Status of pre-compound model and de-excitation module

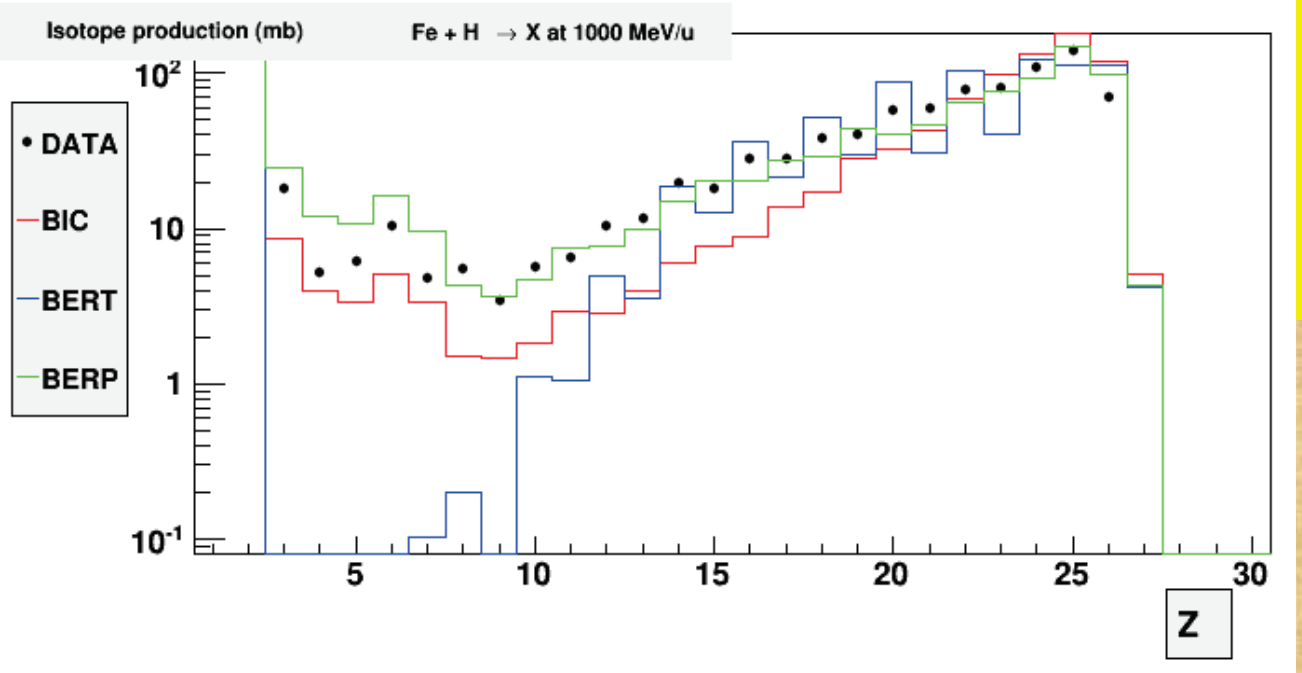
V. Ivanchenko

20th Geant4 Collaboration Workshop
FNAL, Batavia (Illinois, USA)
29 September 2015

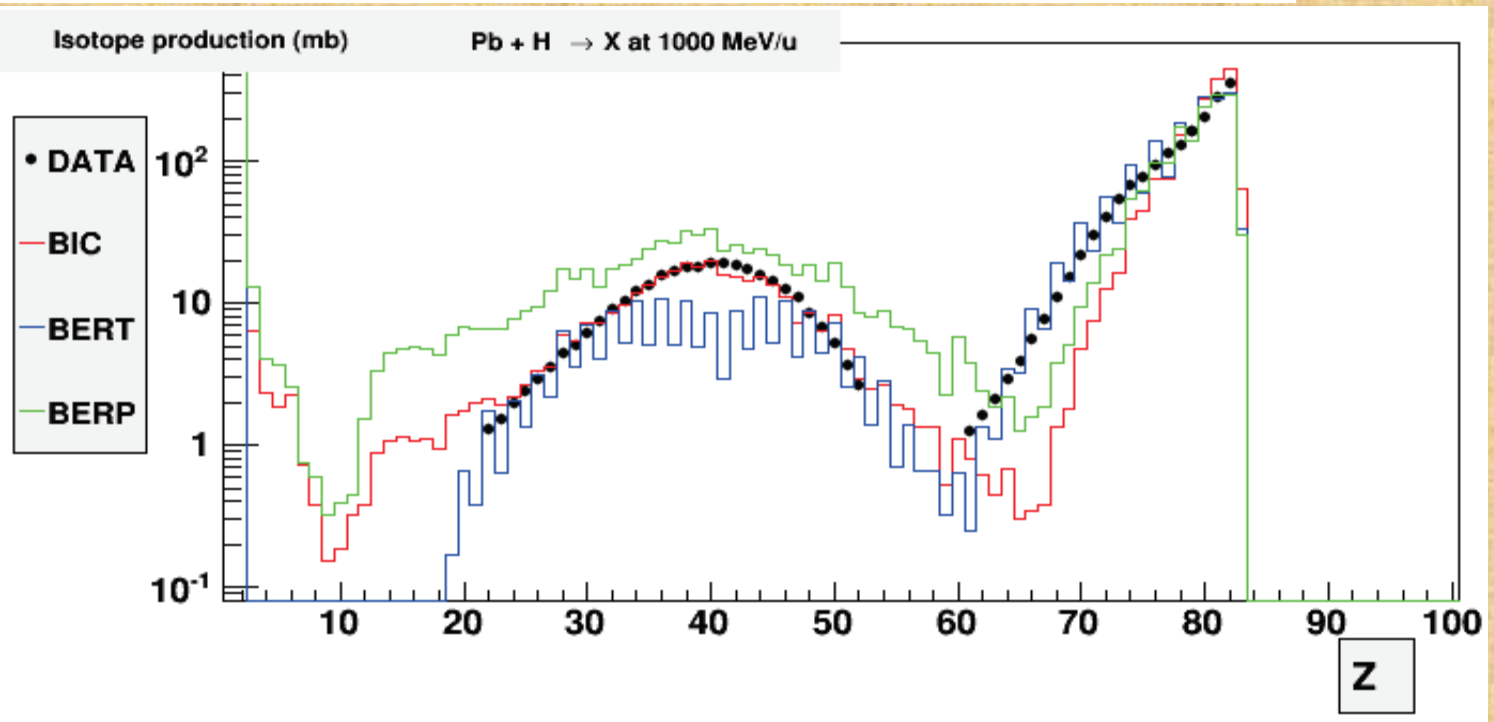
Introduction

- Geant4 pre-compound model is responsible for simulation of pre-equvilibrium emission of neutrons and light ions
  - When excited nucleus reach the equliribrium the pre-compound model call de-excitation module
  - De-excitation module consists of several submodels:
    - Multi-fragmentattion
    - FermiBreakUp
    - Evaporation
    - GEM evaporation
    - Photon evaporation
- Any hadronic model may interface pre-compound model or de-excitation module
  - CPU performance and memory consumption of many of hadronic generators are limited by the performance of pre-compound/de-excitation
- Several years ago Jose-Manuel Quesada have done a detailed review of the pre-compound/de-excitation and achieve situation that physics performance of all sub-models work corresponds to publish theoretical prescriptions for these models
  - At that time we have extended hadronic testiong suite including a lot of data for moderate and low energies to validation low-energy hadronic physics

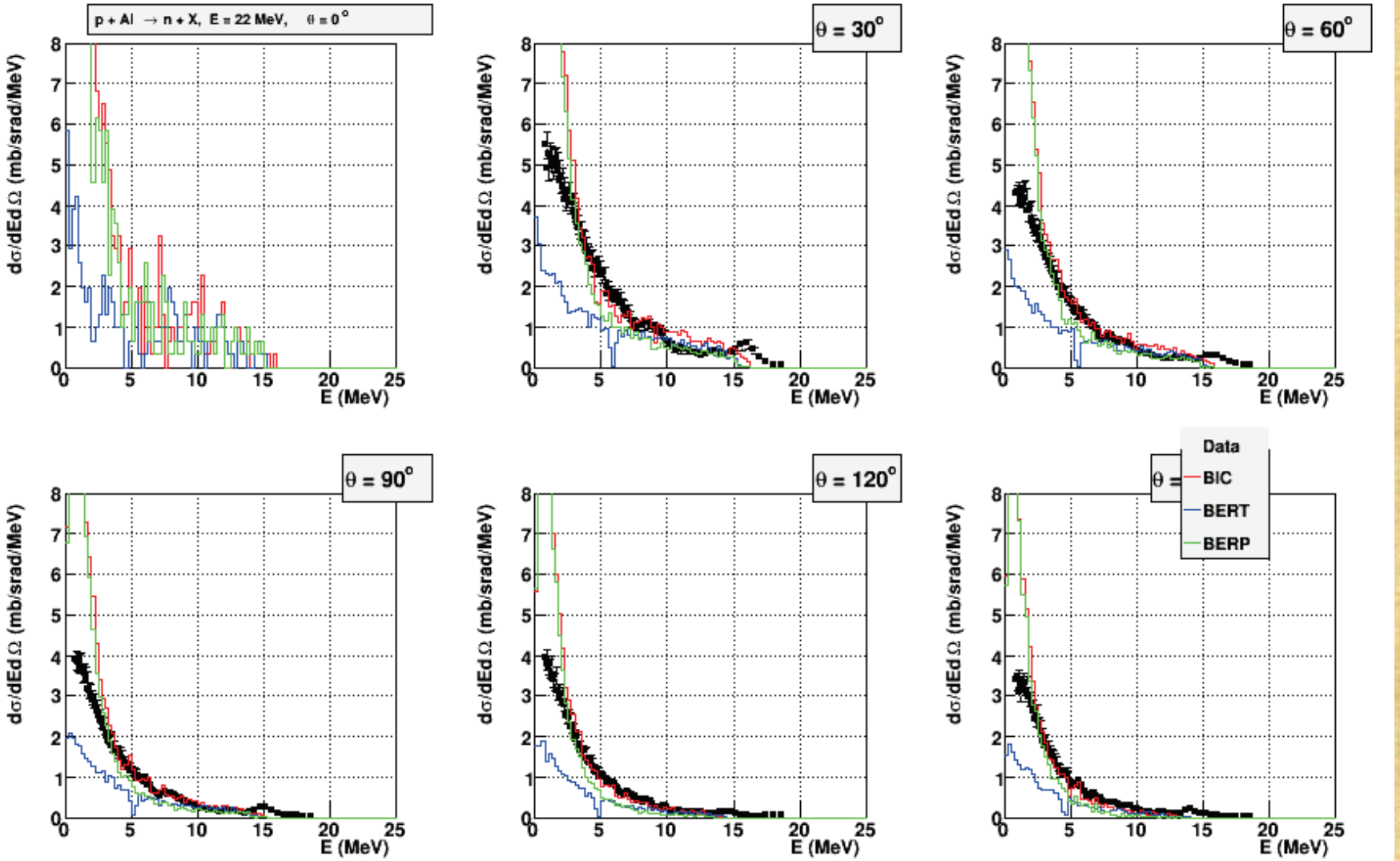
Recent results for isotope production



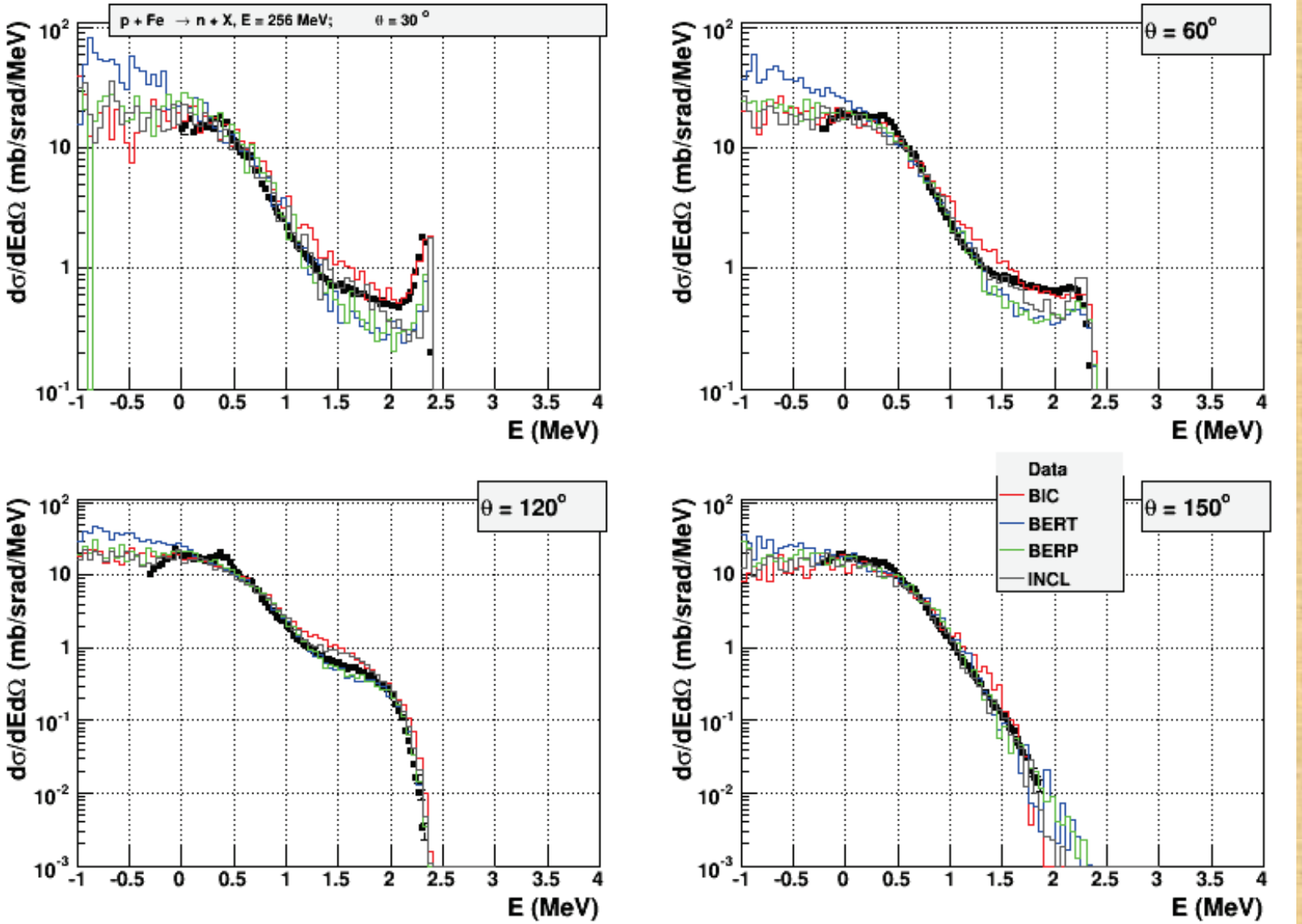
Bertini-PRECO is more accurate for Fe Binary – for Pb



Neutron double differential spectra produced by 22 MeV protons in Al



Neutron double differential spectra produced by 256 MeV protons in Fe



Motivation for upgrade of pre-compound/de-excitation

- These models affect accuracy of hadronic simulation in many application domains
  - CMS report shift of electron/gamma response when Bertini neutron yeild was changed
- CPU and memory profile show significant contribution of pre-compound/de-excitation classes and data structures
  - This is natural because excited nucleus emitting many fragments
  - to sample one emission we need to compute probabilities of all decay channels
    - 68 channels are used by default
- Pre-compound/de-excitation code was created at very early state of Geant4 and initial design/implementation is far not ideal
  - There were a lot of doublicated code
  - Parameters of models are hardcoded in various classes
  - Any tuning of parameters become tecnically very difficult
- During recent releases we are performing adiabatic re-design and cleanup of the code
  - Existing of extended testing suite allows to control modifications

Status of de-excitation module in 10.1

- De-excitation module was revised
  - Optimisation of memory management, reduced memory churn
    - G4Fragment is using G4Allocator
  - Optimisation of data structure
    - FermiBreakUp was redesined and cleaned up
  - Thread safety
  - Nuclear level management for MT (Makoto)
  - Speed up of the code (G4Exp, G4Log, G4Pow + code cleanup)
  - Isomer production introduced
  - Overall CPU performance and memory usage in hadronics were improved
- Number of problems were identified:
  - Non-reproducibility for HEP production
  - Radioactive decay problems:
    - Wrong life time
    - Many fake gamma lines
    - Energy non-conservation in the case of internal conversion to e-

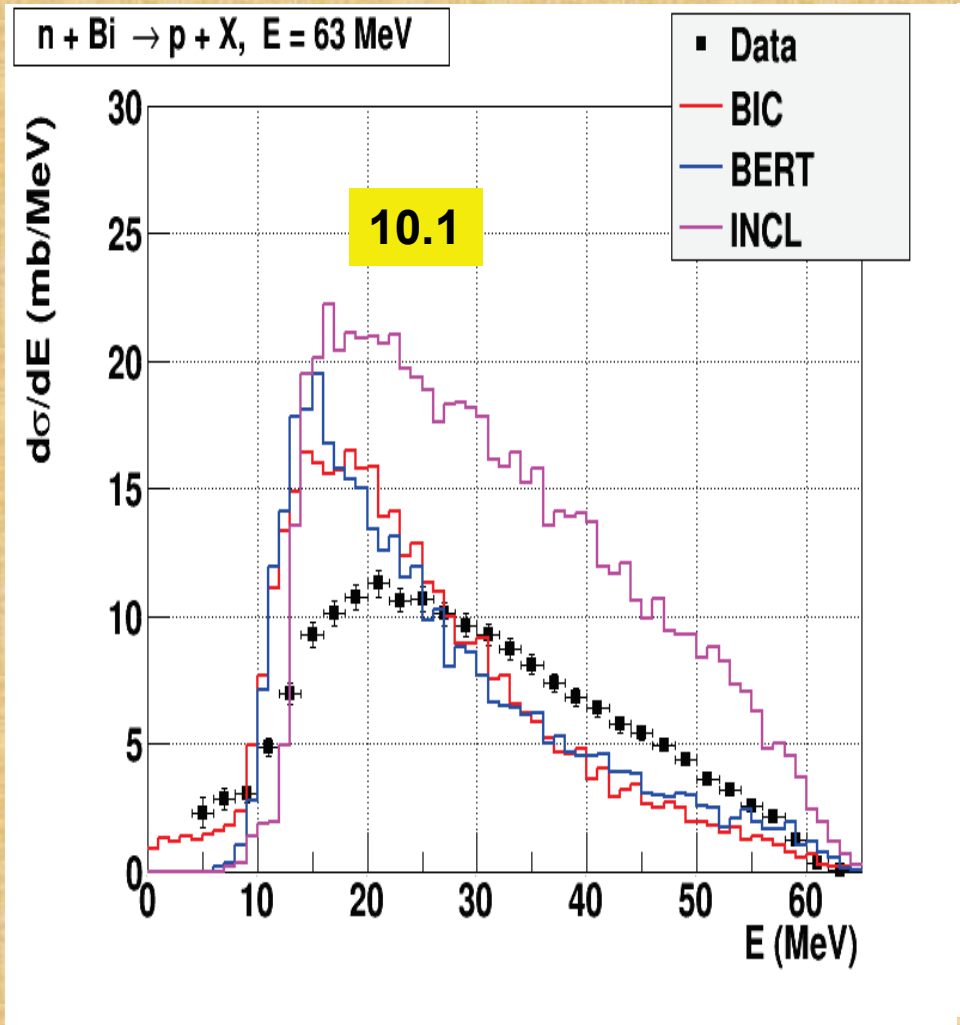
Main problem of 10.1 for de-excitation

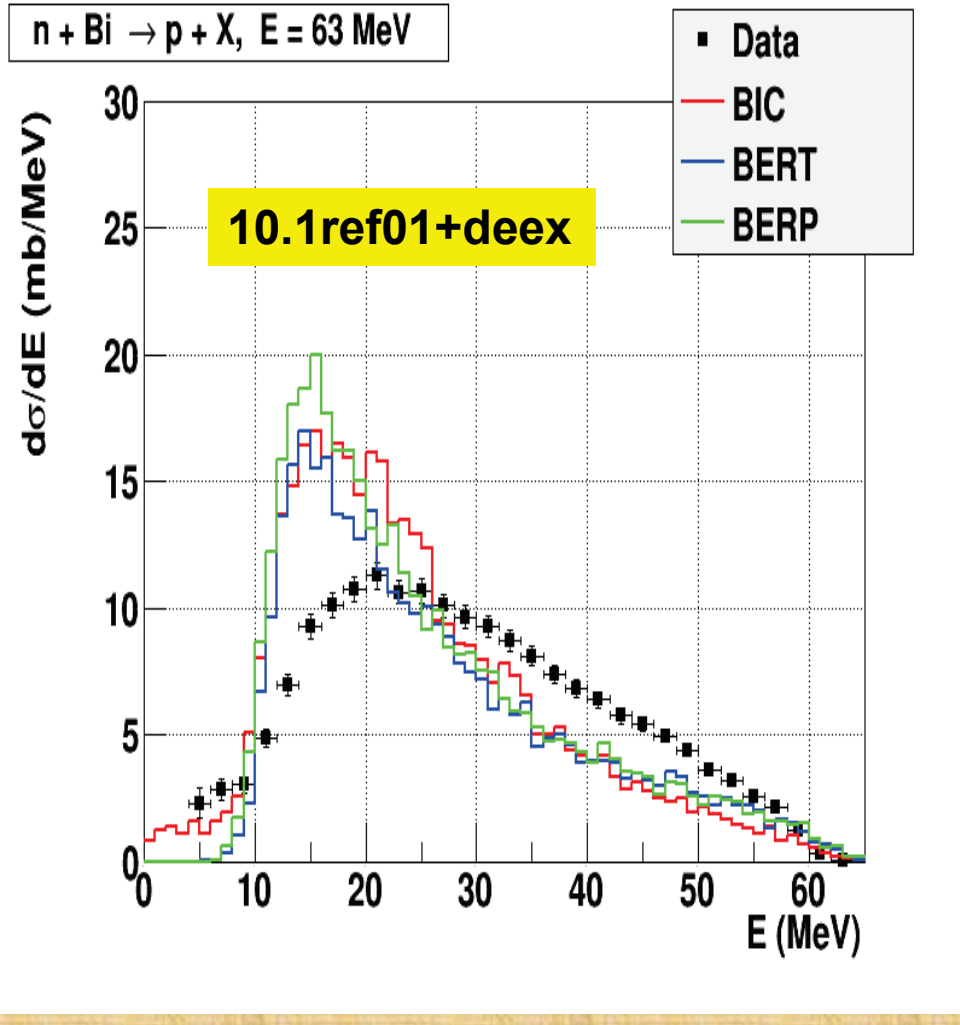
- Various hadronic models use different data on nuclear levels
  - FermiBreakUp
  - GEM
  - Photon evaporation
  - Radioactive decay
  - Isomer table
- There is a tight check on proposed excitation of an isomer: G4IonTable::GetIon(Z, A, Eex)
  - If new isomer is not agree with hardcoded value 2 eV then an unknown new state with zero life time is created

Fixes introduced to 10.1p02

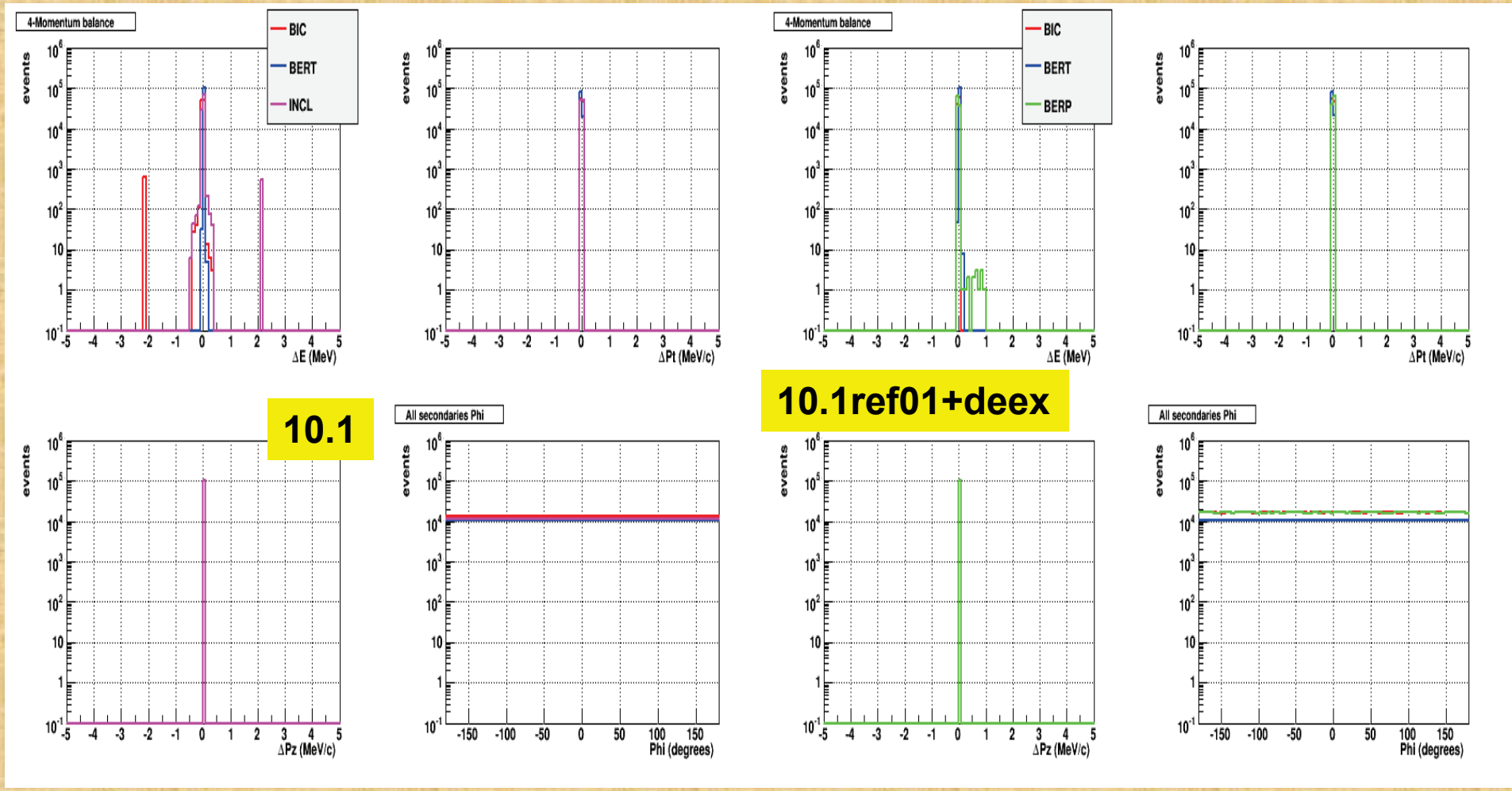
- Isomer production inside de-excitation module is disabled
- If a level has large life time, than sampling of emission is done assuming decay at rest (as it was in 9.6)
  - Time of emitted gamma or electron is sampled within photon evaporation model
  - correction on electron bound energy is applied (L.Desourger)
  - correction on energy of recoil fragment is applied
- Validation was done
  - test30 benchmark: http://vnivanch.web.cern.ch/vnivanch/verification/verification/hadronic/test30/
  - Alberto confirmed reproducibility
  - Dennis confirmed improvements for radioactive decay
  - Recently Michel complained for several use-cases in radioactive decay which were identified by Laurent as a problem of energy tolerance
    - In ref-08 tolerance is reduced to 0.1 keV in all classes of photon evaporation
- Because all decay channels are in competiton this fixes affect all test results

Low-energy proton production

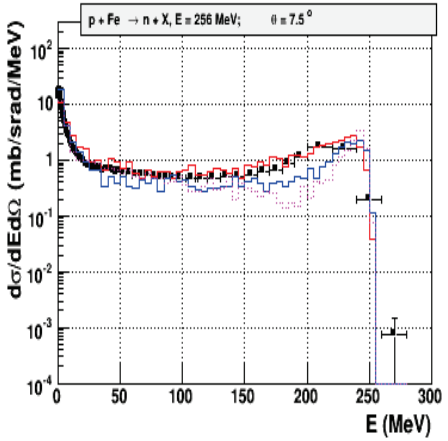


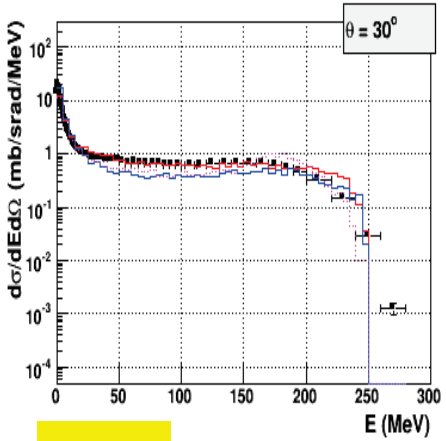


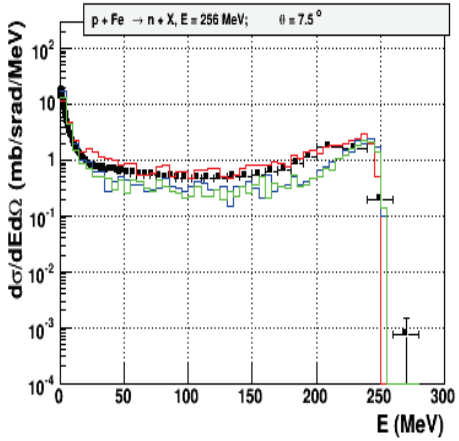
Energy/momentum balance for proton production

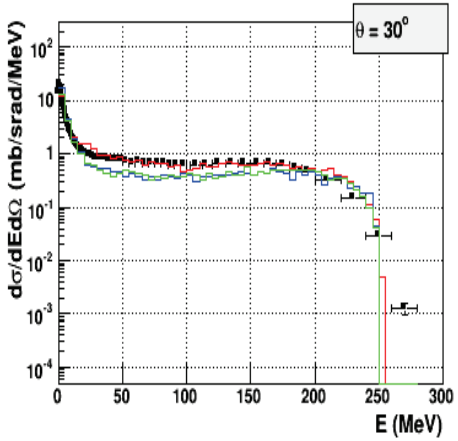


Low-energy neutron production

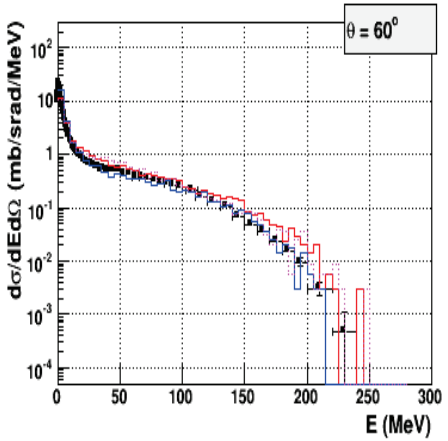


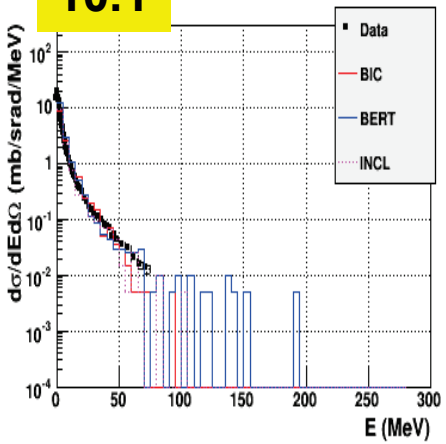




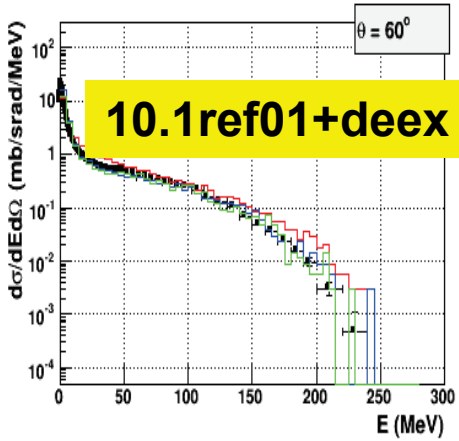


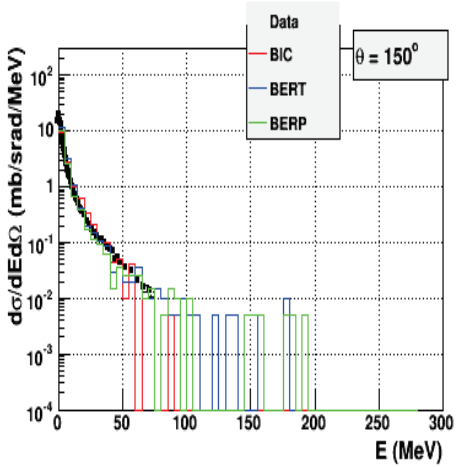
10.1





10.1ref01+deex





Development plan for 10.2 and beyond

- Re-design of inverse cross section computation in pre-compound/de-excitation
- Extract parameters of sub-models and provide mechanism of parameter modification
- Introduce new photon evaporation model and new alternative nuclear level data structure
  - GEM, Evaporation, and FermiBreakUp should be re-designed to use the same nuclear level data
  - Only this approach may gurantee reproducibility of the de-excitation module and corect production ofmeta-stable isomers
- We need ensure coherence of data used by G4IonTable, Radiaocve decay, and by the de-excitation module

Pre-compound/de-excitation code upgrade for 10.2

- Two new utility classes were introduced:
  - G4ChatterjeeCrossSection (used by Opt2)
  - G4KalbachCrossSection (Used by Opt3)
- These classes provides cross sections for light ion emission from excited nuclei
  - Used by both pre-compound and evaporation models
  - Reduced douplicated code
    - instead of 12 places were cross sections were coded now it is implemented in the one place
  - Simplified classes which are using these cross sections
    - Significant code cleanup
- Changed methods for
  - integrated evaporation probability
  - Sampling of final state
  - The goal is efficiency and reduced memory turn

New alternative nuclear level data structure

- De-excitation module requires common source of nuclear level data structure which will be used by all de-excitation sub-models
  - Improving CPU performance and memory
  - Removing fake intermediate states
  - Removing fake gamma lines
  - Providing consistent excitation energy for isomers
- New classes are added:
  - G4NuclearLevelData – pure singleton
  - G4LevelManager – manager class for all excited state of an isotope Z,A
  - G4NucLevel – gamma data for excited states

Alternative photon evaporation

- G4PromptPhotonEvaporation – new class
  - To enable it G4UsePromptPhotonEvaporation environment variable should be defined
- For both photon evaporation classes following options are available:
  - SetIMC(G4bool) – enable/disable internal conversion in gamma de-excitation
    - Not needed for high energy hadron/nuclear interactions
  - RDMforced(G4bool) – flag of radioactive decay
    - If enabled the decay time is not sampled in photon evaporation

Current status and plans

- What is done for 10.2
  - Inverse cross section computations for pre-compound/de-excitation
  - G4PreCompoundParameters data class
  - New nuclear level data structure
  - Alternative photon evaporation
  - Added utility classes for correlated gamma emission simulation
- What may be done for 10.2
  - New photon evaporation to be default
  - GEM and Evaporation models re-design to be based on the new level data
- What should be done after 10.2
  - FermiBreakUp to be base on the new level data
  - Introduce correlated gamma simulation
  - Extract de-excitation module parameters in the parameters class
  - Provide mechanism of parameters modfication for pre-compound/de-excitation
  - Add photon evaporation tests to testing suite
  - Perform tuning of pre-compound/de-excitation
  - Migrate to c++11 and further improve CPU performance
  - Redesin multi-fragmentation model