Recent Developments in Pre-equilibrium and De-excitation Models in Geant4

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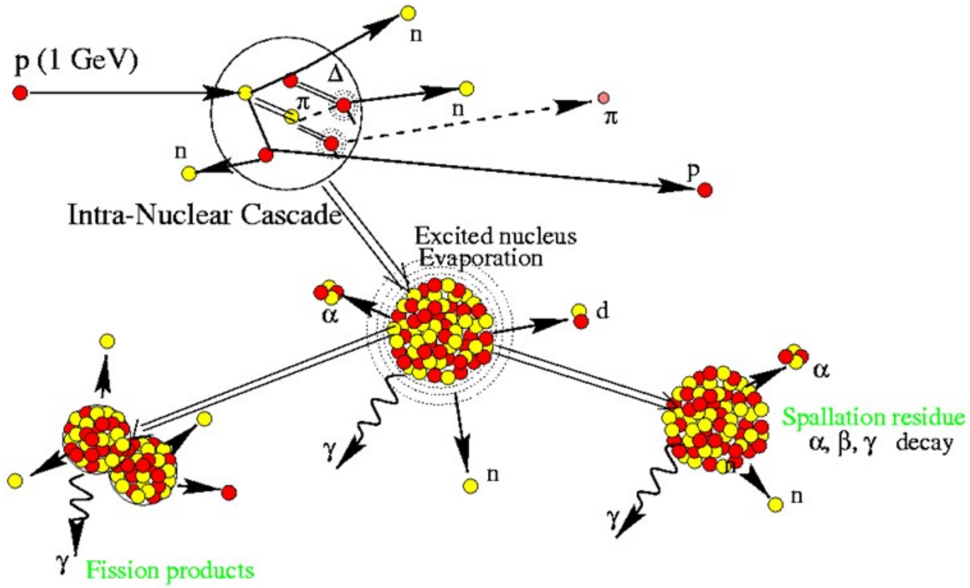
IAEA Benchmark on Spallation Reactions

- The benchmark was organized under the auspices of IAEA
- To assess the prediction capabilities of the spallation models
- To understand the reason for the success or deficiency of the models
- To reach a consensus, if possible, on some of the physics ingredients

Geant4 has participated with two cascade models:

Binary Cascade
Bertini cascade



Geant4 *Low Energy* Hadronic Models

- **Binary Cascade**:
  - a time-dependent model which depends as little as possible on parameterization and therefore can be expected to be more predictive
  - is an *in house* development, including its own precompound and evaporation models.

NATIVE

- **Bertini Cascade**:
  - it came from the INUCL code which was intended as an all-inclusive model
  - it came with its own pre-compound and de-excitation models, which are not very different in origin from those in Binary, but the implementations are different.

IAEA benchmark

- **INCL/ABLA**:
- **CHIPS(Chiral Invariant Phase Space)**
- **QMD (Quantum Molecular Dynamics Model)**

Pre-equilibrium

- After Binary Cascade stage *native* pre-equilibrium follows
- Native pre-equilibrium de-excitation model in Geant4 is a version of standard exciton model.

Competitor processes:

- Internal transition rates:
  - CEM (Cascade Exciton Model, Gudima et al). Default
  - Blann-Machner's parameterization.
- Particle emission rates:
  - Nucleon emission in standard exciton formulation.
  - Complex particle emission (d,t,^{3}He, ^{4}He) from CEM.

Pre-equilibrium: new inverse reaction cross sections

- **Key ingredient**: Inverse reaction cross sections play a mayor role in the calculation of (competing) emission probabilities.

- Theory driven *old* parameterization (Dostrovski et al, 1959) (kept as option)

- **NEW**: More realistic parameterization of reaction cross sections (after release 9.2)
  - Chatterjee at al: Calculated with global optical model potentials, in turn fitted to reproduce available experimental data
  - Kalbach's retuning (PRECO code)
  - Wellisch's parameterization of proton reaction cross sections by direct fitting to experimental data
  - **Default option** combines the best combination of inverse cross sections (Wellisch's parameterization for protons and Kalbach's one for the rest)

Pre-equilibrium: transition to De-excitation

- The transition from pre-equilibrium to equilibrium de-excitation should take place when:

$$\lambda_+(p,h,E) = \lambda_-(p,h,E) \quad (1)$$

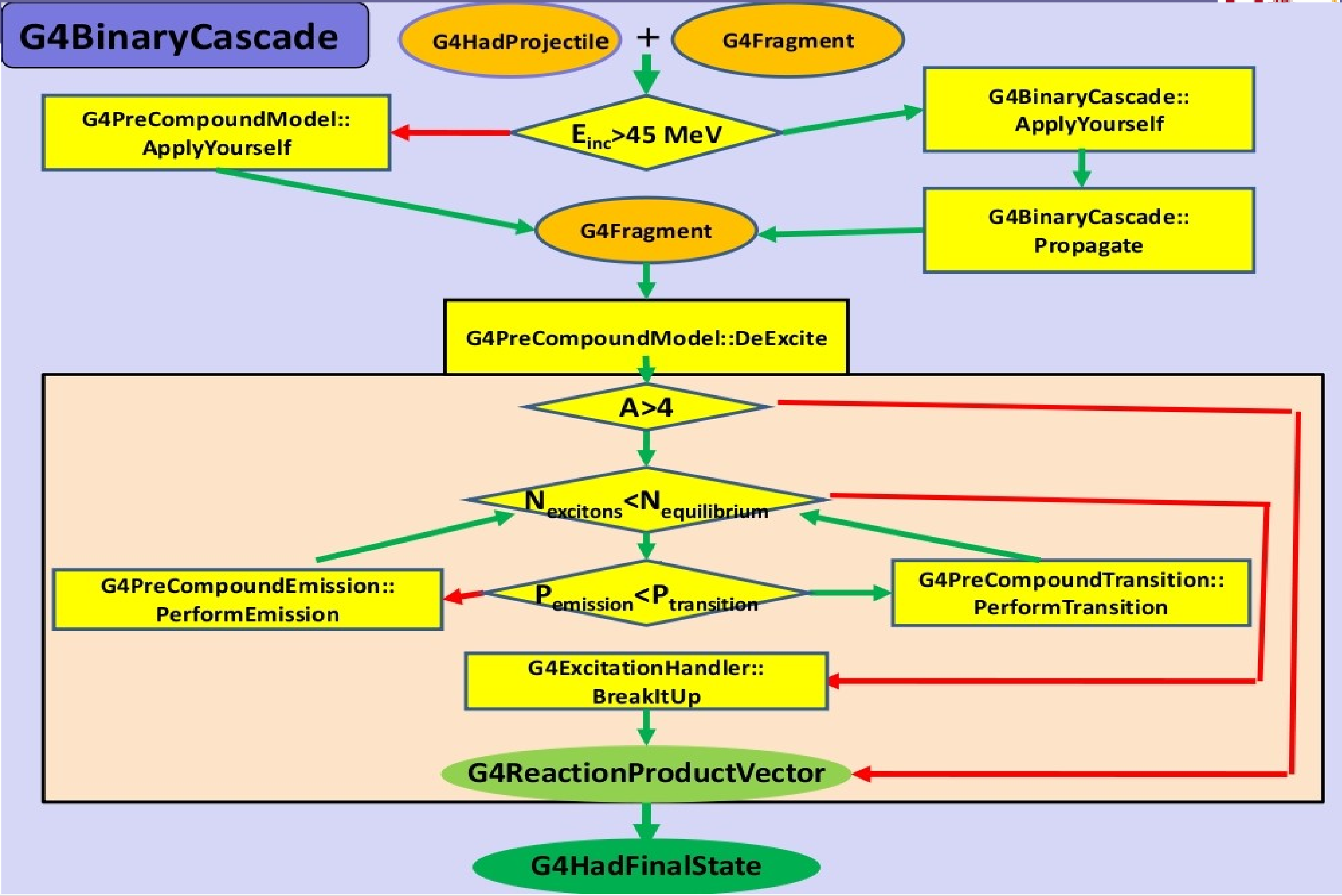
- Which can be roughly estimated as:

$$n_{eq} = \sqrt{2gE^*} \quad (2)$$

(initially in G4PreCompoundModel)

- **NOW** the more physically consistent condition (1) has been implemented by means of the appropriate algorithm .

Pre-equilibrium



Equilibrium De-excitation

Five processes are considered:

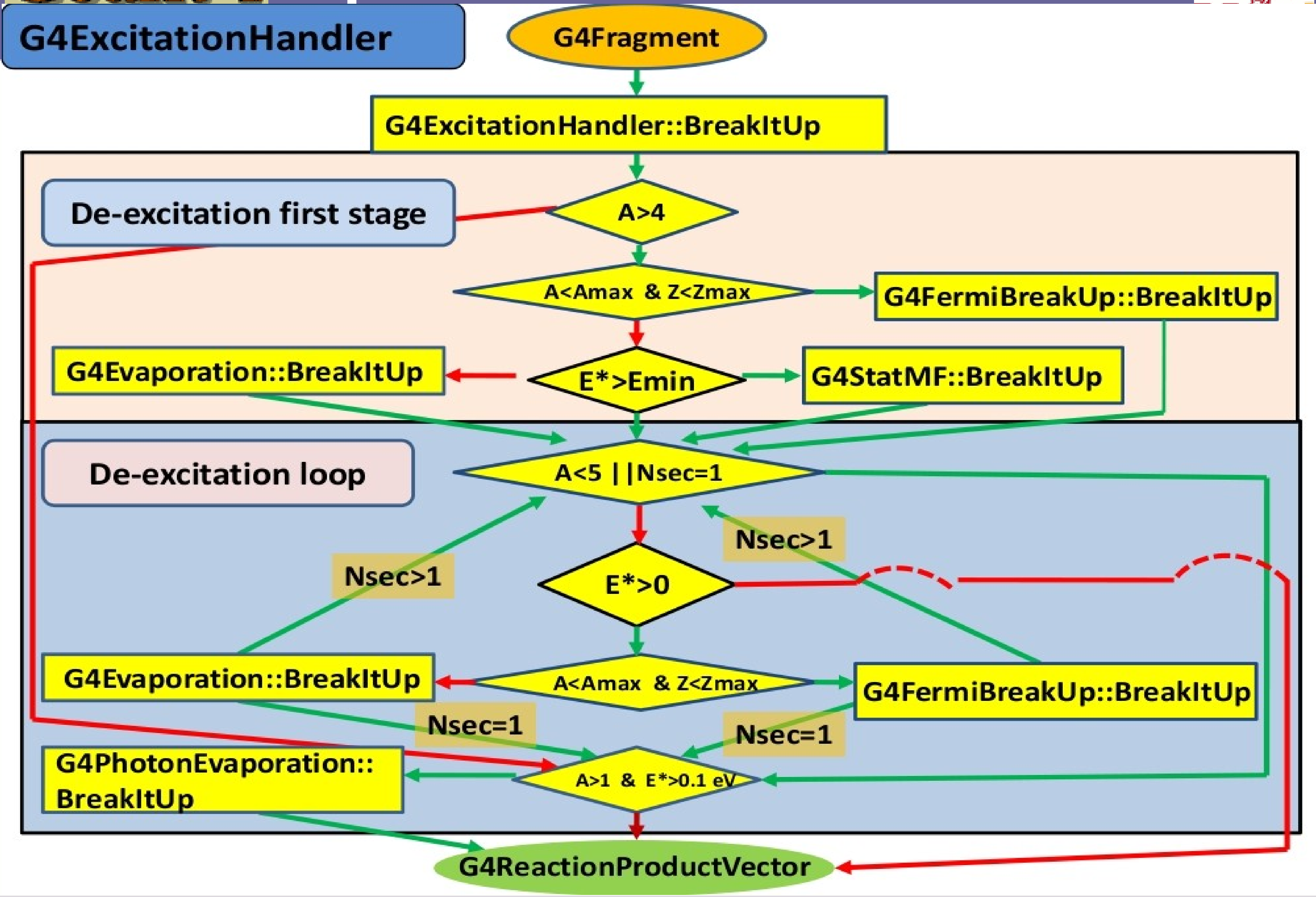
Alternates:

- **Fermi Breakup , for Z<9, A<17 (Botvina *et al*)**
- **Statistical Multifragmentation, for E*/A > 3 MeV (Botvina *et al*)**

Competitors:

- **Fission (Bohr-Wheeler model + Amelin prescript.)**
- **Particle Evaporation:**
  - **Evaporation Model (Weisskopf-Ewing) : n,p,d,t,3He, alphas)**
  - **Generalized Evaporation Model (Furihata) : Z<13 , A<29 .**
- **Photon Evaporation:**
  - **Discrete (tabulated E1,M1, E2)**
  - **Continuum (GDR strength)**

Equilibrium De-excitation



Situation in AccApp'09 Conference

(related to geant4.9.2p01 official release results)

- No *ad hoc* tuning of level density parameter ratio a_{fis}/a_{evap}. (preliminary trials show that it is critical, as reported in previous works).
- No *soft transition* from pre-equilibrium (i.e. increment of equilibium at the expenses of pre-equilibrium) .
- Very important: parameters tuned in a “model suite” shouldn’t be assumed to work in a different *environment*, i.e. with different *coupled* models.

↓

Ad hoc tuning of parameters was clearly necessary in order to reproduce fission data. (Done in next release geant4.9.3)

Progress after AccApp'09 Conference

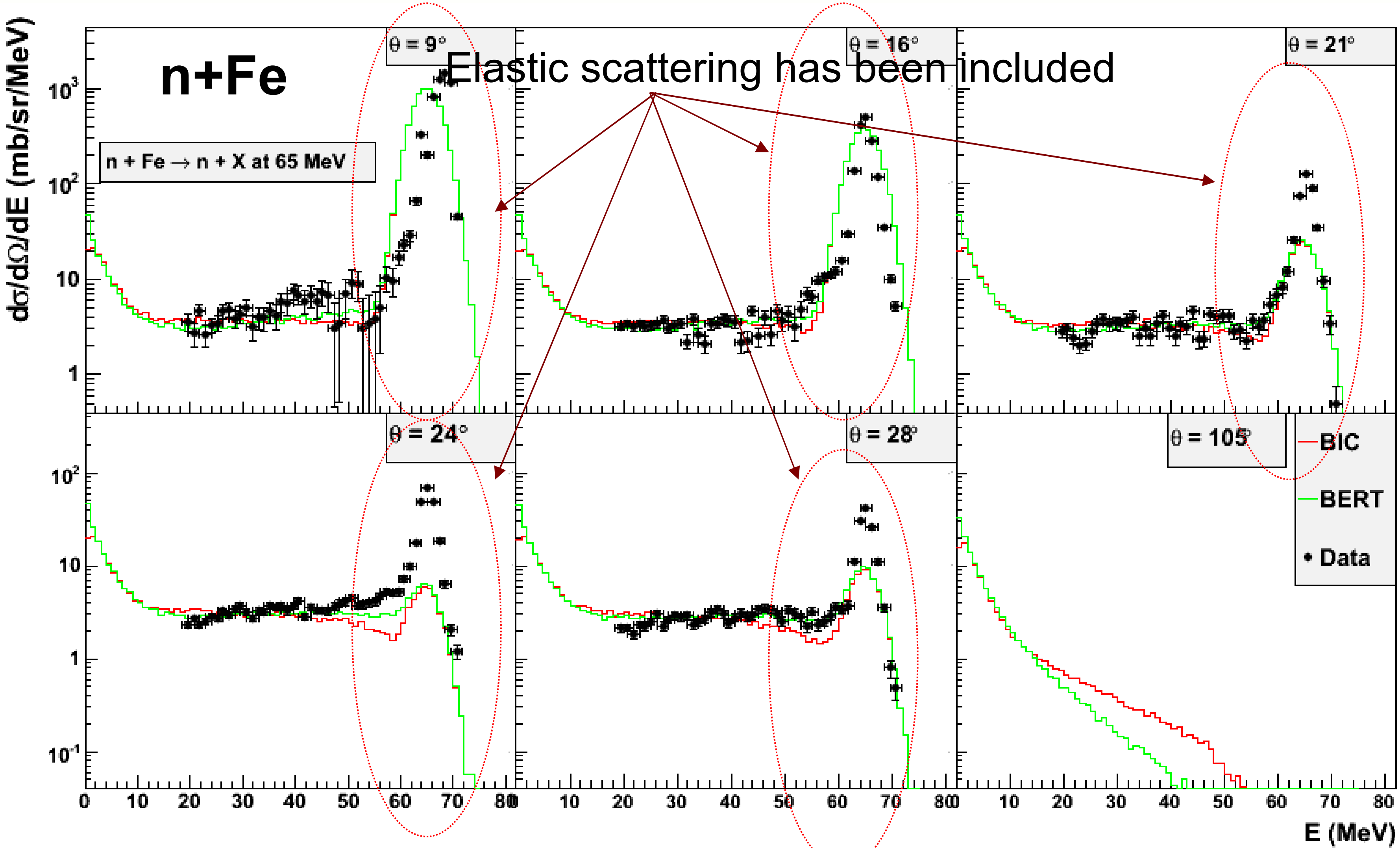
(included in geant4.9.3 official release)

- Transition probabilities at pre-equilibrium (exciton model) have been calculated according to CEM
- NEW: Combined WE-GEM model has been implemented in de-excitation (allows description of IMF production)
- First retuning of parameters :
  - Tuning of level density parameter ratio a_{fis}/a_{evap}.
  - Tuning of the width of symmetric component of fission fragment distribution

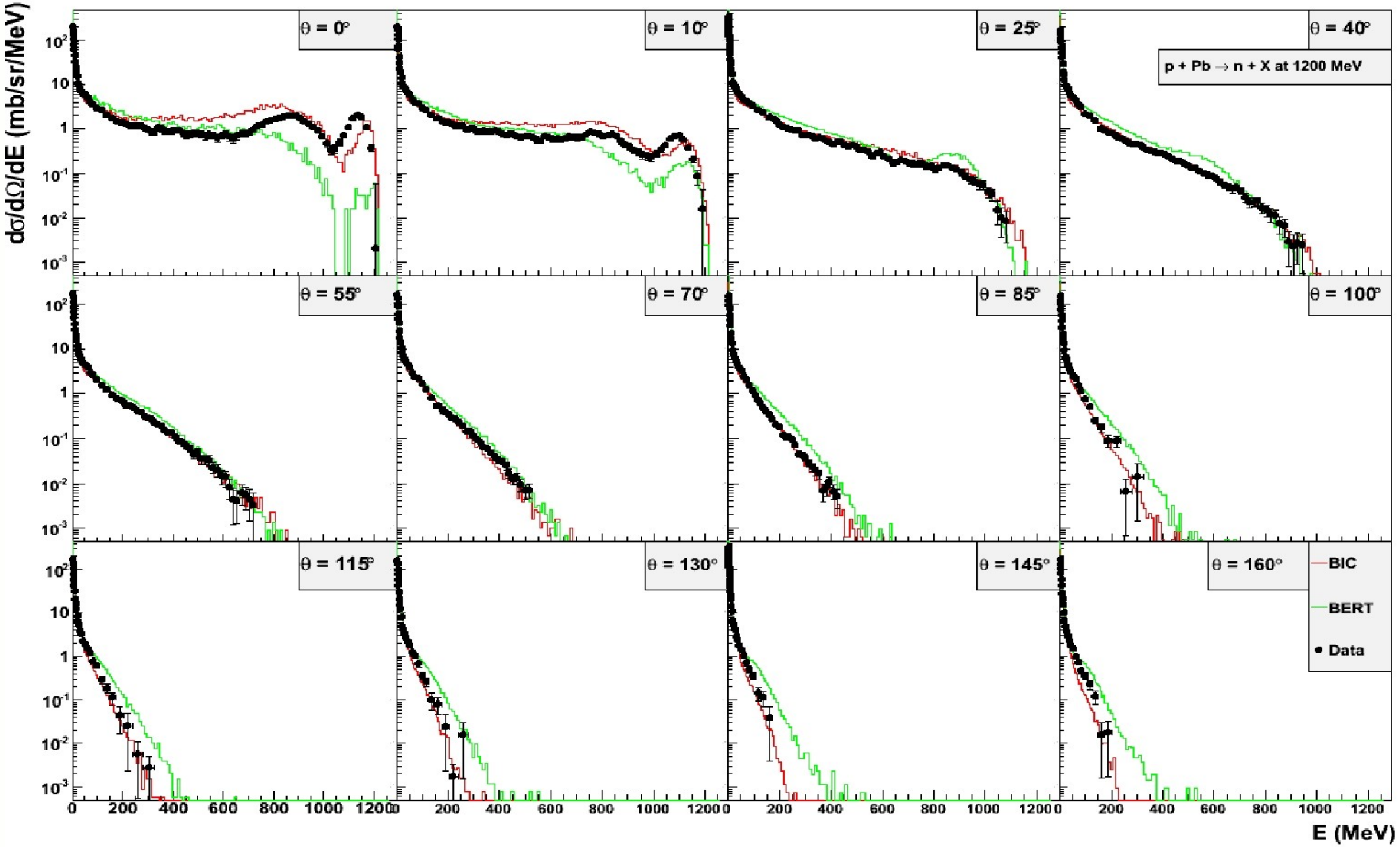
RESULTS

(geant4.9.3)

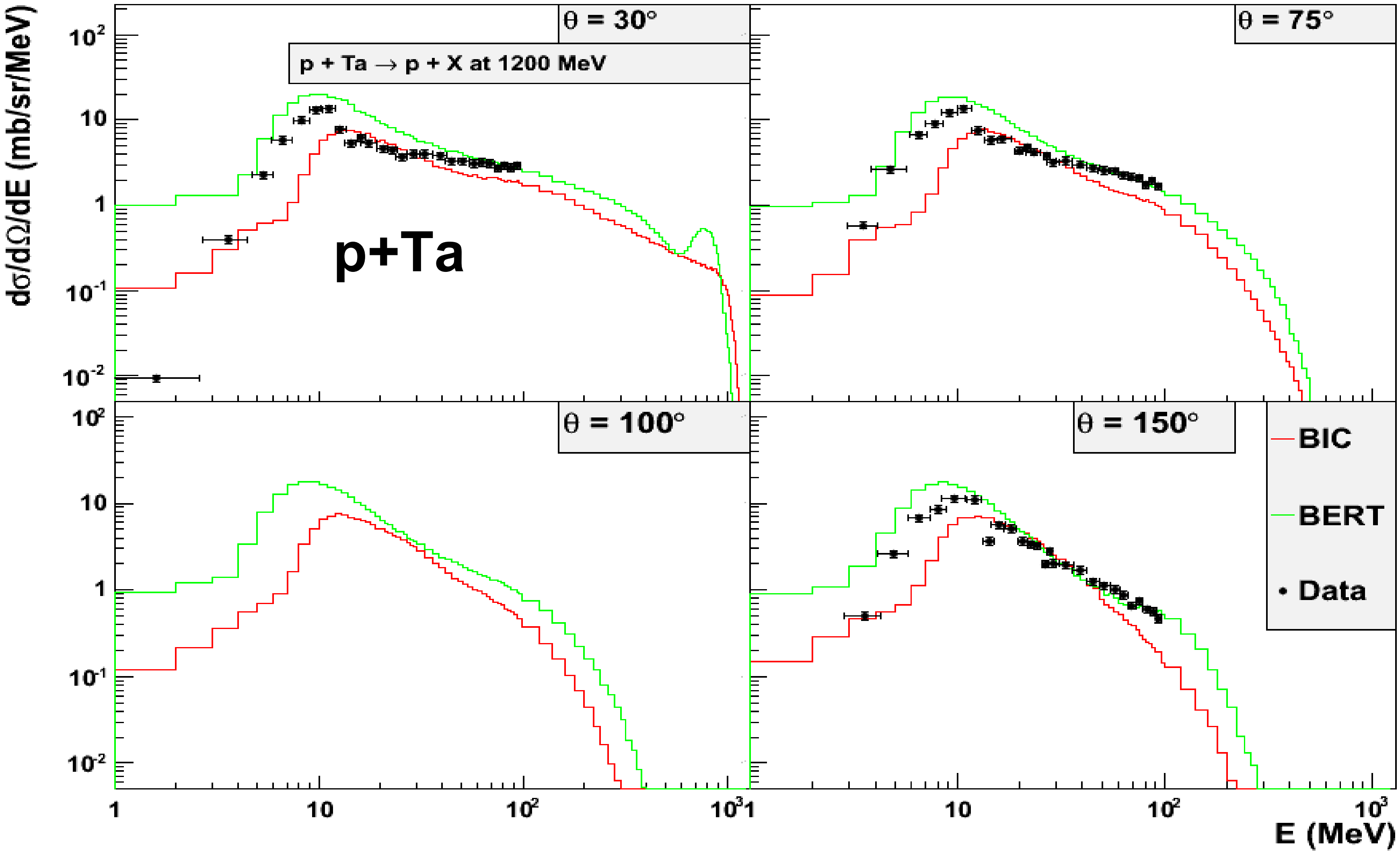
Neutron production at 65 MeV



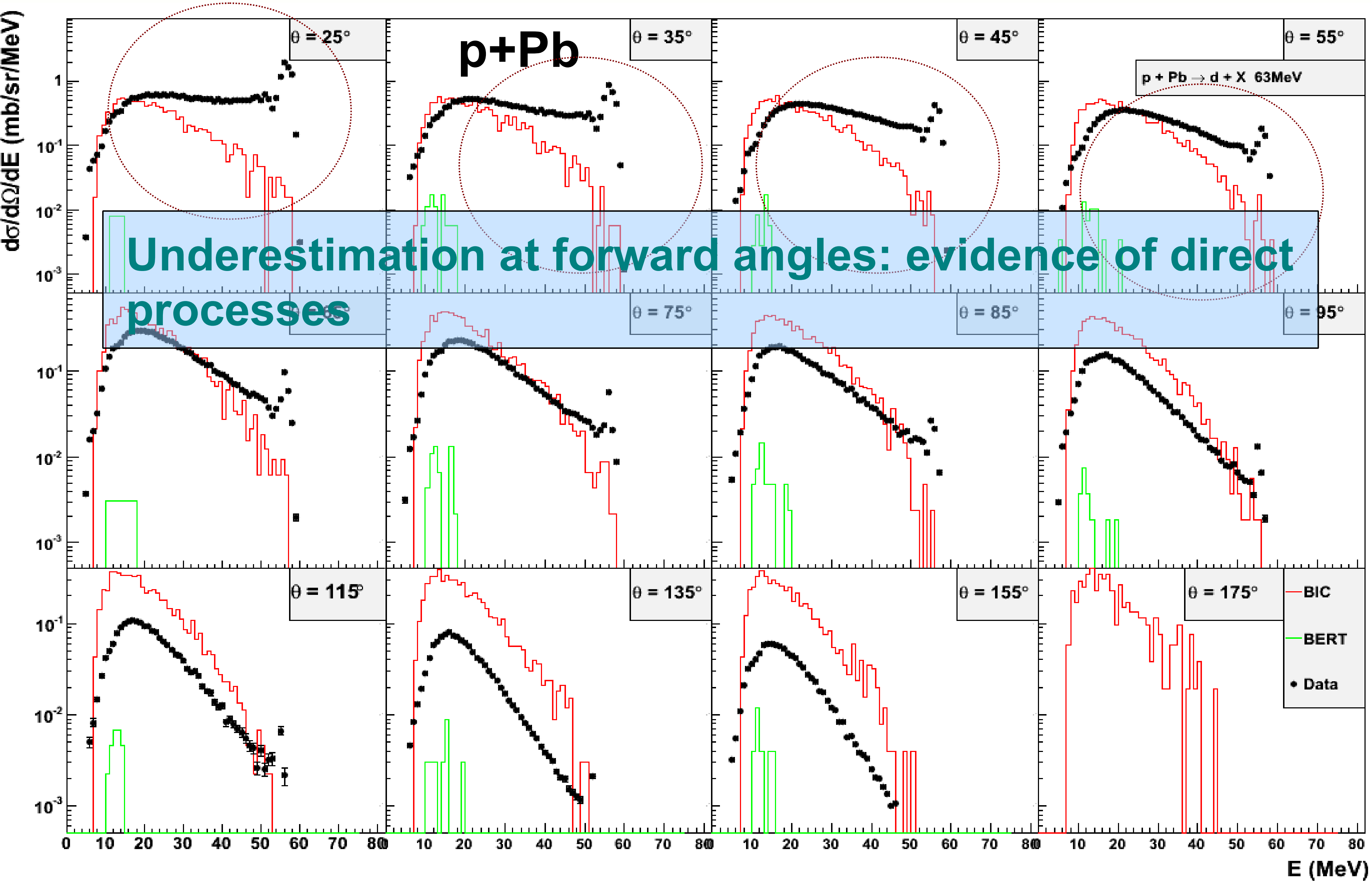
Neutron production at 1200 MeV



Proton production at 1200 MeV

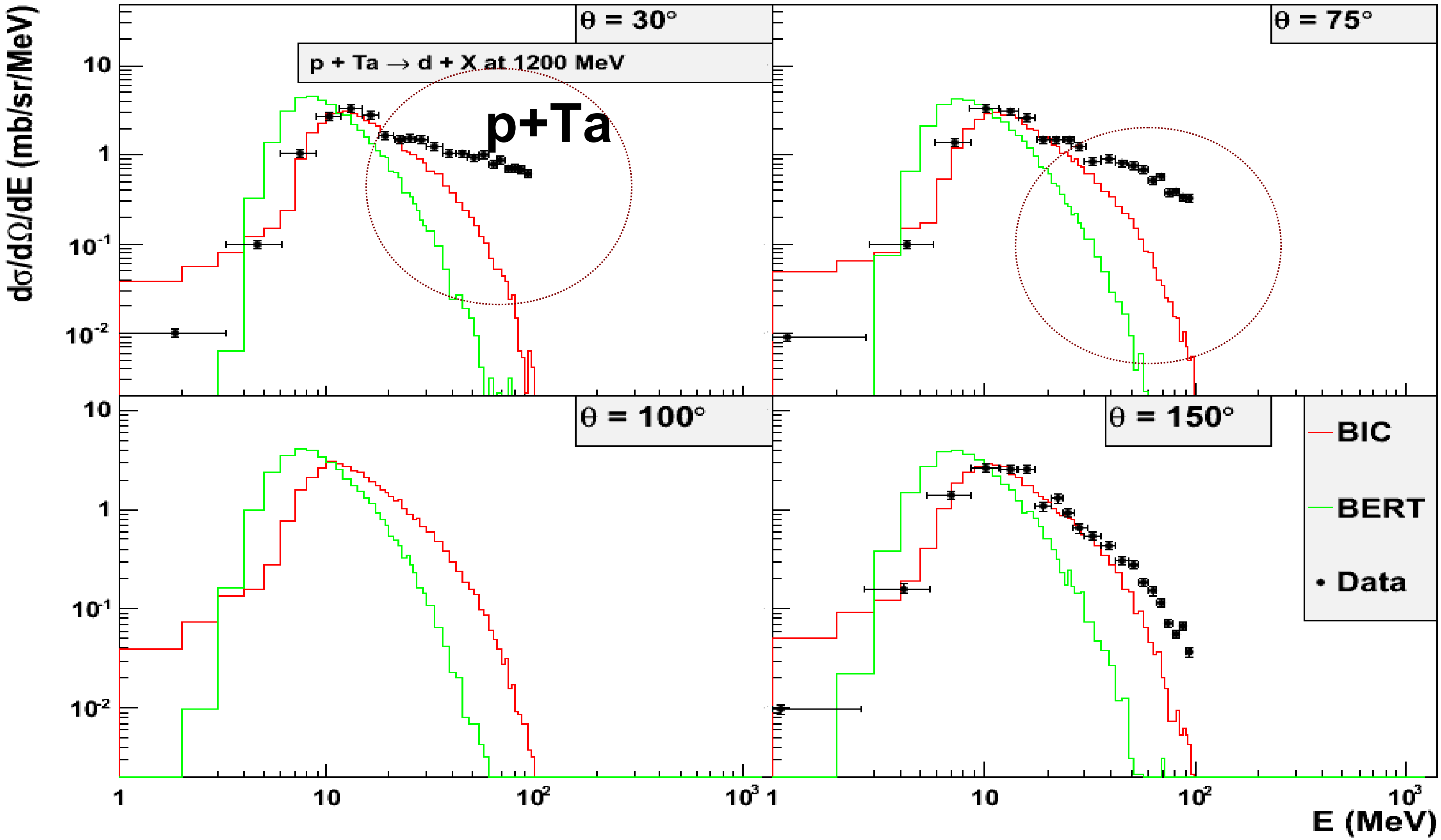


Deuteron production at 63 MeV

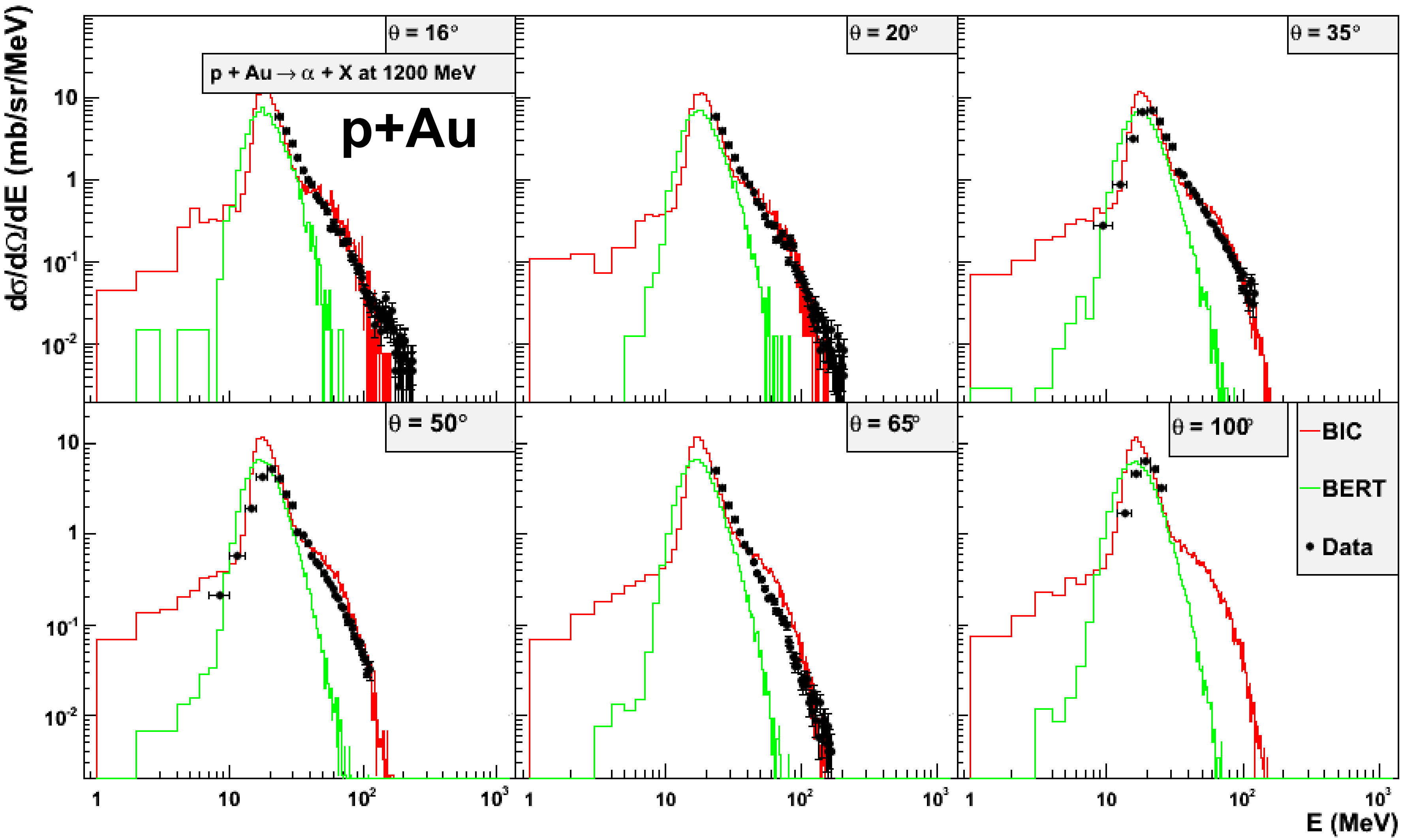


Underestimation at forward angles: evidence of direct processes

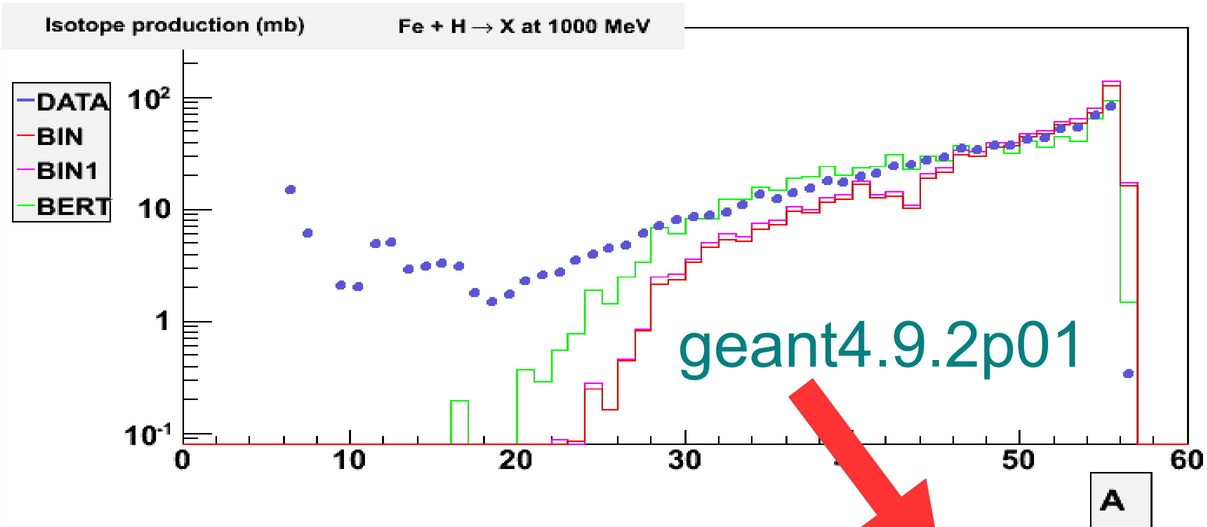
Deuteron production at 1200 MeV



Alpha production at 1200 MeV

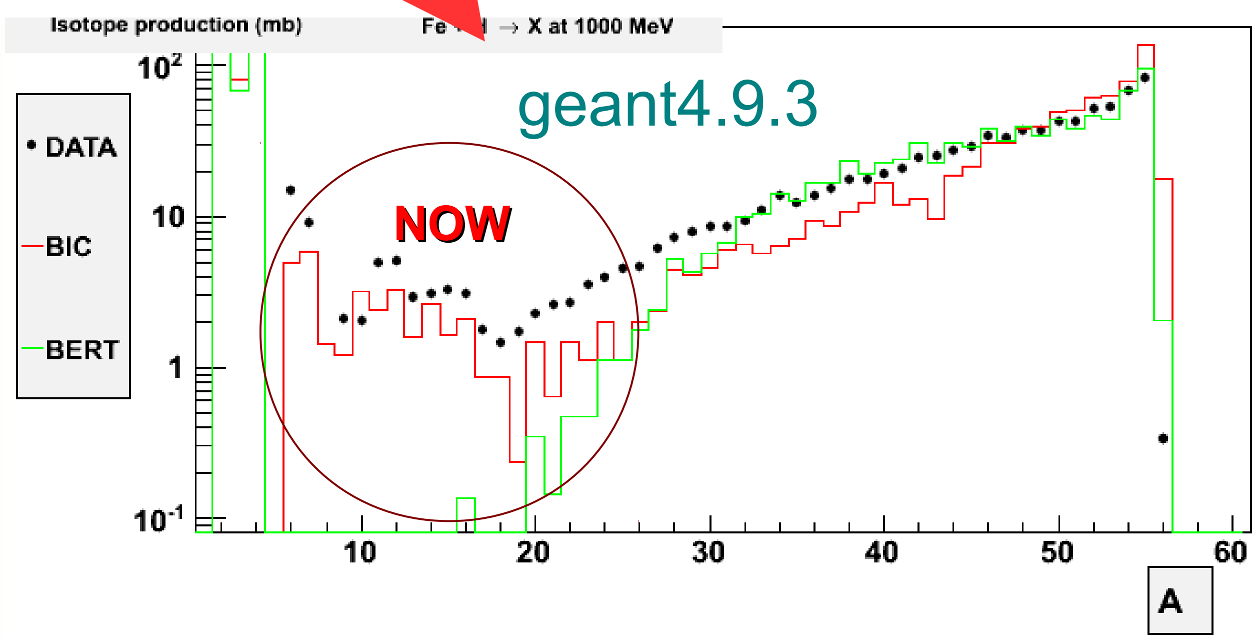


Isotopic distibution at 1 GeV

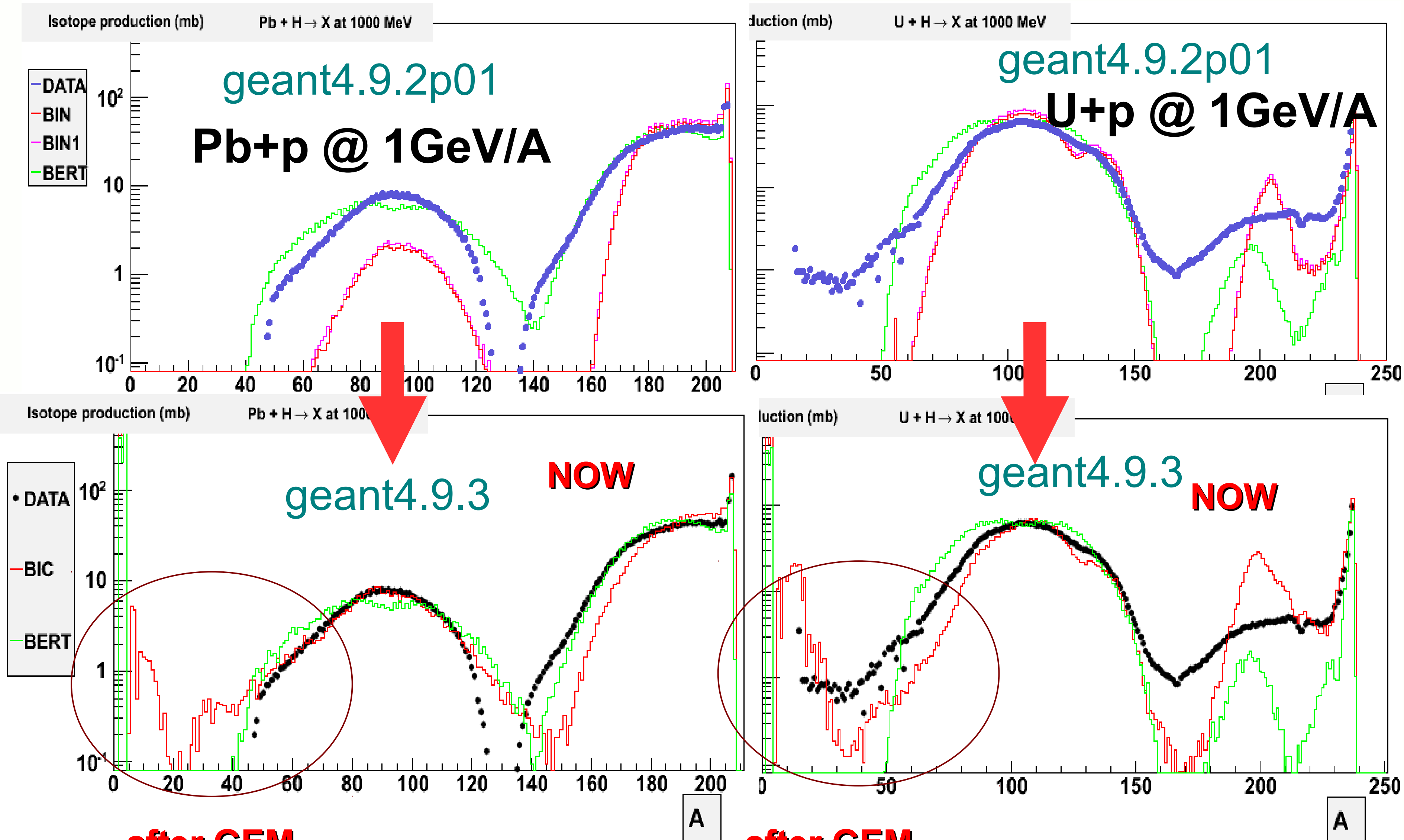


Fe+p @ 1GeV/A

after GEM inclusion



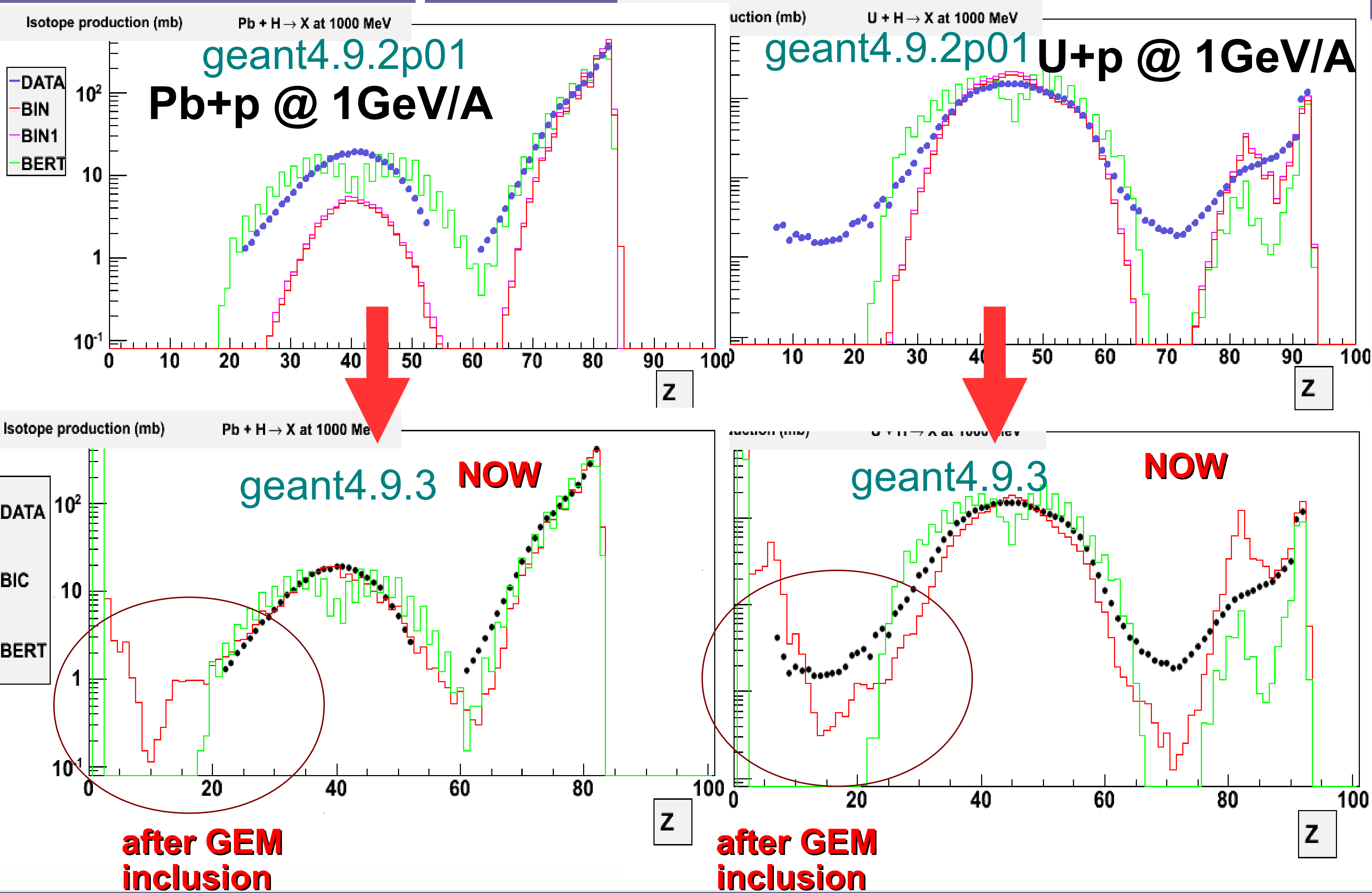
Isotopic distibution at 1 GeV



after GEM inclusion

after GEM inclusion

Isotopic distribution at 1 GeV



Work in progress

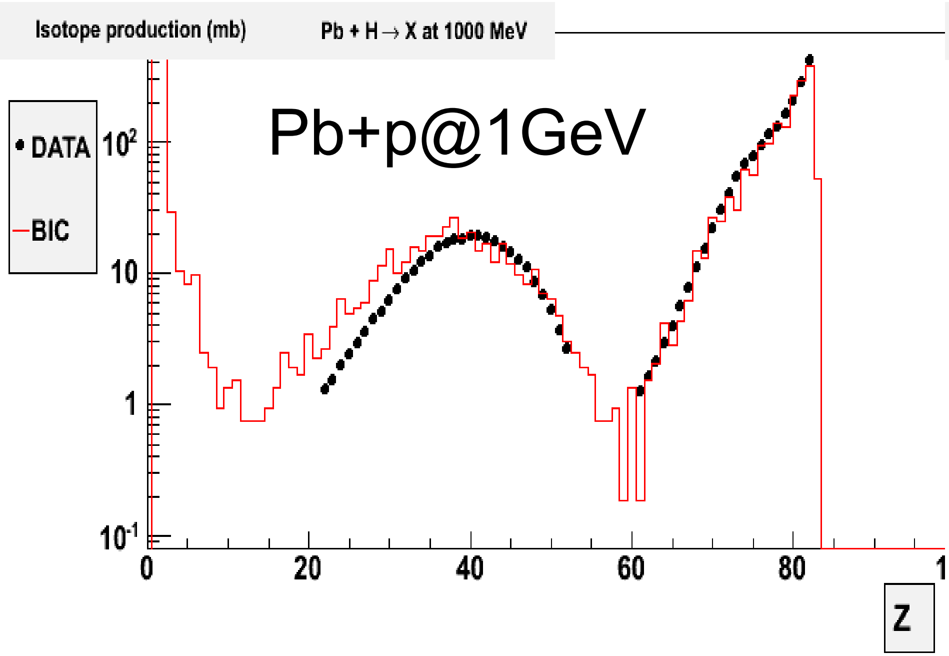
(in development version, yet under testing)

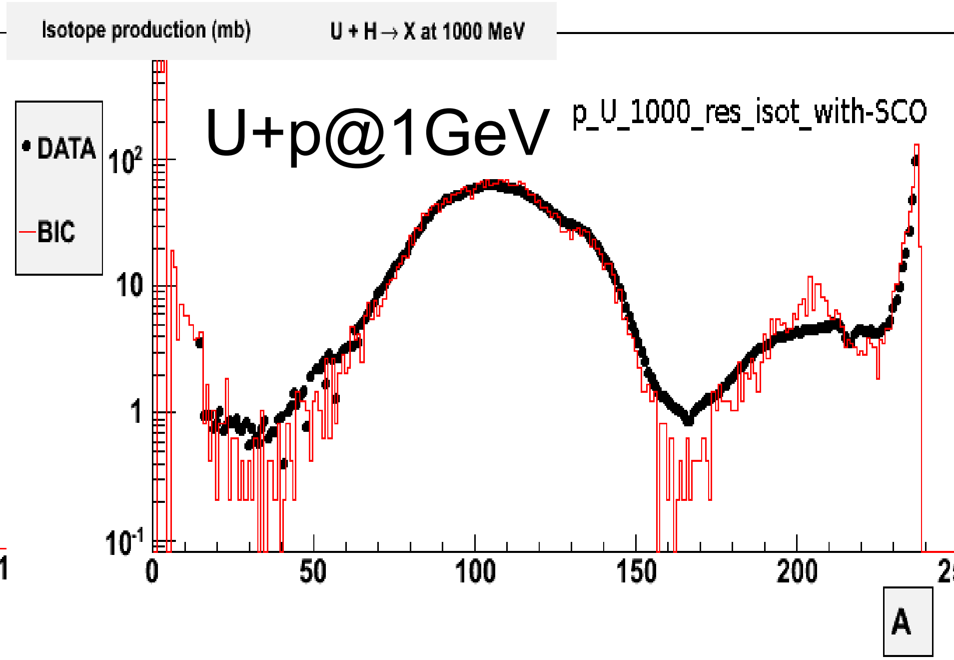
- *Soft cut-off* transition from pre-equilibrium partially cures this problem, but, in our case, it worsens performance at fission and at pre-equilibrium
  - A new version of the s*oft cut-off* algorithm with n_{eq} strictly calculated according to

$$\lambda_+(p,h,E) = \lambda_-(p,h,E)$$

  - The *diffusivity* of the transition has been drastically reduced
- No chance for a global set of parameters (optimal for any combination of models)
  - Different sets of fission parameters were fitted for each choice (with/without soft cut-off) .

Development version





- “soft cut-off” ON
- Fission parameters have been fitted
- The situation at pre-equlibrium is quite the same
- CPU time increase (factor ~ 1.5)

Conclusions

- The review of the native pre-equilibrium and de-excitation models of Geant4 recently performed has led to an overall satisfactory reproduction of experimental data set of IAEA nuclear spallation reactions benchmark thanks to recently made improvements to :
  - Pre-equilibrium
  - Evaporation
  - Fission
- Additional development work is in progress:
  - Transition to de-excitation and fine parameter tuning (specific interest: spallation reactions)
  - Fermi Breakup and Photon Evaporation (specific interest: Hadrontherapy)
  - CPU performance and code cleanup (interest: all applications)

Thanks for your attention