PRE-COMPOUND/ DE-EXCITATION MODELS AND HADRONIC FRAMEWORK

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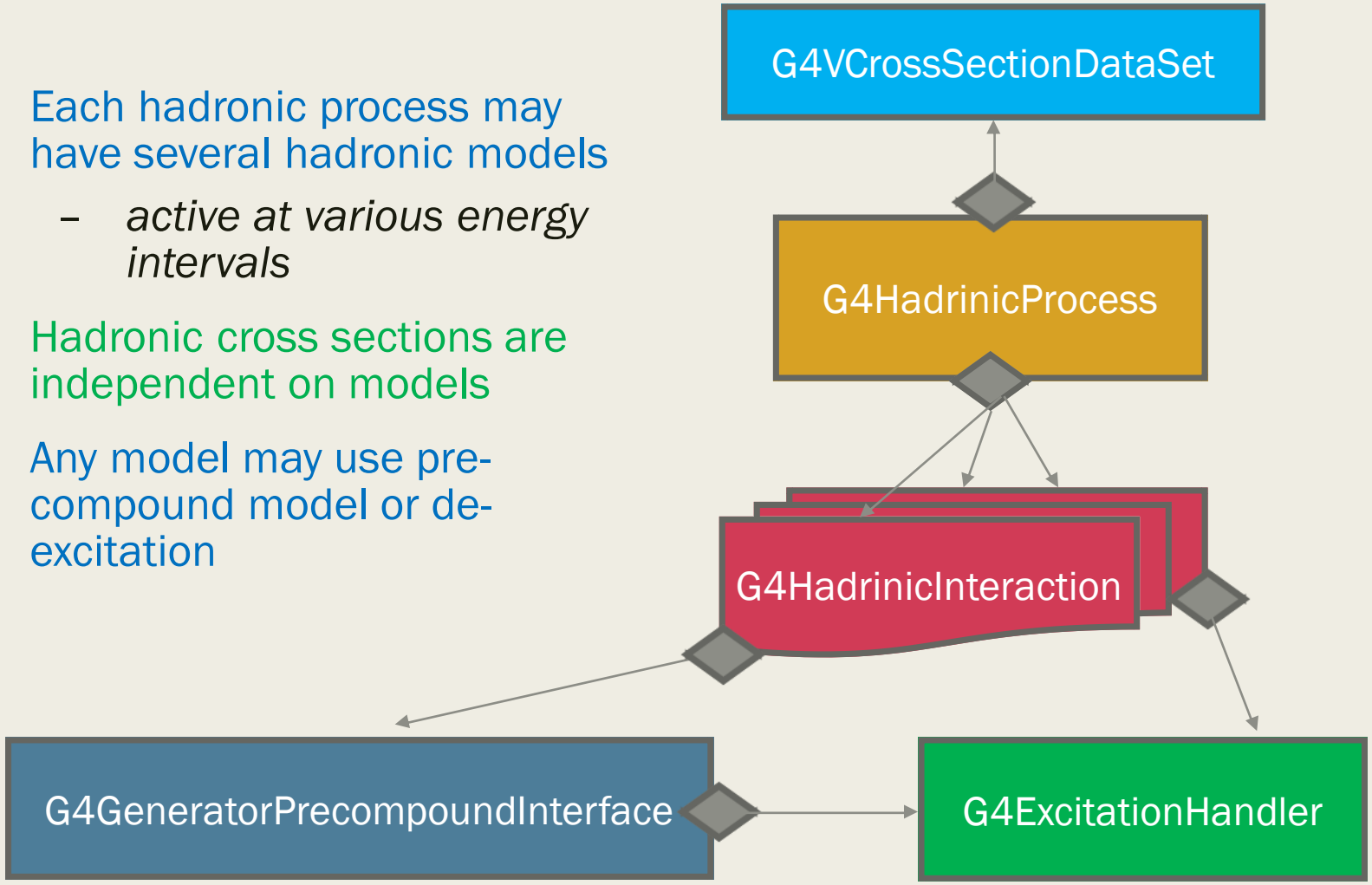
Outline

- Design of pre-compound/de-excitation
- G4HadronicProcess updates for 10.6
- Precompound/deexcitation update for 10.6
- Some validation results

Geant4 hadronic physics design

- Each hadronic process may have several hadronic models
  - *active at various energy intervals*
- Hadronic cross sections are independent on models
- Any model may use pre-compound model or de-excitation



Native pre-compound model

- Is based on K.K. Gudima, S.G. Mashnik, V.D. Toneev, Nucl. Phys. A401 (1983) 329
- In the model two processes are sampled:
  - *creation of extra excitons*
  - *emission of nucleons and light fragments*
  - *when the transition probabilities for increasing and decreasing the exciton number become approximately equal the equilibrium condition is met*
    - De-excitation module is called for further sampling of decay at equilibrium state
- The interface:
  - *G4PreCompoundModel::DeExcite(G4Fragment&)*
- G4Fragment is the main object of the de-excitation module
  - *Container of excited nucleus parameters*
  - *Including number of holes and excitations*
  - *Optionally including nuclear polarization state*
- Complete list of references see in J. Allison et al., Nucl. Instr. Meth. A 835 (2016) 186

Native de-excitation module

- Equilibrium de-excitation is sampled as a completion of several decay channels according to their probabilities:
  - *Photon evaporation*
  - *Fission*
  - *Light fragment evaporation (Weisskopf-Ewing)*
  - *Medium fragments (GEM model)*
- Two special models may be applied:
  - *High excitation state – multifragmentation (Barashenkov)*
    - Disabled by default, limited by excitation energy per nucleon
  - *Low Z – FermiBreakUp model*
- Some key publications:
  - *J.P. Bondorf et al., Phys. Rep. 257 (1995) 133*
  - *A.S. Iljinov et al., Nucl.Phys. A543 (1992) 517*
  - *V.E. Weisskopf, D.H. Ewing, Phys. Rev. 57 (1940) 472.*
  - *S. Furihata et al., JAERI-Data/Code 2001-015, Japan Atomic Energy Research Institute, 2001*
  - *Several preprints in Russian*

Modifications on level of G4HadronicProcess

- Problem #2175: in ion-ion interaction neutrons are produced out of the mass shell and fail to decay
  - *The problem is fixed in the method where we convert hadronic secondaries into G4DynamicParticle*
  - *We force particle to be on mass shell if mass deviation is above 10 keV (in 10.6beta it was 1.5 MeV)*
  - *G4IonBinaryCascade rarely generates particles with deviation for few MeV*
- Random rotation of secondaries is removed completely
  - *It was checked, that all hadronic models of today making proper random directions of secondaries*
  - *It allows a possibility to simulate reactions of polarized particles*
- Try/couch pattern is removed from GetMeanFreePath(..)
  - *G4HadronicException is removed from cross sections*

Pre-compound model development

- Extra parameter is added PrecoMaxEnergy
  - *If excitation of a fragment > A*PrecoMaxEnergy fragment is passed to the de-excitation model, no pre-compound decay simulated*
  - *Current default 100 MeV/u*
  - *For today it provides annoying frequent warnings which should be suppressed for 10.6*
    - The problem is inside FTFP, which produces very excited light fragments
  - *We may reduce this value for 10.6 but remove the warning*

De-excitation module in 10.6beta

- G4DeexPrecoParameters – addressed #2098
  - *Verbose() is added and is used in all de-excitation module classes*
  - *The default is 1 (only a table of parameters is printed)*
- G4FermiBreakUpVI
  - *Fixed Coulomb Barrier correction – may affect medical tests*
- G4PhotonEvaporation
  - *Fixed #2124 – limit value for IC probability*
  - *Fixed #2123 – if no data for a given level make transition to the closest one*
- G4Evaporation
  - *Simplified method of integration of differential inverse cross section and sampling of final state*

G4ExcitationHandler developments

- Only 1 loop of de-excitation remains
  - *Second loop for photon cascade never called now*
- Slightly changed logic to choose FermiBreakUp or Evaporation
  - *Only fragments, which have decay channels in FermiBreakUp and have excitation below FBUEnergyLimit are sent to FermiBreakUp*
    - Current limit is 20 MeV
  - *All other fragments are sent to Evaporation*
  - *De-excitation is stopped if final G4Fragment do not have any decay channel within the time limit*
    - Default 1000 second, if RadioactiveDecay is active the limit is changed to one of G4NuclideTable (1000 ns)

G4FermiBreakUpVI model

- Old G4FermiBreakUp model was based on hard-coded data
  - *A pool of 112 states, Z < 9, A < 17*
  - *Precomputed probabilities of decay of each state from this pool into 2-, 3-, 4-body final state from this pool*
- New G4FermiBreakUpVI model fully based on data of G4GAMMALEVELDATA
  - *A pool of 260 states from data files and 399 reactions, Z < 9, A < 17 (10.4)*
  - *A pool of 380 states from data files and 991 reactions, Z < 9, A < 17 (10.5)*
    - Maximal excitation energy 20 MeV
  - *Only binary decay chains are considered*
    - A standard Coulomb barrier computation is used
  - *An extra set of 80 unphysical fragments not known from data in 10.5*
    - Including very exotic intermediate states like H_8 or He_2
    - Will be removed in 10.6 – decay of unphysical fragments will be delegated to Evaporation
  - *Probability of the first decay is computed on fly if initial excitation of the primary fragment is not equal to one of known levels*
  - *The second and others decay probabilities are precomputed*
  - *Final product is always a list of states from the main pool, which has no Fermi decay channel (may have gamma transition)*

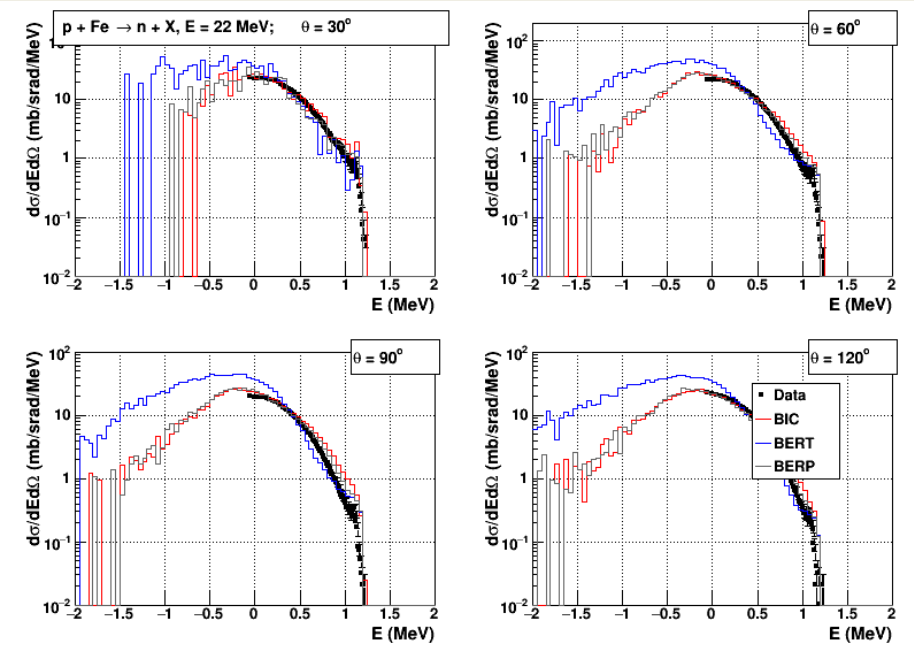
G4Evaporation developments

- Stop of de-excitation loop inside G4Evaporation happens if
  - *G4Fragment is stable*
  - *G4Fragment has FermiBreakUp decay channels and excitation energy below FBUEnergyLimit*
- If G4Fragment is not known to Geant4 level DB and it has no opened decay channels it is marked as unphysical
  - *G4UnstableFragmentBreakUp is used*
  - *We force disintegration of unphysical fragments by forced emission of neutron or light ion*
  - *We are speaking on abnormal He2, H6… objects*
  - *If final fragment is "physical" it continues decay within evaporation loop*

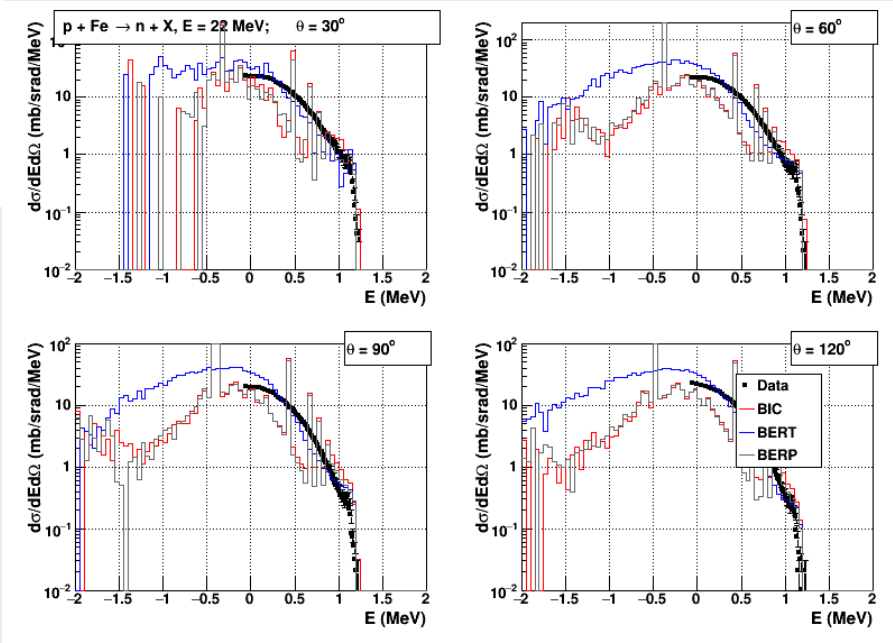
De-excitation module in 10.5ref08

- General clean-up of classes and addition of C++11 patterns is being performed
  - *It was triggered by needs of the new GEM model and concerns from medical community*
  - *Any modification is validated using test30*
- Introduced a possibility (optional), forcing final state after each evaporation to correspond to one of level for given isotope
  - *There is a problem, which not allows making this the default*
  - *Extra flag should be added to G4DeexPrecoParameters*
  - *This issue needs further study*
  - *may be activated together with Radioactive decay*

Proton 22 MeV scattering of Fe

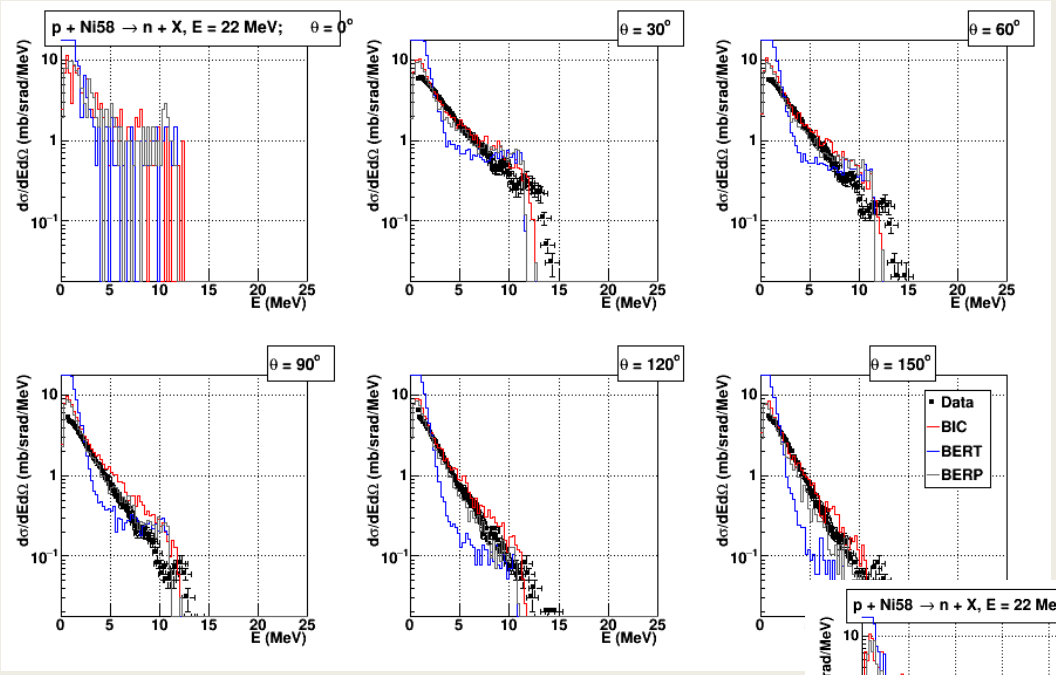


10.5



New results have peaks, not supported by data

Proton 22 MeV scattering of Ni58



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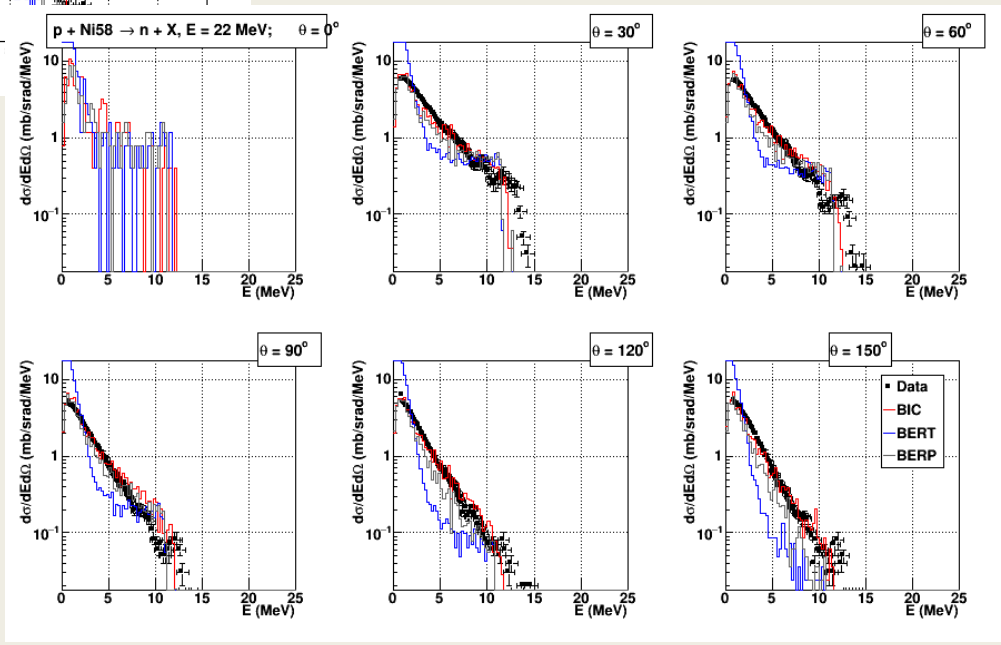


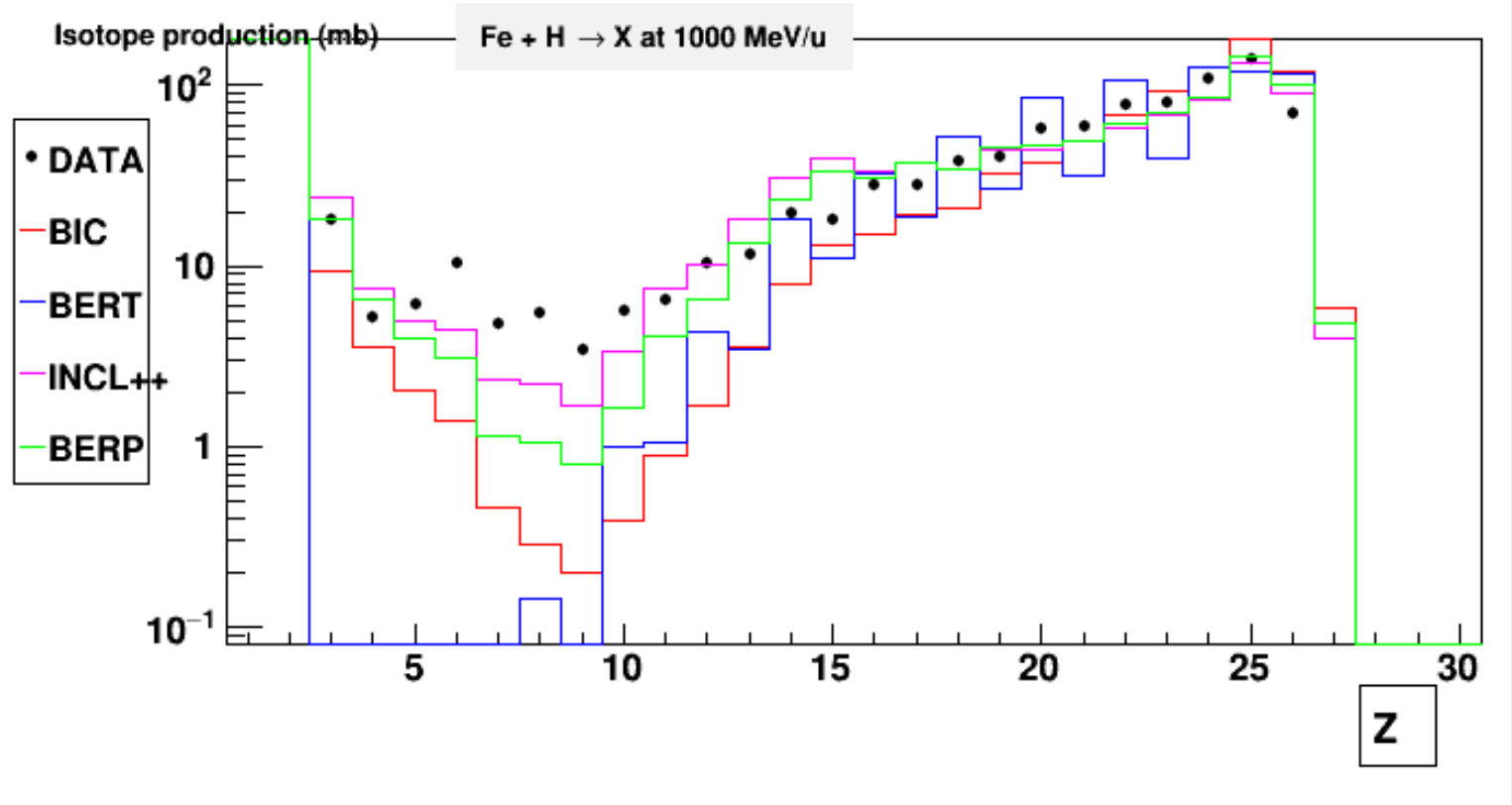
New looks fine
Probably good data
for isotopes involved
in this test

De-excitation module: parameterisation of level density

- For long time a simplified level density parameterization was used: Ld = 0.1*A
- In literature several fits to nuclear level data are published
- For Geant4 10.5 a variant was chosen from A.Mengoni and Yu. Nakajima, JNST 31 (1994) 151
  - $Ld = \alpha \bullet A \bullet (1 + \beta/A^{1/3})$
    - Where parameters are different for odd-odd, odd-even, and even-even fragments
  - It turned out, that in order to have reasonable results, the same parameterisation should be used in evaporation, fission, photon evaporation
  - There is a new option in G4DeexPrecoParameters Get/Set LevelDensityFlag
  - The default Ld = 0.075*A
- We cannot enable this parameterization by default so far, because we need to be sure, that all results are OK

Isotope production by 1 GeV protons in Fe target

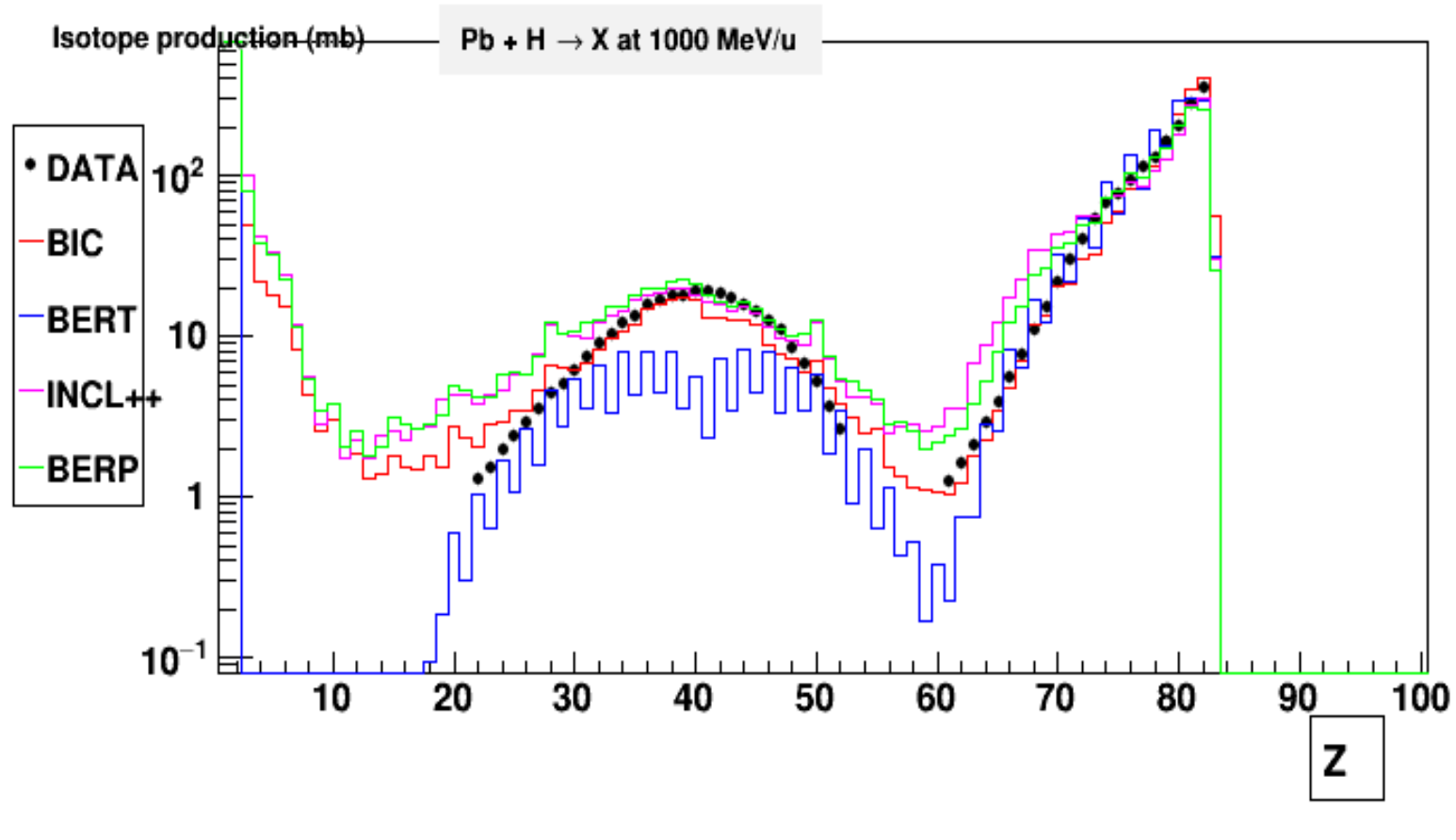
C.Villagrasa et al., AIP Conference Proceeding 769 (2005) 842



- At this and previous plots INCL++ demonstrates more accurate simulation for ion components
- The binary cascade predictions improves when multi-fragmentation sub-model is enabled

Isotope production by 1 GeV protons in Pb target

C.Villagrasa et al., AIP Conference Proceeding 769 (2005) 842



- For Pb target isotope production is better by the Binary cascade
- The Bertini cascade is not accurate for fission

Summary

- Pre-compound/de-excitation were improved in 2019
  - *Number of problem reports were fixed*
  - *Remaining problem reports can be fixed is data files will be improved/extended*
- Few relatively simple developments mentioned in this talk need to be addressed for 10.6
- Detailed validations including full G4MSBG are required
- Some options are promising but cannot be default in 10.6
  - *Extended density level parameterization*
  - *Discrete final states in evaporation*
  - *new GEM model*