Status of pre-compound model and de-excitation module

V. Ivanchenko, CERN & Geant4 Associates International

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Outline

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- Preco/deex parameters
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Motivations

- Geant4 pre-compound model is responsible for simulation of pre-equilibrium emission of neutrons and light ions
  - When excited nucleus reach the equilibrium the pre-compound model call de-excitation module
- De-excitation module consists of several sub-models:
  - Multi-fragmentation
  - Fermi Break-up
  - Evaporation
  - GEM evaporation
  - Photon evaporation
- Any hadronic model may interface pre-compound model or de-excitation module
- Recently a process of review and redesign of pre-compound/de-excitation is started due to following reasons:
  - Provide thread safe and effective code
    - CPU performance and memory consumption of many of hadronic generators are limited by the performance of pre-compound/de-excitation
  - Sub-models use hardcoded nuclear level energies and other parameters
    - not possible guarantee reproducibility
  - There were a lot of duplicated code
  - Memory was used not in an optimal way
    - Overheads in MT mode
  - It was difficult to add new features
    - For example, correlated gamma emission

Strategy

- Updated pre-compound/de-excitation module fully based on $G4GAMMALEVELDATA
  - New data structure developed by Laurent Desorgher provides coherent nuclear data for Ion table, Radioactive decay and gamma levels
- G4PhotonEvaporation was updated first in 10.2 and in 10.2patch02 known problems were fixed
  - Now it is working coherently for Radioactive decay and hadron interactions
  - Correlated gamma emission should be available in 10.3
- G4ExcitationHandler use G4IonTable data
  - In 10.2 it does not generate isomere states but always ground state isotope is emitted
  - The goal to produce meta-stable isomeres still pending for 10.3
- For 10.3 new models are prepared
  - G4FermiBreakUpVI and G4GEMChannelVI
- Code cleanup is done whenever code is modified
  - Elements of c++11 are included
  - Optimal data handling
  - Thread safety

Preco/deex parameters

- A new class is added G4DeexPrecoParameters
  - Access: G4NuclearLeveldata::GetInstance()->GetParameters()
  - The class is shared between threads
  - It keeps currently 22 parameters
  - const Get methods
  - const Dump methods
  - Set methods are active only in the master thread in G4State_PreInit
- G4PreCompoundModel and all updated de-excitation sub-models are fully migrated to this scheme
- There parameters are useful for
  - sub-model development and tuning
  - advance users for low-energy applications
  - transparent documentation/dump of pre-compound/de-excitation configuration

Gamma evaporation

- There are 3 use cases:
  - Hadron inelastic interaction
    - no atomic shell, single de-excitation or full deexcitation chain to be simulated
  - Neutron capture
    - atomic shell exist, full chain gamma cascade to be simulated
  - Radioactive decay
    - atomic shell exist, single gamma transition to be simualted
- Normally the same instance or few different instances of the photon evaporation per thread may be used
  - A concumer model should Set flags to G4PhotonEvaporation
    - void SetMaxHalfLife(G4double lifetime);
    - void SetICM(G4bool flag); // enable internal conversion
    - void RDMForced(G4bool flag); // set flag of radioactive decay
- For simulation of correlated gamma emission the polarisation should be known
  - G4Fragment has now a pointer to G4NuclearPolarization
  - It is nullptr by default – no penalty for HEP

Jason Detwiler: IT Multipole expansion for correlated gamma emission

- For a particular value of M_1, consider the transition:

$$|J_1^{\pi}, M_1\rangle \rightarrow |J_2^{\pi'}, M_2\rangle + |L, M\rangle$$

- In this transition, the amplitude for photon emission in direction ***k*** is

$$\text{Amplitude}(\mathbf{k}) = \sum_{M_2, L, M} A_{J_1, M_1, \pi, J_2, M_2, \pi', L, M} \, T_{J_1, J_2, L} \, D_{L,M}(\mathbf{k})$$

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Clebsch-Gordannery

Nuclear Data

Spherical Harmonics

Jason Detwiler: new code required for correlated gamma simulations

- Utility classes already added to Geant4
  - G4Clebsch (Wigner6J and Wigner9J functions, etc.)
  - G4LegendrePolynomial
    - N-th coefficient, associated Legendre polynomial evaluation
  - G4PolynomialPDF
    - set coefficients, randomly sample
  - G4NuclearPolarization: the “statistical tensor”
    - data object attached to G4Fragment
  - G4PolarizationTransition
    - samples angles and modifies the G4NuclearPolarization after decay
- Extended gamma level data
  - To be added L, L’, δ to each gamma level
  - Laurent Desorgher has prepared a new data extended data set for 10.3
    - Data reader should be updated and the data should be released
- Correlated gamma emission will be enabled via G4PrecoDeexParameters
  - The algoristhm to sample final state with polarisation should added additionally to the defaults one

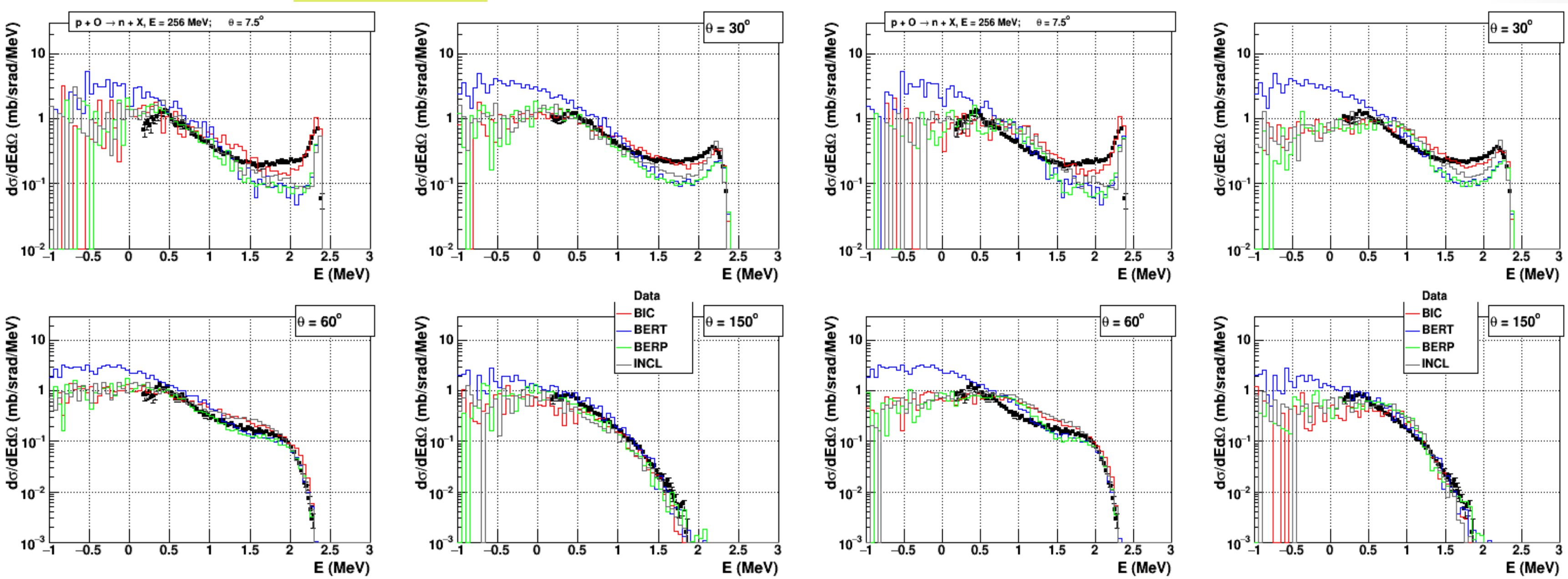
Fermi Break-up model

- Old G4FermiBreakUp model was based on hadrcoded 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, Z < 9, A < 17
  - An extra set of 80 unphysical fragments not known from data
    - Including very exotic states like H_8 or He_2
  - Only binary decay chains are considered
    - A standard Coulomb barrier computation is used
  - The probability of the first decay is computed on fly because initial excitation of the primary fragment is not fixed
  - The decay product may be as a state from the main pool or from the extra set
  - The second decay probabilities are precomputed
  - Final product is always a list of states from the main pool whihc have no Fermi decay channels
    - Ground states or excited states which have only gamma decay
- The new model is slightly slower than the old one but is more correct physically

Validation and tuning of the new model

10.3beta

10.2ref07

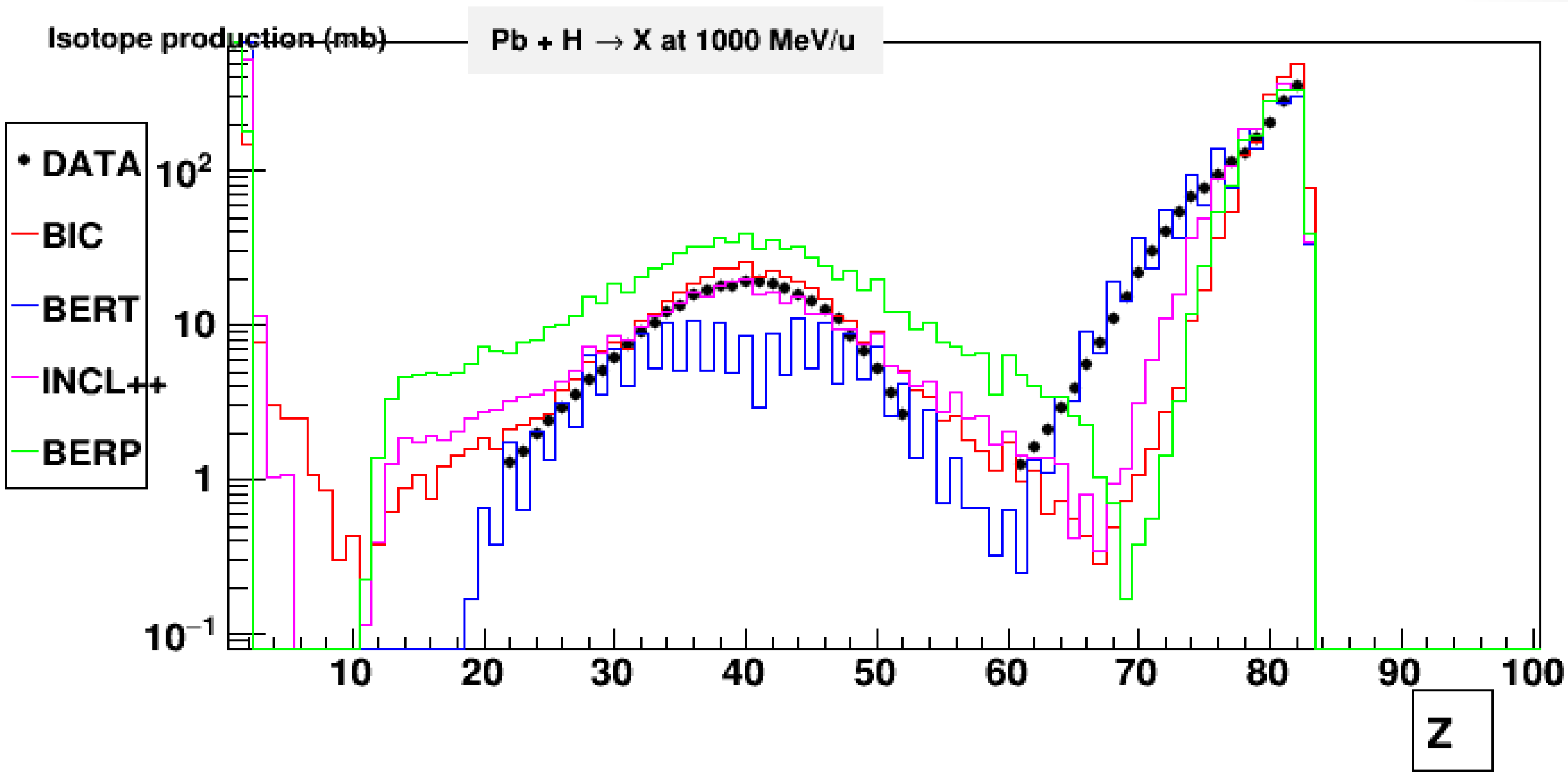


- We have limited data for the case Z < 9 and A < 17
    - In test30 there are data for p interaction with C, O, Li at relatively high energy
- The only one model parameter Elim=30 MeV (max excitation of the initial state) was tuned

GEM evaporation

- Old GEM evaporation model describing 66 decay channels into hardcoded states with Z < 13 (Mg)
  - GEM decay assumes emitted state from the hardcoded list
  - Residual isotope assumed to have a random excitation
  - There are separate classes for probability and Coulomb barrier for each channel
- The new model is implemented in one class
  - A set of 79 channels is red from G4GAMMALEVELDATA for Z < 13
  - Emitted fragment may have excitation known from the data or has a higher excitation
  - The residual G4Fragment may have an excitation corresponding to the data or be higher
  - The standard Coulomb barrier class is used
- Validation and tuning of model parameters is not yet done

Isotope production in p+Pb at 1 GeV

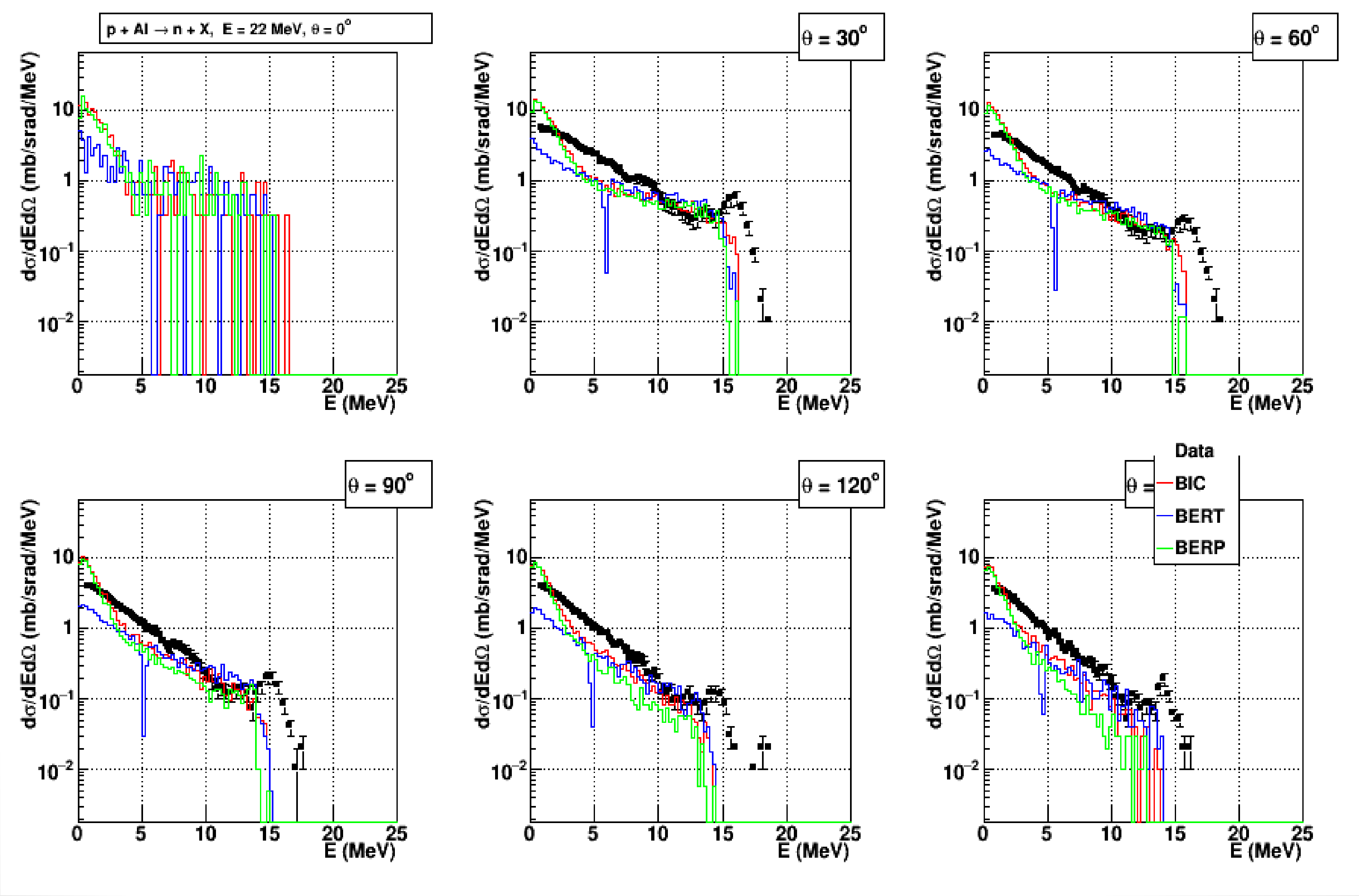


- Binary and INCL++ describe fission well
- Bertini is better to describe spallation
  - BERP does not describe well both spalation and fission
- Usage of GEM does not improve the situation
- Usage of multi-fragmentation provides a bit better agreement for the Binary cascade
- The goal of the new GEM model is an improvement of isotope production.

TEST30 RESULTS ON DOUBLE DIFFERENTIAL CROSS SECTIONS OF NEUTRON PRODUCTION

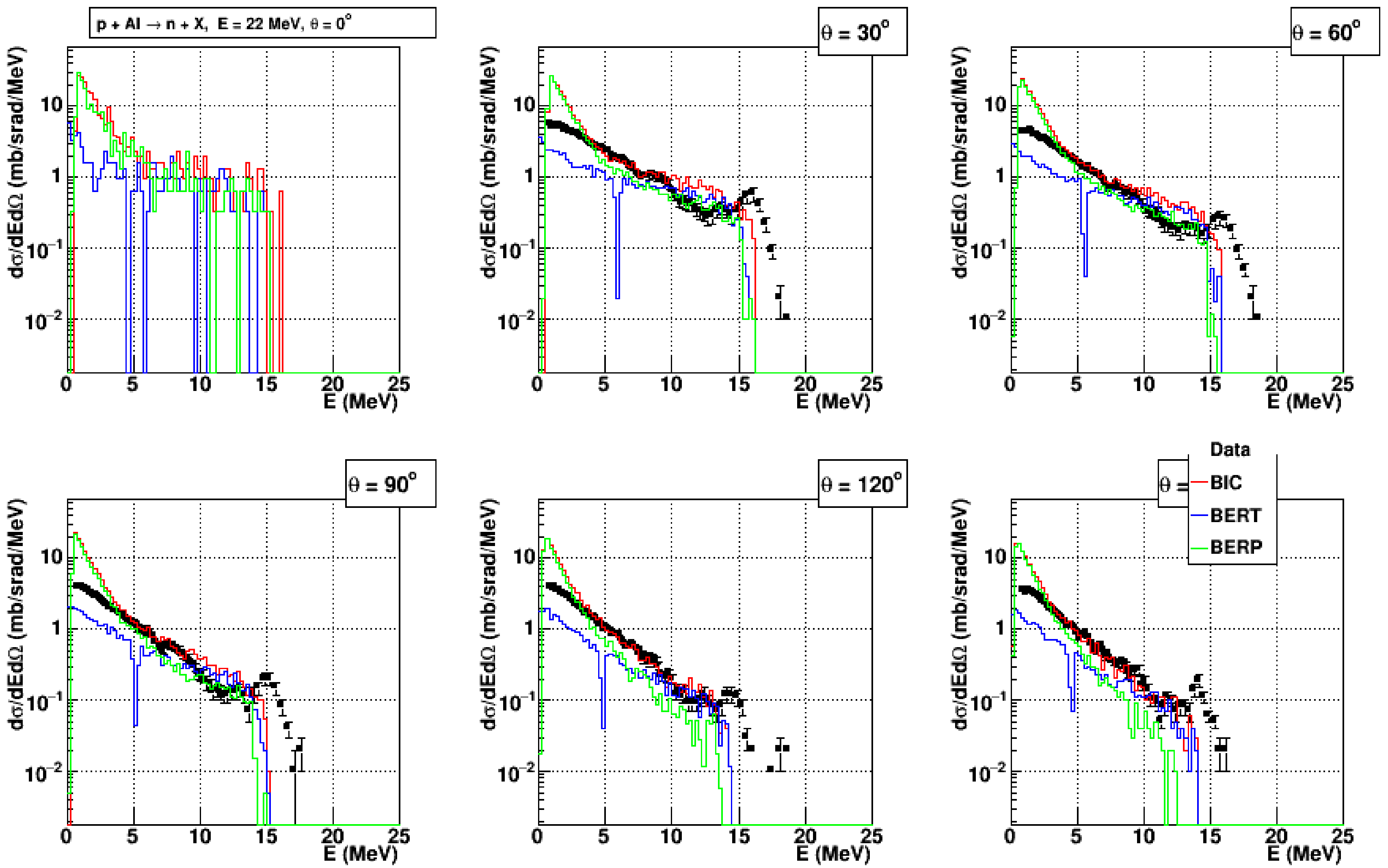
10.1p03 versus 10.2ref07

Double differential p+Al at 22 MeV 10.1p03

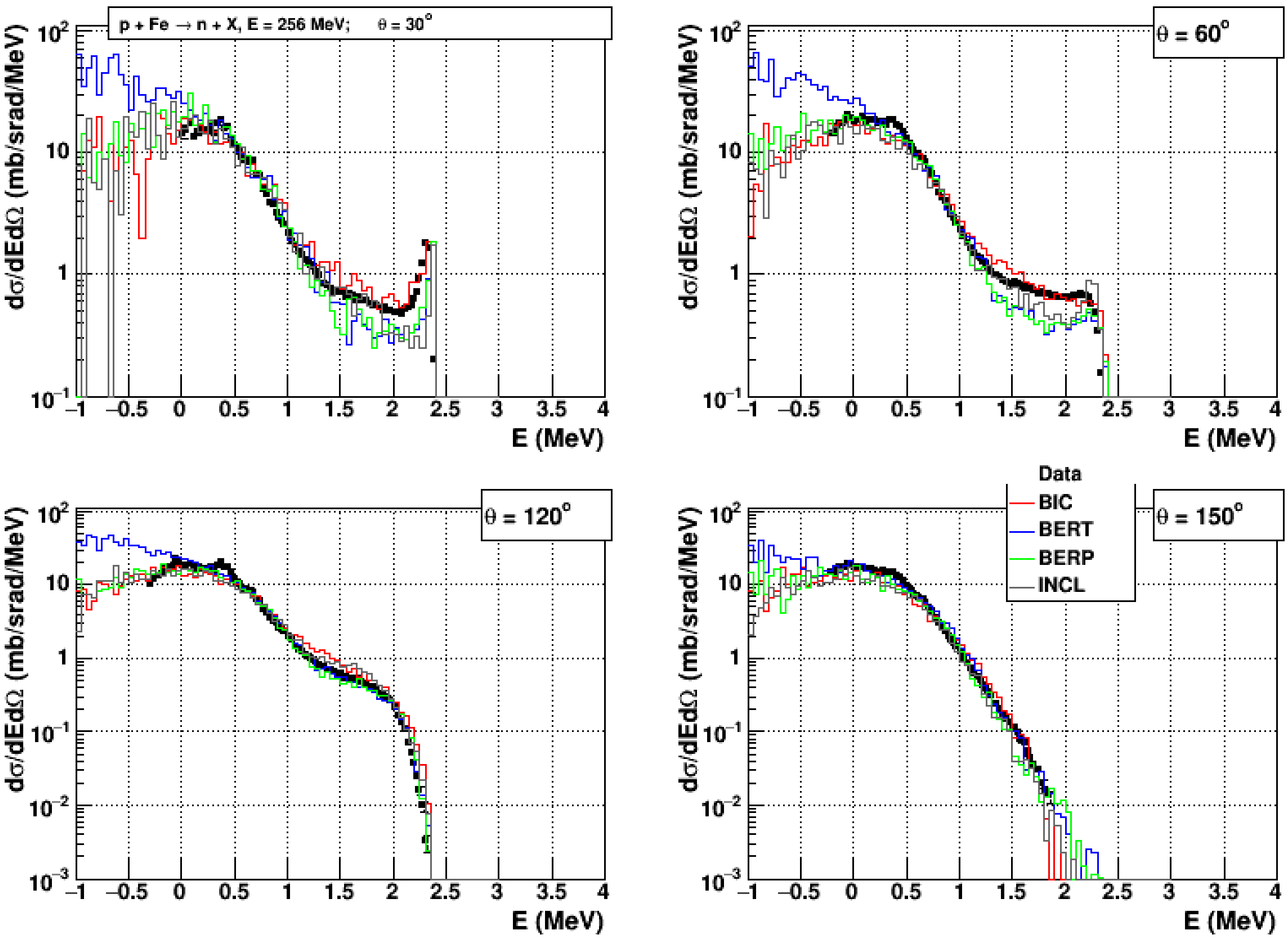


V. Ivanchenko, "Pre-compound/de-excitation" 21th G4 Workshop, 15 Sept 2016, Ferrara, Italy

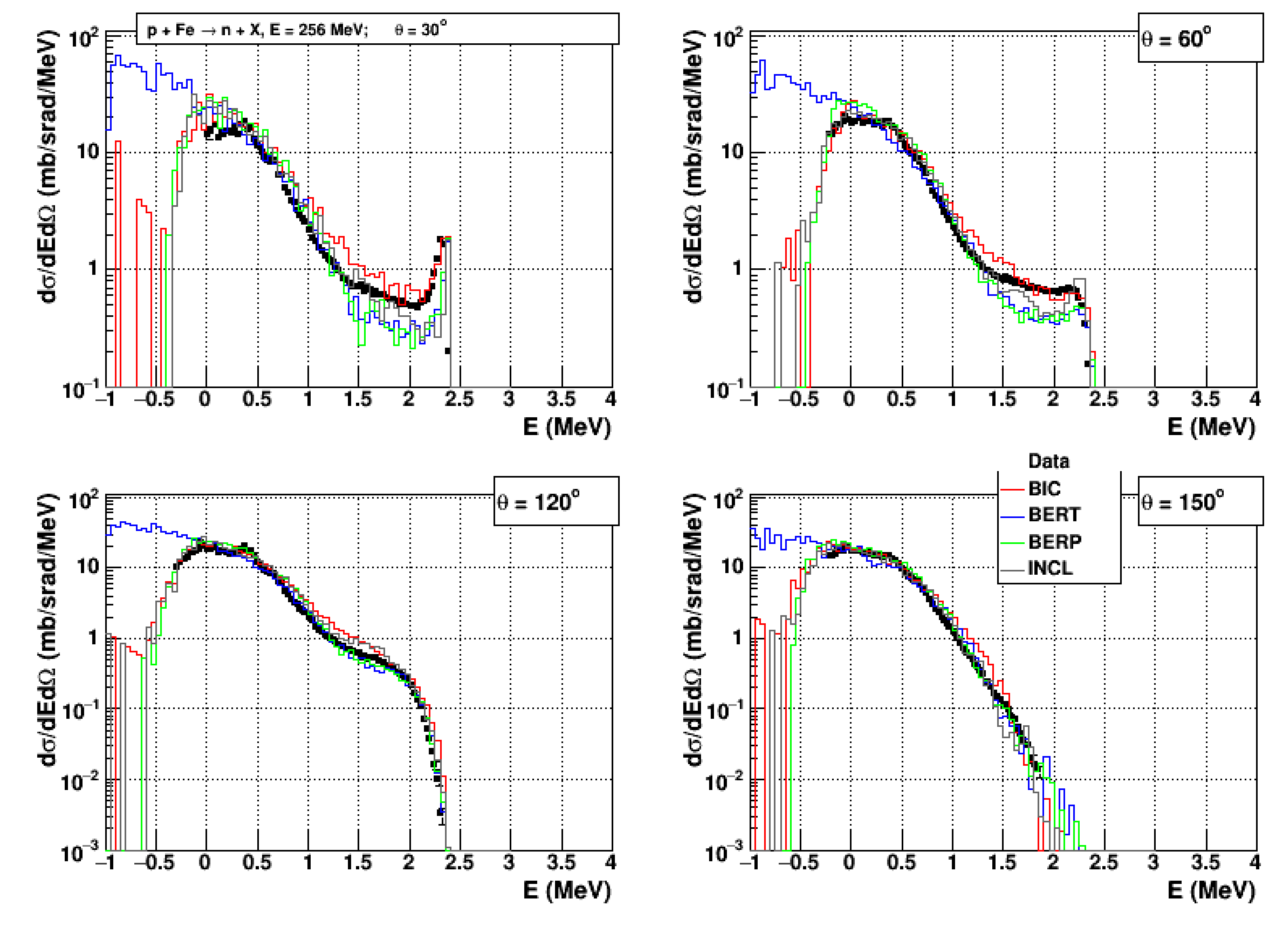
Double differential p+Al at 22 MeV 10.2ref07



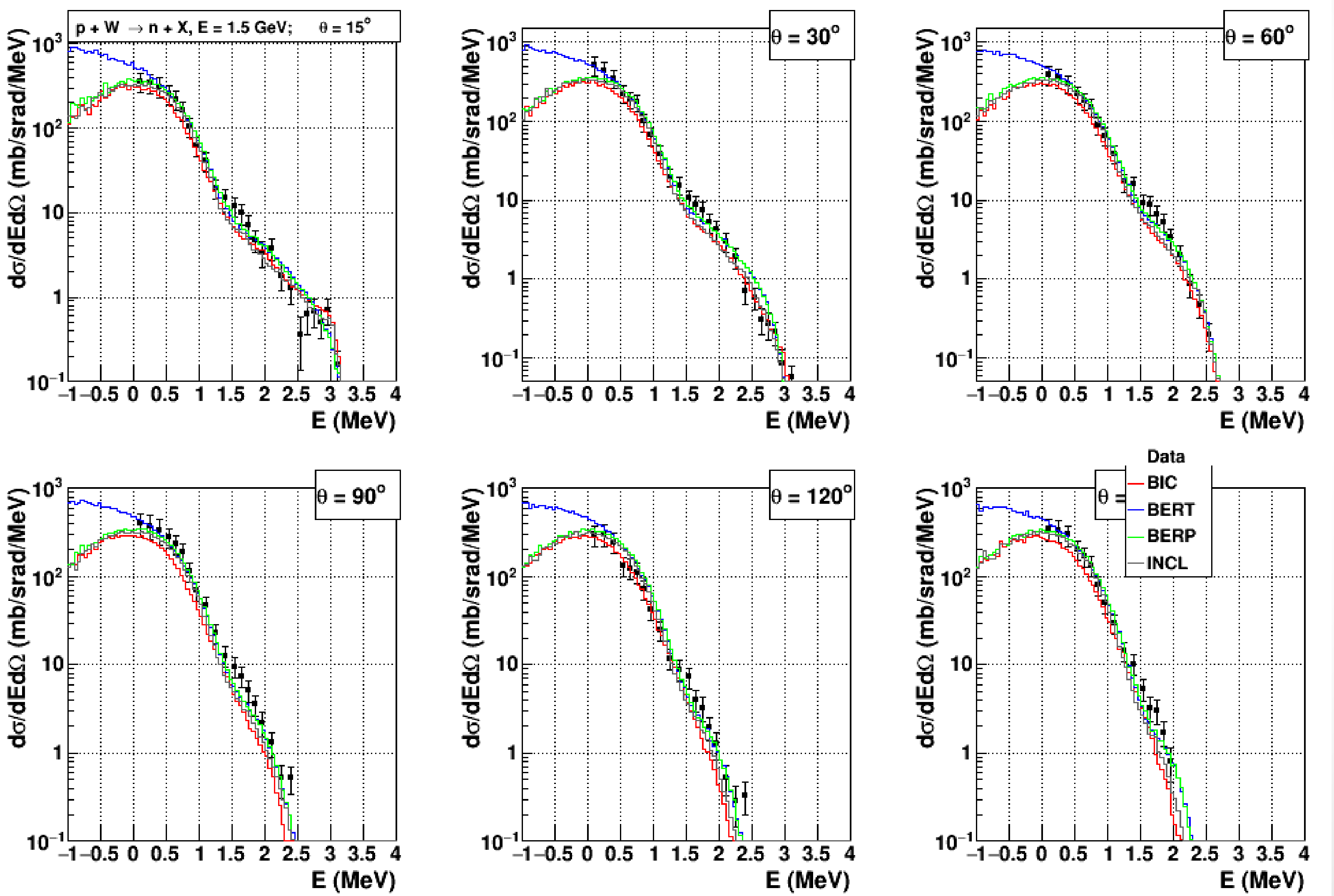
Double differential p+Fe at 256 MeV 10.1p03



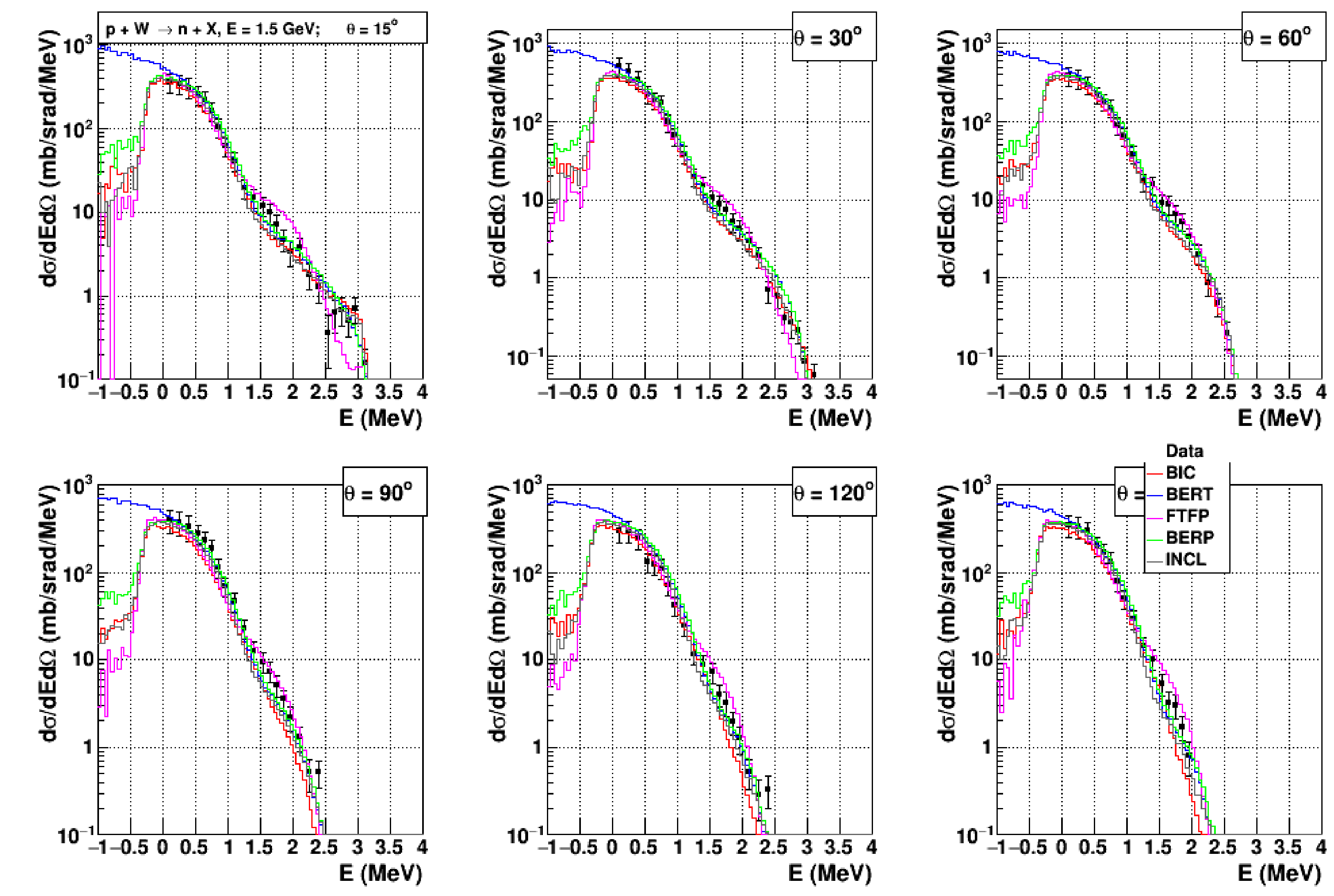
Double differential p+Fe at 256 MeV 10.2ref07



Double differential p+Pb at 1.5 GeV 10.1p03



Double differential p+Pb at 1.5 GeV 10.2ref07



CPU in test30 for 256 MeV proton interaction in thin target

Target	Model	CPU 10.0 (sec)	CPU 10.1 (sec)	CPU 10.2beta (sec)	CPU 10.2ref07 (sec)
Al	Binary	117	106	100	97
	Bertini	16	16	17	16
	Bertini+ Preco	38	27	23	17
	INCL++				88
Pb	Binary	470	413	356	331
	Bertini	45	45	46	45
	Bertini+ Preco	210	145	111	56
	INCL++				578

Summary

- A general redesign of the de-excitation module is ongoing
  - The module includes c++11 elements
  - Performance is improved
  - Bertini cascade will have similar CPU performance if use standard pre-compound/de-excitation
- There are several developments for 10.3 which not yet done
  - Adoptation of the new data structure prepared by L.Desorgher
  - Enabling correlated gamma emission
  - Validation and tuning of the new GEM model
  - Enabling of isomere production
- Validation results are stable in general
  - There are some plots with improvemets
  - There are some plots with slight degradation
  - Neutron spectra below 0.5 MeV is strongly supressed in the new model
    - This requires evaluation and further tuning