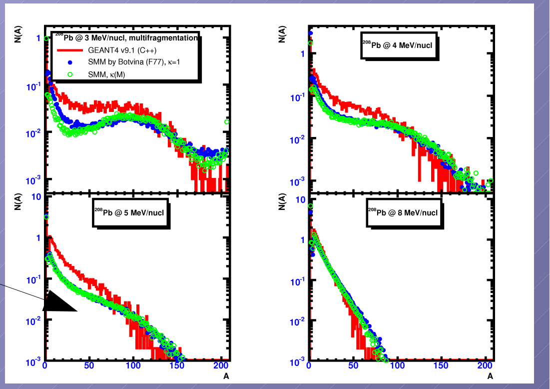
The fragment mass distributions agree well both for ^{20}Ne and ^{208}Pb!

It is advisable to use κ(M) in calculations (actually default option in G4).

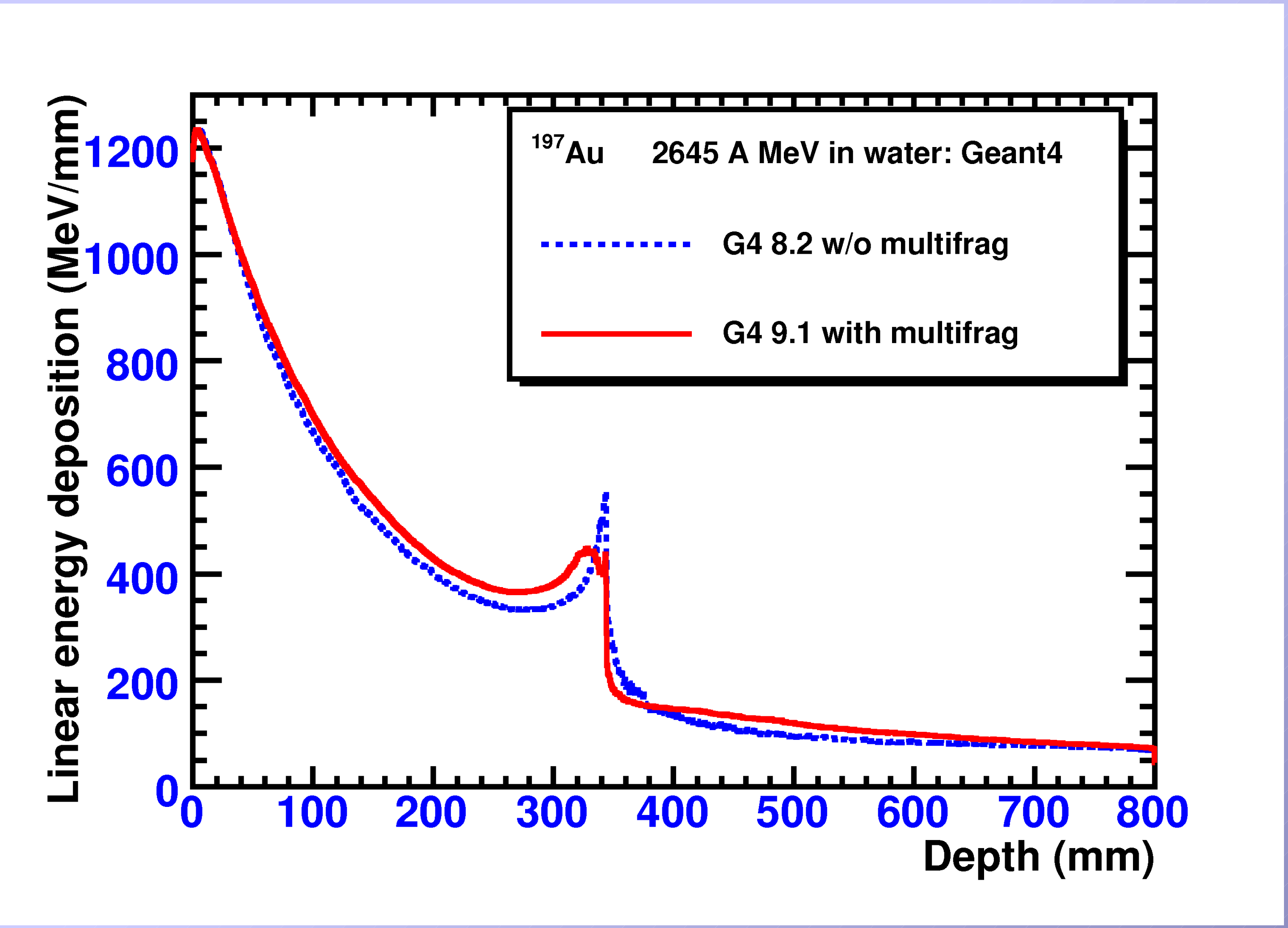




It is much better now than before!



High-energy Au ions in water: impact on depth-dose curve



The Bragg peak is due to primary Au. The beam is attenuated due to fragmentation

The tail beyond the peak is due to light fragments (p, d, He).

Multifragmentation gives fragments between p and Au. A bump is seen.

To be validated with experimental data!

Conclusions and suggestions:

- To the best of our knowledge, the only transport code which includes multifragmentation is Geant4. (Only Fermi break-up of light nuclei in FLUKA)

- Multiframentation is important to describe nuclear fragmentation properly.

- Currently multifragmentation is initialized “off” in the constructor of G4ExcitationHandler.

- G4 Binary cascades makes it own ***private*** instance of ExcitationHandler – no way to switch it on.

- On the contrary, Wilson Abrasion model creates a ***public*** instance of G4ExcitationHandler and users are allowed to control the de-excitation submodels.

- To speed up the calculations multifragmentation can be off, but for isotope production it should be on – please allow the user to decide, e.g. to use with new models like G4 QMD

Thank you for attention!

Back-up slides I:

Details on proposed corrections to G4StatMF

Details on introduced corrections:

- **1.** When the chemical potential μ is calculated as a root of the equation $F(\mu)=0$, the initial guess sometimes hits the target in G4StatMFMacroMultiplicity.cc. In some of such cases the length of the interval where a root of the equation is located is less than the requested tolerance as a result of the successful bracketing procedure. In such cases false errors were reported by G4Solver::SetIntervalLimits: "Interval must be wider than tolerance."

  Now this problem is fixed by introducing of an additional check for the bracketing success.

- **2**. An infinite loop in G4StatMFMacroCanonical.cc for proton-only initial systems (Z=A) has been detected. In the original version, the channels containing at least one "fragment" with protons only (Z=A) were disregarded. This resulted to an infinite loop to find a proper channel if the initial system was a proton-only one.

  Now Z=A fragments are admitted if the energy conservation permits such configuration.

Corrections introduced - II:

- **3.** It was found that for relatively cold proton-reach nuclear systems a huge number of trials (up to 10^5) in G4StatMF.cc can be required to find a decay channel with a valid temperature. One can avoid this problem by imposing a restriction not to apply the SMM at low excitation energies, below 3 MeV/nucleon, to light and medium proton-reach systems and to heavy proton-reach systems below 5 MeV/nucleon. Below these excitation energy limits the calculations for nuclei with $A/Z<1.2$ are very slow, as only a small part of decay configurations satisfy energy conservation.

  It is advisable to use evaporation model for systems with low excitations and low neutron-to-proton ratios. Appropriate changes in G4ExcitationHandler have to be made for this purpose.

Corrections introduced - III:

- **4.** The channel for which the attempt to find the temperature failed has to be deleted to release the memory used. Otherwise, as explained above, in the case of the proton-reach nuclei it would lead to memory leak due to large number of iterations. The object "theChannel" is created in G4StatMFMacroCanonical::ChooseZ(), but have to be deleted when not in use in G4StatMF.

  Fixed by introducing a *delete* statement.

- **5**. An infinite loop in G4StatMFChannel.cc is possible:

```
do
  {
   CosTheta1 = 1.0 - 2.0*G4UniformRand();
  }
while (CosTheta1*CosTheta1 < CTM12);
```

as soon as CTM12 becomes closer to 1, e.g. 0.9999993. G4UniformRand() provides numbers in the interval [0.,1.), and the last point is excluded.

Fixed, see the revised version of G4StatMFChannel.cc

Corrections introduced - IV:

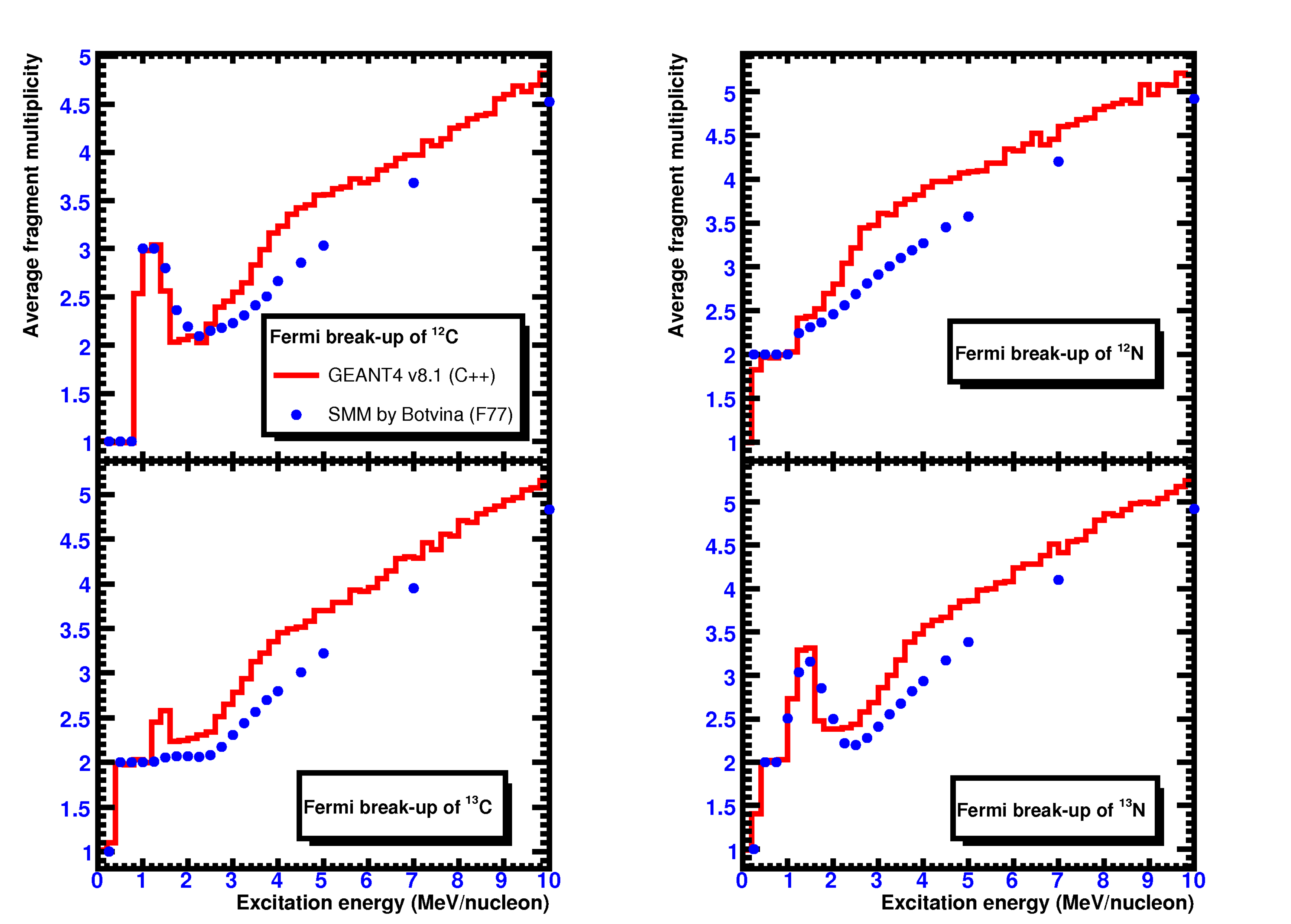
- **6.** The calculation of the fragment symmetry energy has been fixed in G4StatMFMacroMultiNucleon. This restored the agreement with the Fortran SMM model of Alexander Botvina with respect to the average partition temperature and fragment mass distributions for nuclei like ^{50}Ne, ^{140}Sn.

This bug was hidden in calculations of stable nuclei decay (e.g. ^{20}Ne, ^{112}Sn) due to low contribution of the symmetry energy term for such nuclei.

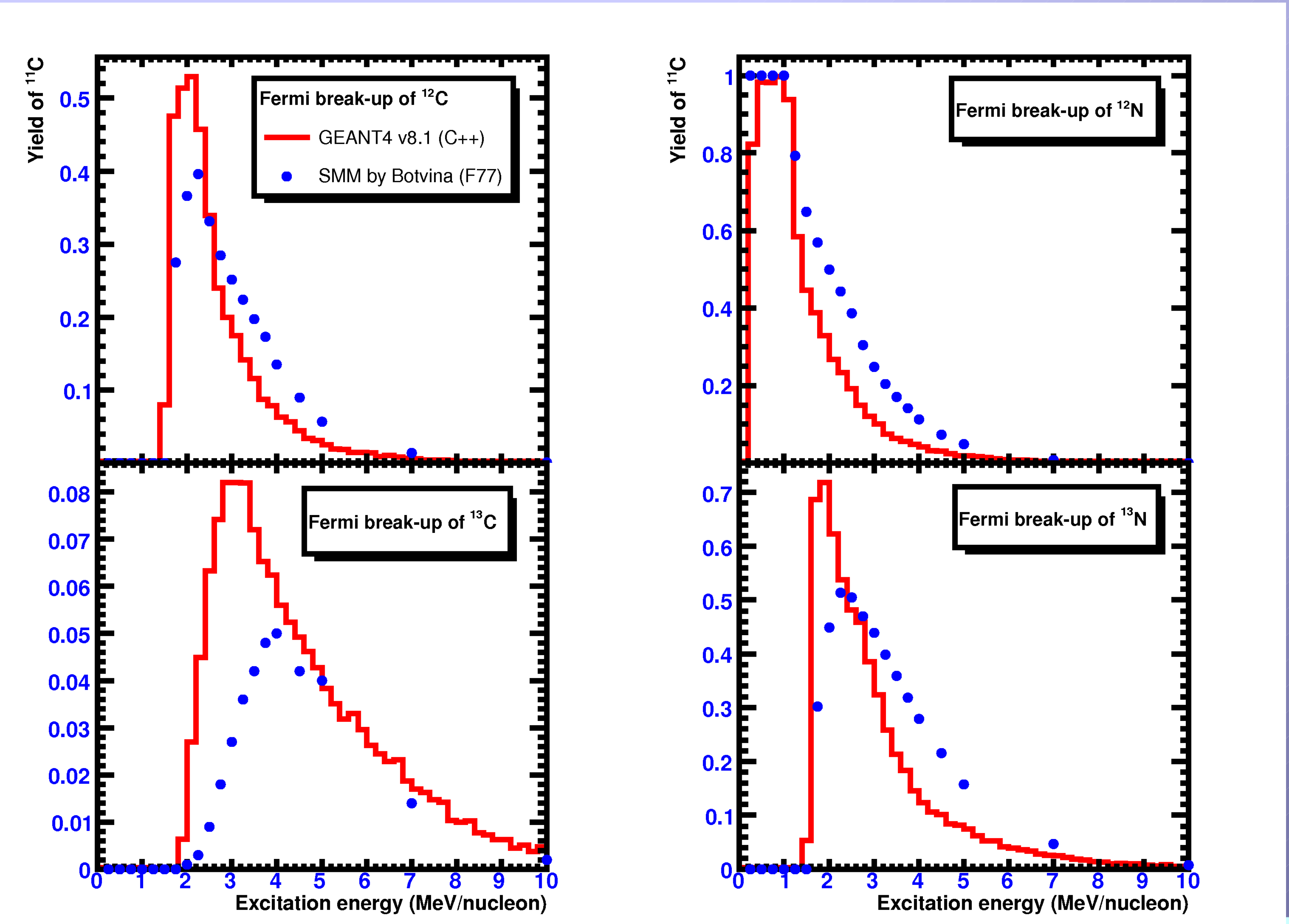
Back-up slides II:

Validation of Fermi break-up model for simulating decay of highly excited light nuclei

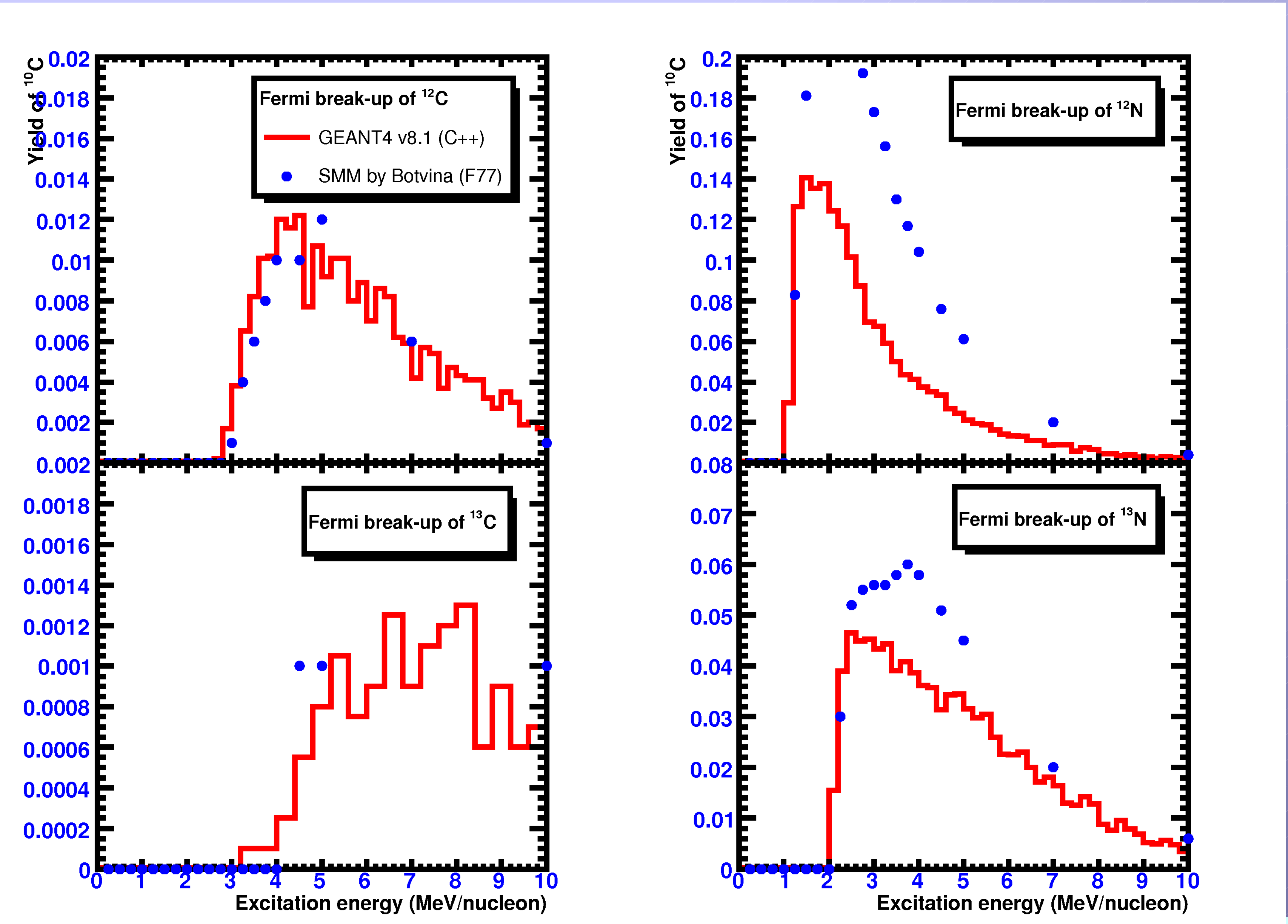
Fermi break-up model for decay of light nuclei – average multiplicity



Fermi break-up model for decay of light nuclei – production of ^{11}C

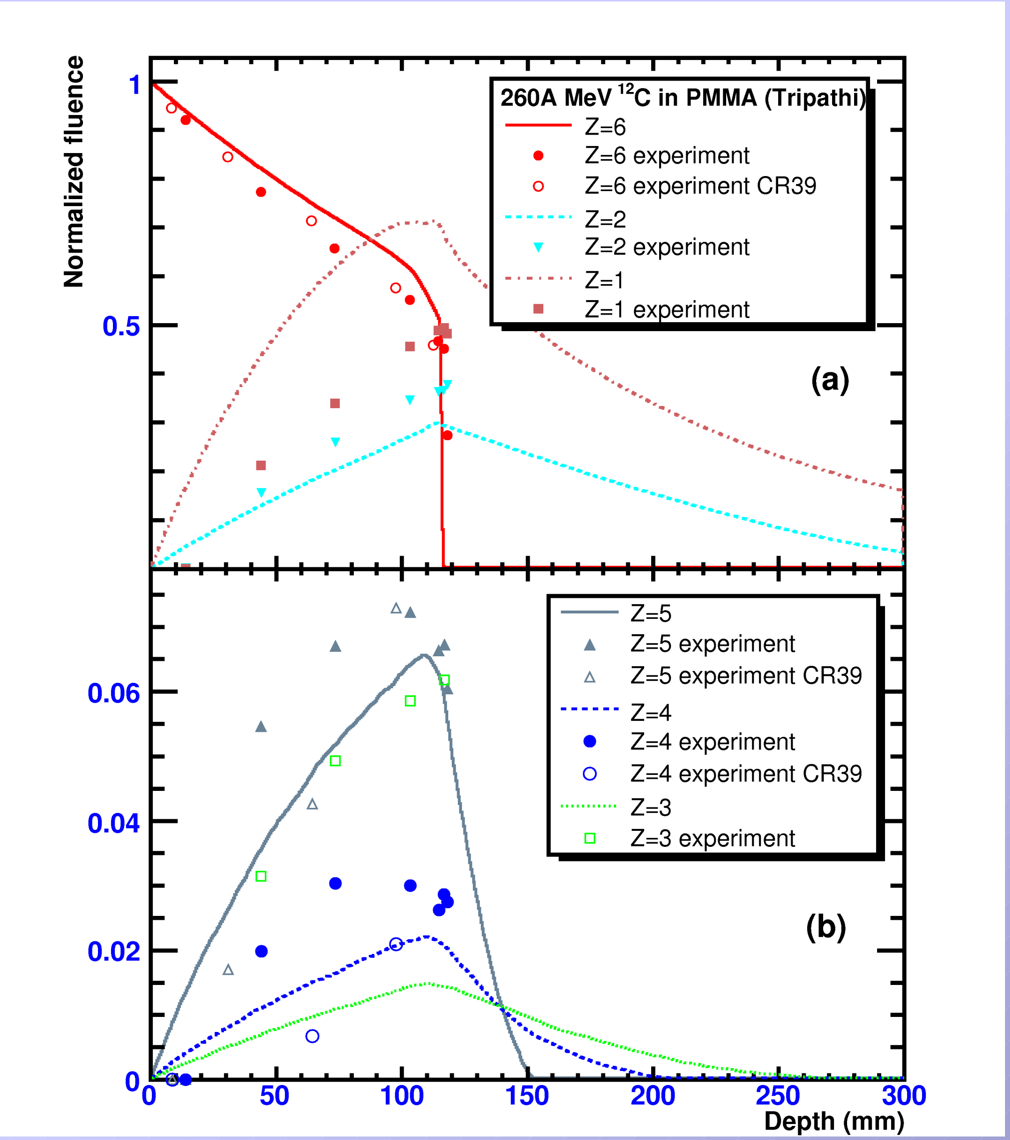


Fermi break-up model for decay of light nuclei – production of ^{10}C

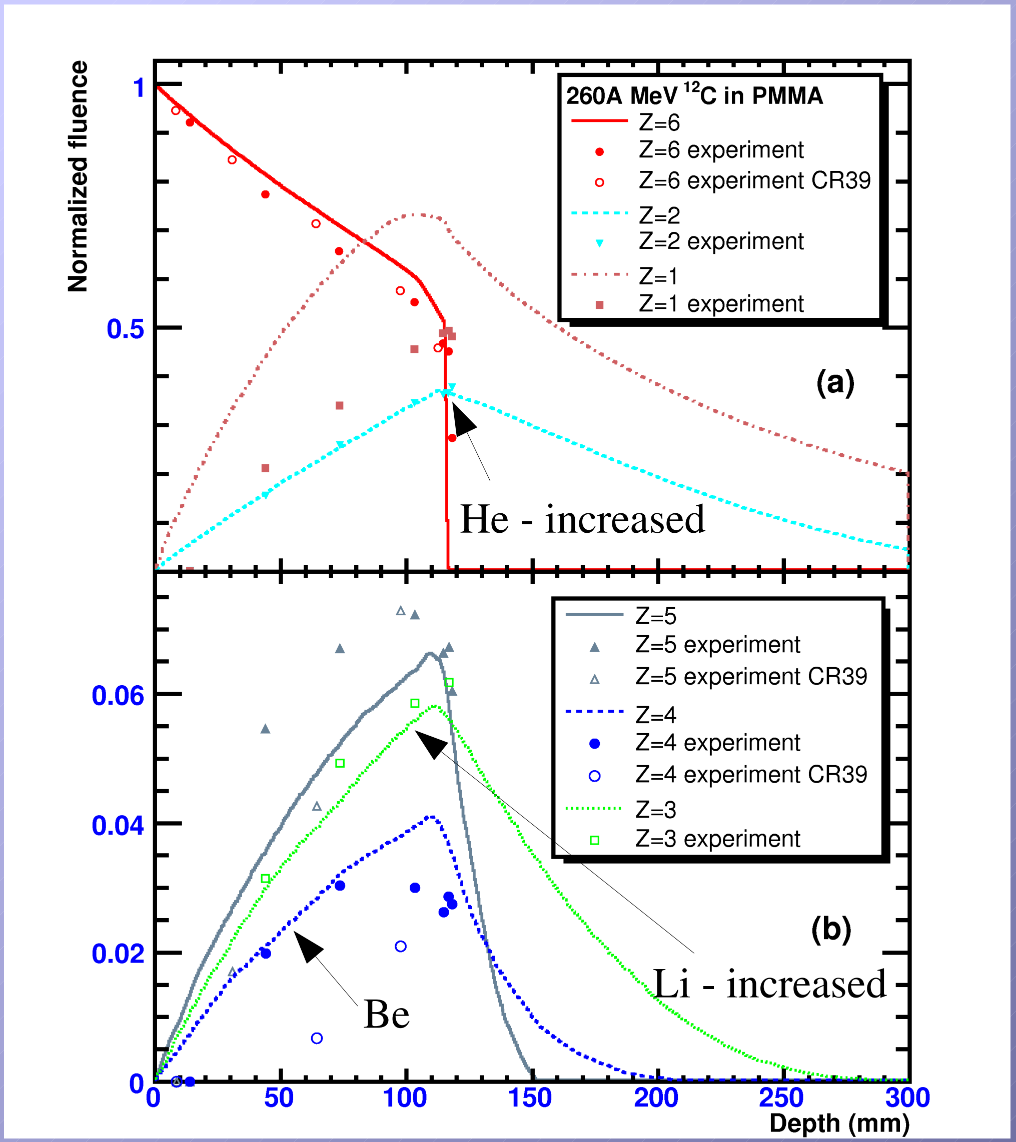


Secondary fragments: Fermi break-up at work

Without Fermi break-up



With Fermi break-up



Fermi break-up model predicts more IMF fragments: He, Be and Li – closer to data !