GEANT4 PRE-COMPOUND MODEL AND NUCLEAR DE-EXCITATION MODULE

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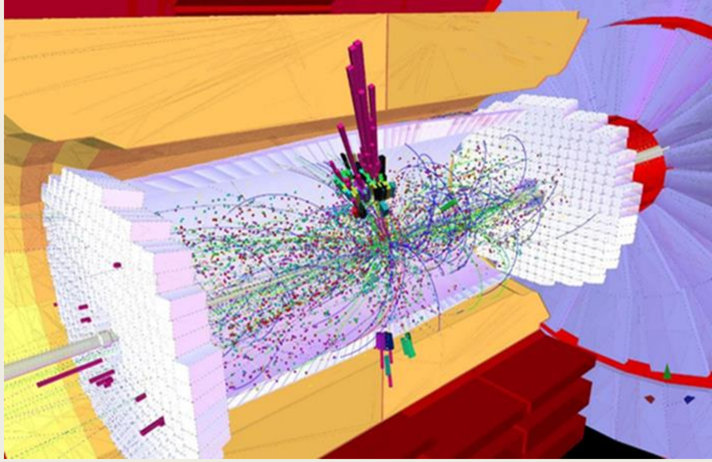
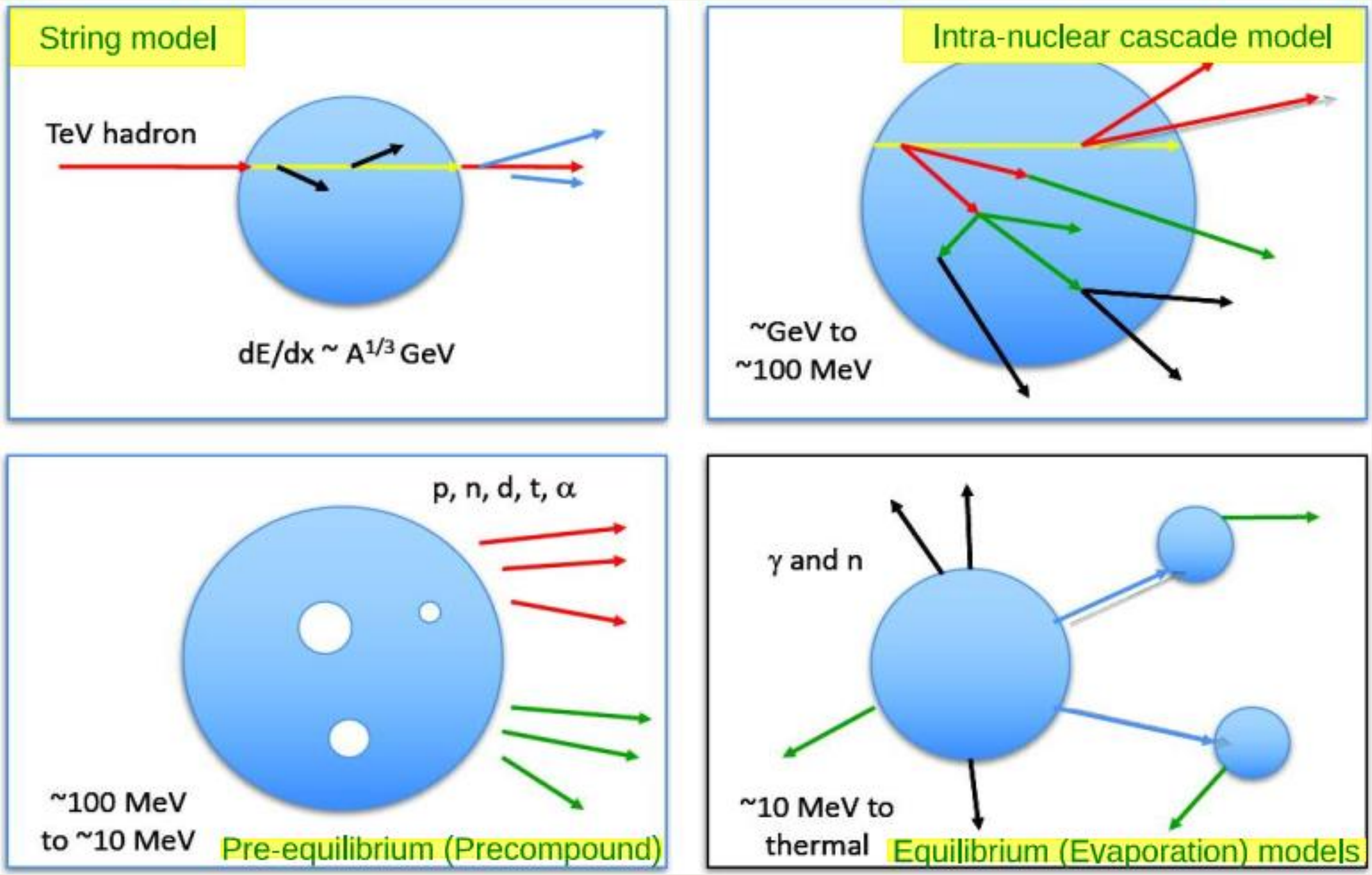
Introduction



- Geant4 hadronic working group is focused first of all on simulation for experiments at LHC
  - *~100 B events are already simulated for LHC detectors*
- LHC results are sensitive to systematic uncertainty of Monte Carlo
- Low-energy component of hadronic shower affect results for
  - *Simulation of calorimeter responses*
  - *Simulation of background for tracking detectors*
- Requirements for low-energy hadronic models
  - *Provide correct energy deposition and fluctuation*
  - *4-momentum balance in each interaction*
  - *CPU and memory efficiency*

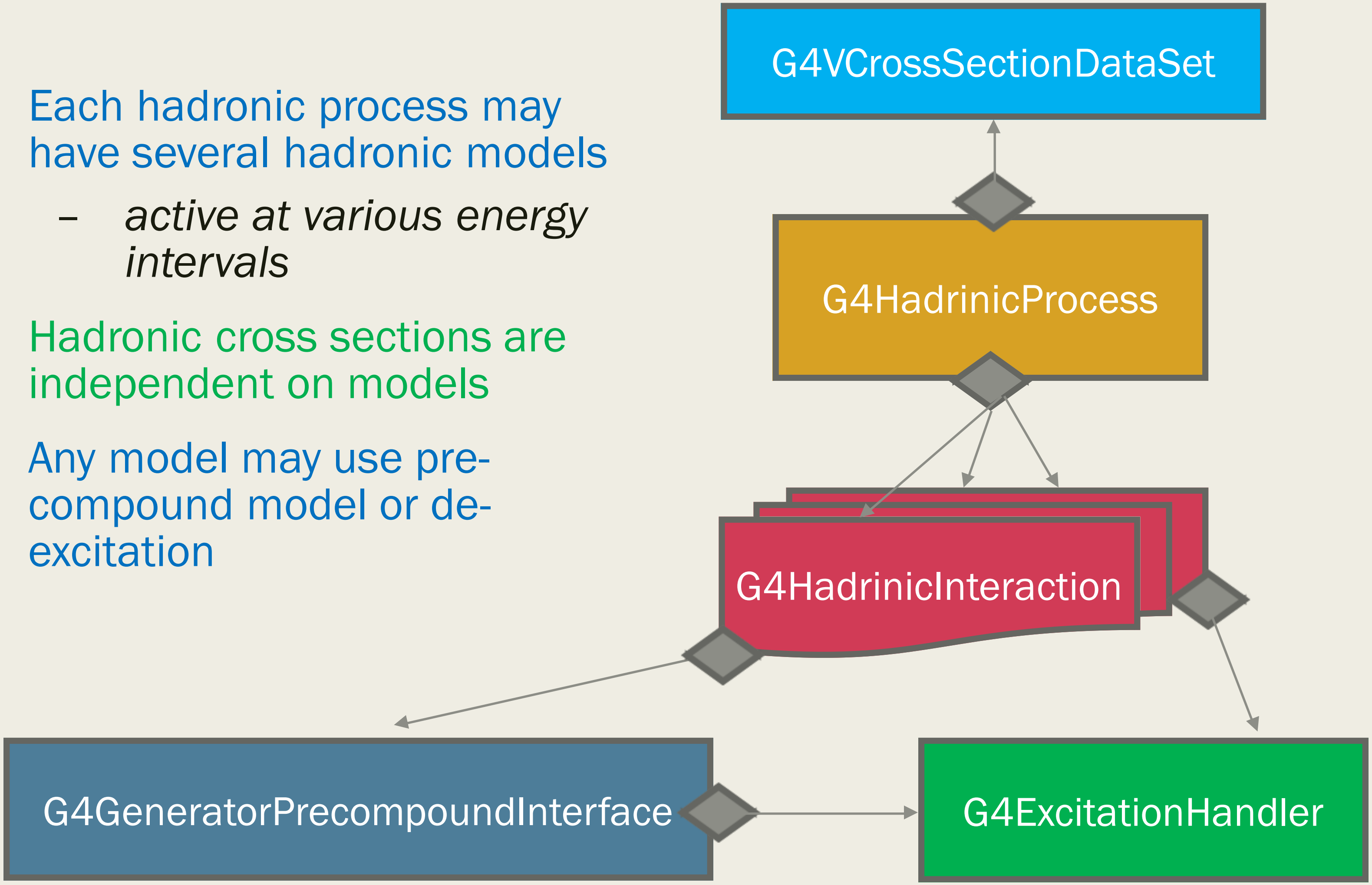
Hadron nucleus interaction



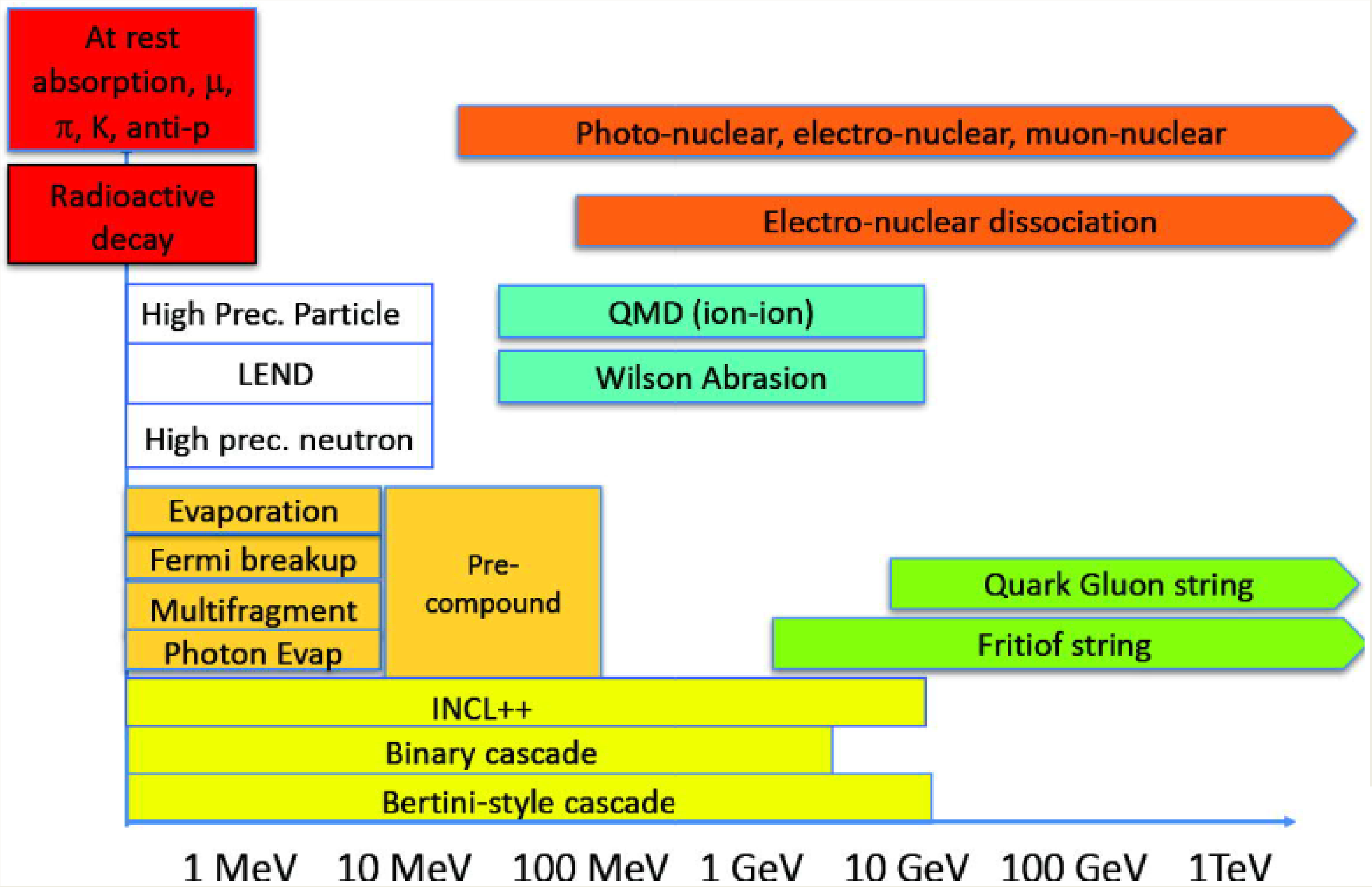
Geant4 hadronic physics design

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



Geant4 hadronic models



Native Geant4 pre-compound and de-excitation models

Native Geant4 pre-compound and de-excitation models

- Native pre-compound model and de-excitation module were created for the first Geant4 releases
- These models are the main part of simulation for HEP experiments
- Starting from 2008 Jose Manuel made general clean-up of these models
- Since that time these models correspond to theoretical prescriptions

Jose Manuel Quesada Molina
Sevilla University, Spain

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*

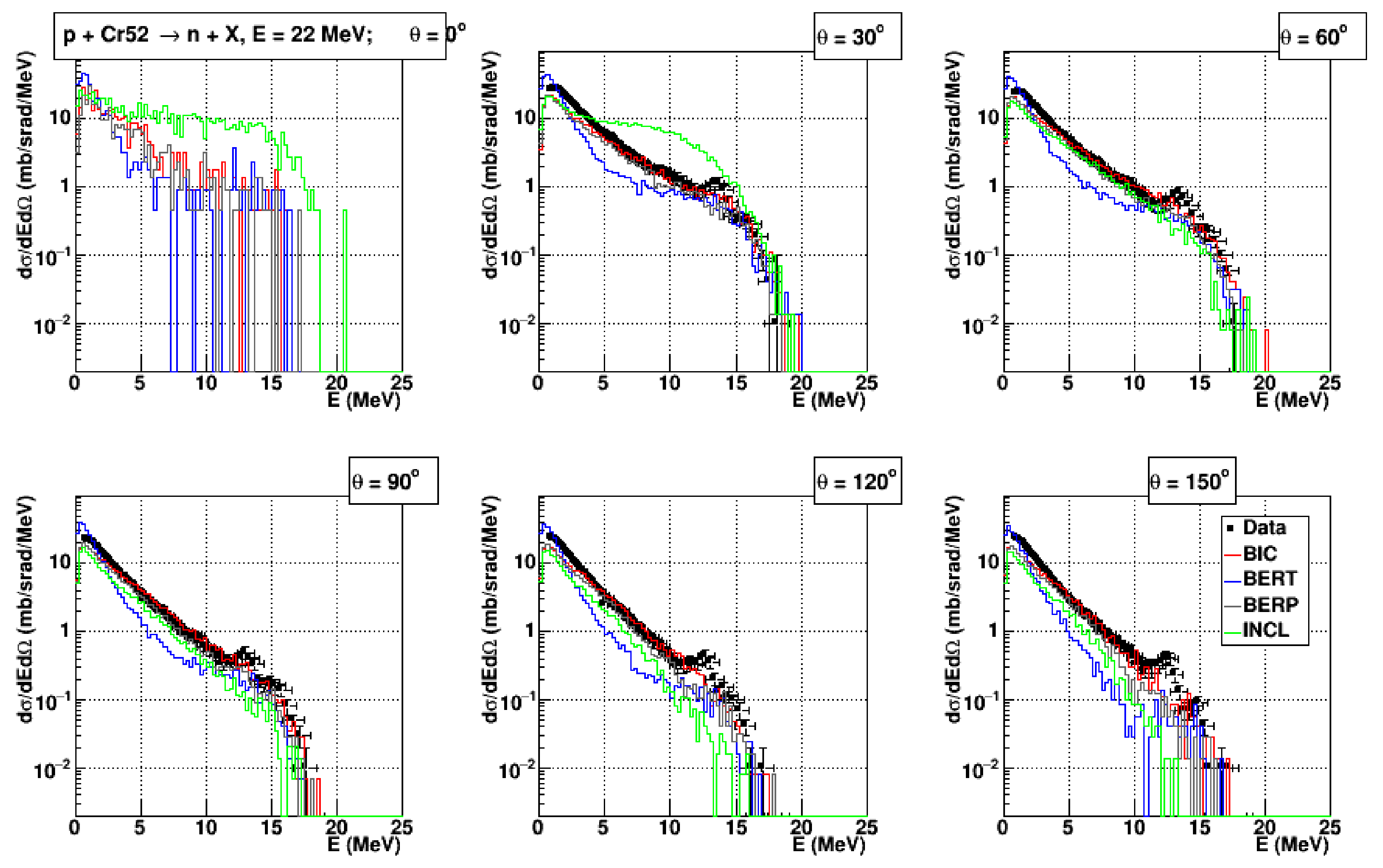
Selected validation results

Nuclear de-excitation in the main hadronic models

- QGS and FTF string models directly use native pre-compound model
  - *Potentially they may uses the Binary cascade but this combination is less tested and is not ready for production*
- The Binary cascade uses native pre-compound model
- The Bertini cascade by default uses its own de-excitation module
  - *The default de-excitation of Bertini is faster but less accurate*
  - *There is an interface to the native pre-compound*
- INCL++ has its own de-excitation module ABLA
  - *by default uses native de-excitation module*
- QMD uses native de-excitation module
- ParticleHP models uses native photon evaporation model

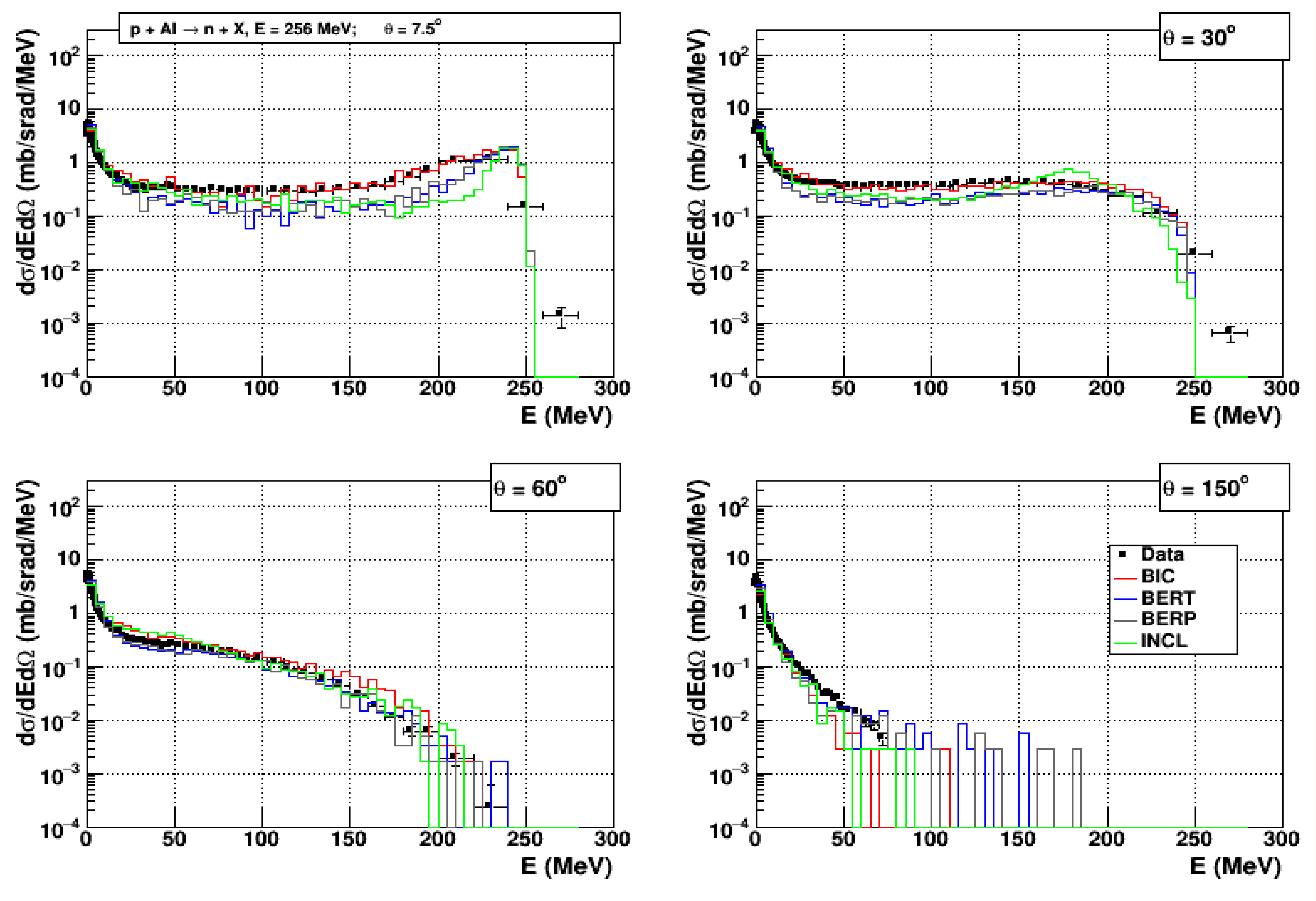
Double differential neutron production cross section for 22 MeV protons in ^{52}Cr target

N.S.Biryukov et al., Sov. J. Nucl. Phys. 31 (1980) 3



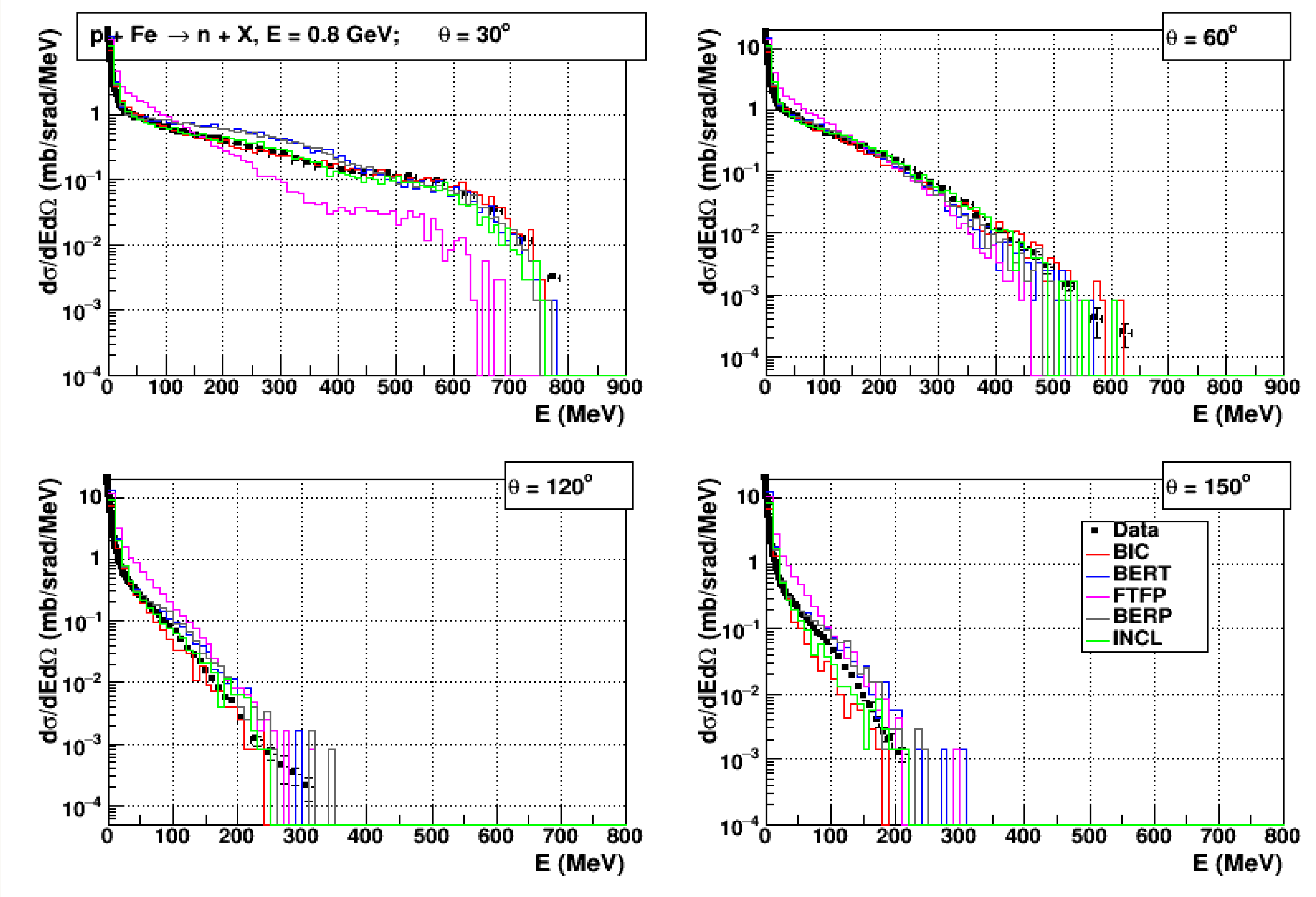
Double differential neutron production cross section for 256 MeV protons in Al target

M.M.Meier et al., Nucl. Sci. Engeneering 110 (1992) 289



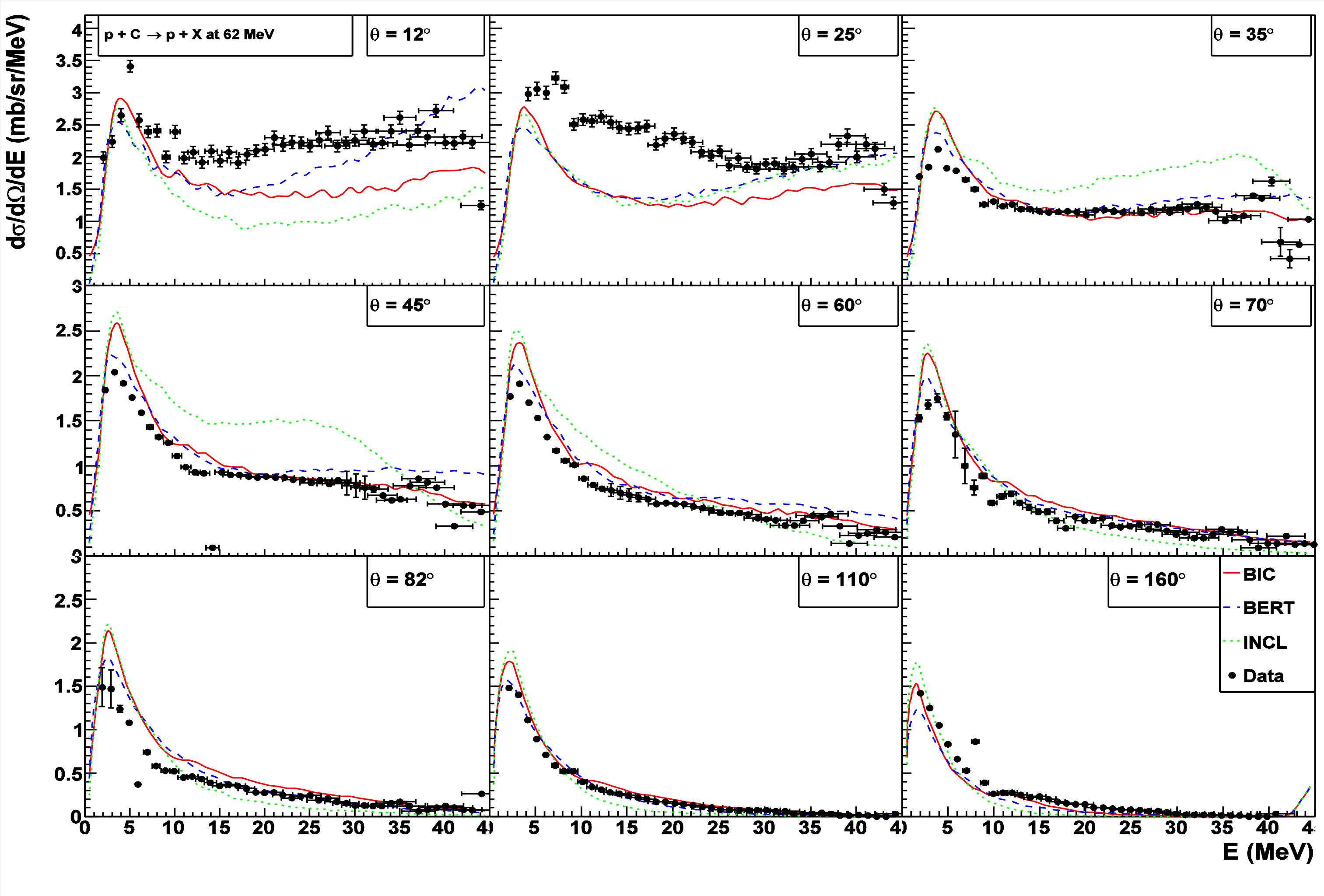
Double differential neutron production cross section for 800 MeV protons in Fe target

W.B.Amian et al., Nucl. Sci. Engeneering 112 (1992) 78



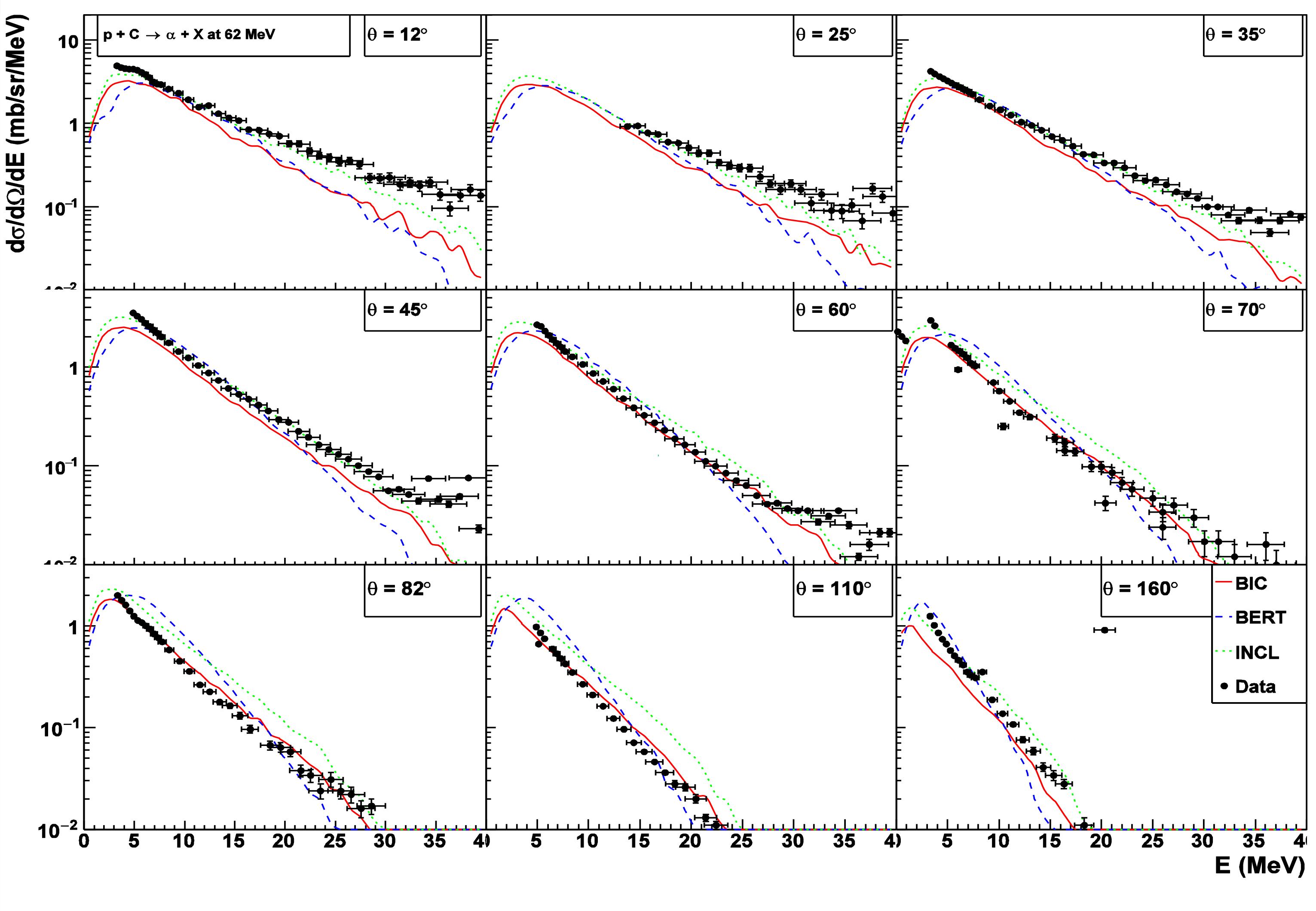
Double differential proton production cross section for 62 MeV protons in carbon target

F.E.Bertrand & R.W.Peelle, Phys. Rev. C 8 (1973) 1045



Double differential alpha production cross section for 62 MeV protons in carbon target

F.E.Bertrand & R.W.Peelle, Phys. Rev. C 8 (1973) 1045



Theory based models versus data driven models

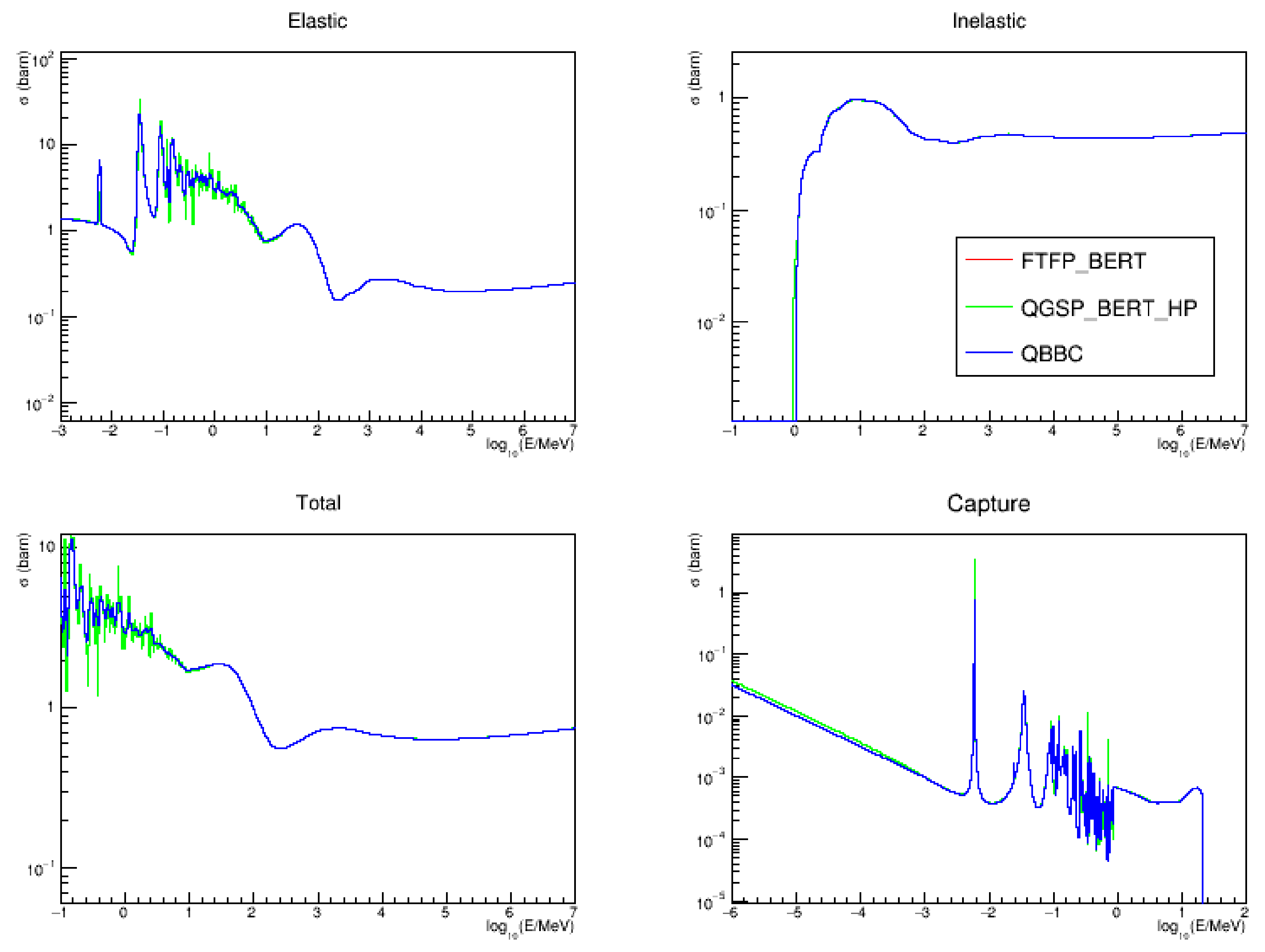
Set of NeutronHP and ParticleHP models

- NeutronHP and ParticleHP models and cross sections are fully based on data
  - *Total cross sections*
  - *Partial cross sections*
  - *Inclusive spectra*
  - *G4NDL, G4TENDL, LEND data sets*
- Native pre-compound/de-excitation are based on phenomenological models, however, a lot of data are also used
  - *Nuclear level database*
  - *Radioactive decay data*
  - *Total cross sections at low energies G4PARTICLEXS1.1 are derived from G4NDL and G4TENDL data sets*

G4PARTICLEXS1.1

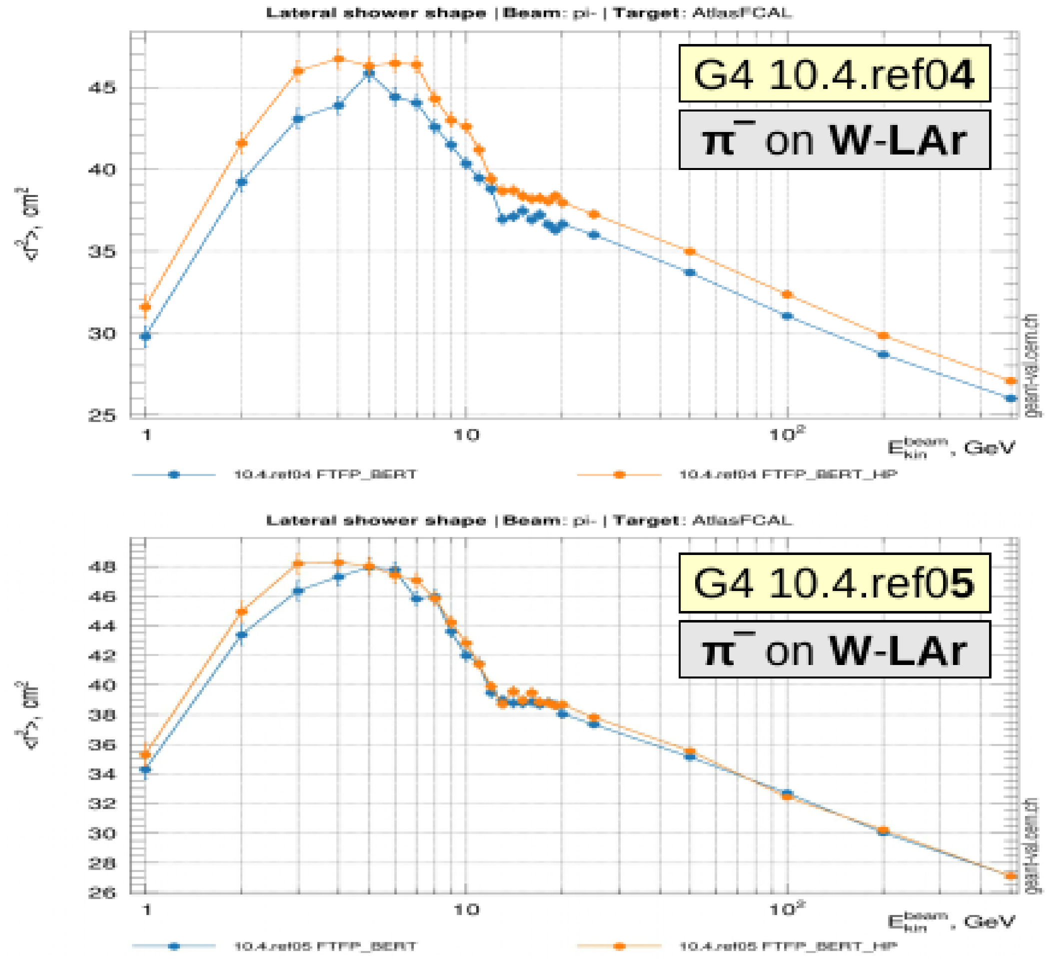
- New development available with Geant4 10.5
- Structure of the data set is change because of particle HP
  - *Separate directories for n, p, d, t, he3, he4 cross sections*
  - *Element x-sections from threshold to max hadronic energy (100 TeV)*
    - Physics data tables shared between threads extracted from ParticleHP
    - Glauber Gribov cross section above 20 GeV for p and n
    - Glauber Gribove cross sections above 20 MeV for , d, t, he3, he4
- Added extra isotope data for 11 more elements (was 17 before)
  - *Ne, Mg, S, Cl, K, Sc, Ti, Ga, Pd, In, Pt*
  - *Limit on isotope abundance is reduced to 0.001 (was 0.01)*
- Fixed discontinues in last bins
  - *Isotope data only for E < 20 MeV*
- Fixed G4CrossSectionDataStore code
  - *Isotope selection*
  - *Integral approach*

Neutron x-sections in Aluminum



G4PARTICLEXS1.1 for hadronic shower

Lateral Shape : FTFP_BERT *vs* FTFP_BERT_HP



FTFP_BERT is closer to FTFP_BERT_HP in Ref05 than in Ref04

Recent developments for the native pre-compound/de-excitation

Motivation for internal re-design of pre-compound/de-excitation

- For long time different components of de-excitation where independent:
  - *RadioactiveDecay, PhotonEvaporation, FermiBreakUp, GEM models had hard-coded:*
    - List of nuclear levels
    - Coulomb barrier parametersations
    - Level density
    - ….
- It make a serious problem with multi-threading
  - *different model produced incompatible excited states*
- After Geant4 10.2 a redesign of the de-excitation module was performed
  - *A strong requirement: do not change HEP calorimetry responses*

General development topics

- Established set of model parameters for PRECO and DEEX and user interface to these parameters
- Renewed internal data structure for nuclear levels
  - *G4ENDSFSTATEDATA, G4LEVELGAMMADATA, G4RADIOACTIVEDATA are coherent*
  - *New data format was introduced in Geant4 10.3*
  - *All components of PRECO and DEEX use this data and not hard-coded numbers*
- Provided long-lived isomer production
  - *Added floating level states*
  - *Long lived isomers may be tracked by Geant4*
- Provided correlated gamma emission for radioactive decay
  - *Is disabled by default but may be enabled by a flag*
- Make code to be more efficient
- Added c++11 coding style where possible
- It was completed in general for Geant4 10.4
  - *However, some fixes and improvements are still added in 10.5*

Parameters for pre-compound/de-excitation

- G4DeexPrecoParameters scheme
  - *Printout of all important parameters values at initialisation*
  - *Modification of parameters allowed only at G4State_PreInit*
  - *New boolean parameters are added recently allowing disable DEEX or PRECO*
- How it can be used?
  - *G4DeexPrecoParameters* param=*
    G4NuclearLevelData::GetInstance()->GetParameters();
  - *param->StoreStoreICLevelData(true);*
  - *param->SetCorrelatedGamma(true);*
  - *param->SetInternalConversionFlag(true);*
  - *param->SetDeexChannelType(fGEM);*
  - *……….*
  - *param->Dump();*
- G4ExcitationHandler has public Set methods
  - *This interface is left in order to allow creation of custom handler*
  - *Normally parameters should be set via G4DeexPrecoParameters class*

Nuclear level data

- Only one singleton class G4NuclearDataStore left with static data shared between all threads
  - *No thread local data anymore*
  - *Access to*
    - G4DeexPrecoParameters
    - Nuclear level data
    - G4PairingCorrections
    - G4ShellCorrections
- Transient data structure may include internal conversion (IC) data
  - *SetStoreICLevelsData() flag enable/disable storing of internal conversion data*
    - If true the full data size 56 M (radioactive decay enebles)
    - If false – 8 M (HEP case)
  - *IC is controlled by InternalConvertionFlag()*
    - If false – only gammas produced
    - If true – electrons produced even if IC data are not stored
    - For some levels no gamma transitions data only IC performed

Isomere production

- Deexcitation of any excited nuclear fragment is stopped if
  - *Excitation energy below 10 eV*
  - *Life time of the fragment below time limit*
    - 10^3 s by default to reduce number of extra objects in HEP simulations
    - 10^{-6} s if radioactive decay is enabled
- List of possible excited state is synhkronized between the deexcitation module and G4NuclideTable
  - *Additionally to simple excited isometers floating level isomeres may be produced*
    - +X,+Y,+Z,+U, +V,+W,+R,+S,+T,+A,+B,+C
- After each de-excitation reaction the time is defined
  - *For radioactive decay no extra sampling*
  - *Alternatively sampled decay time according to the life time of the level*
- Information on time and creator model is propagated to G4HadronicProcess
  - *Allowing proper checks of charge and energy conservation*
    - Emision of Auger electrons is allowed

New Fermi Break-up model

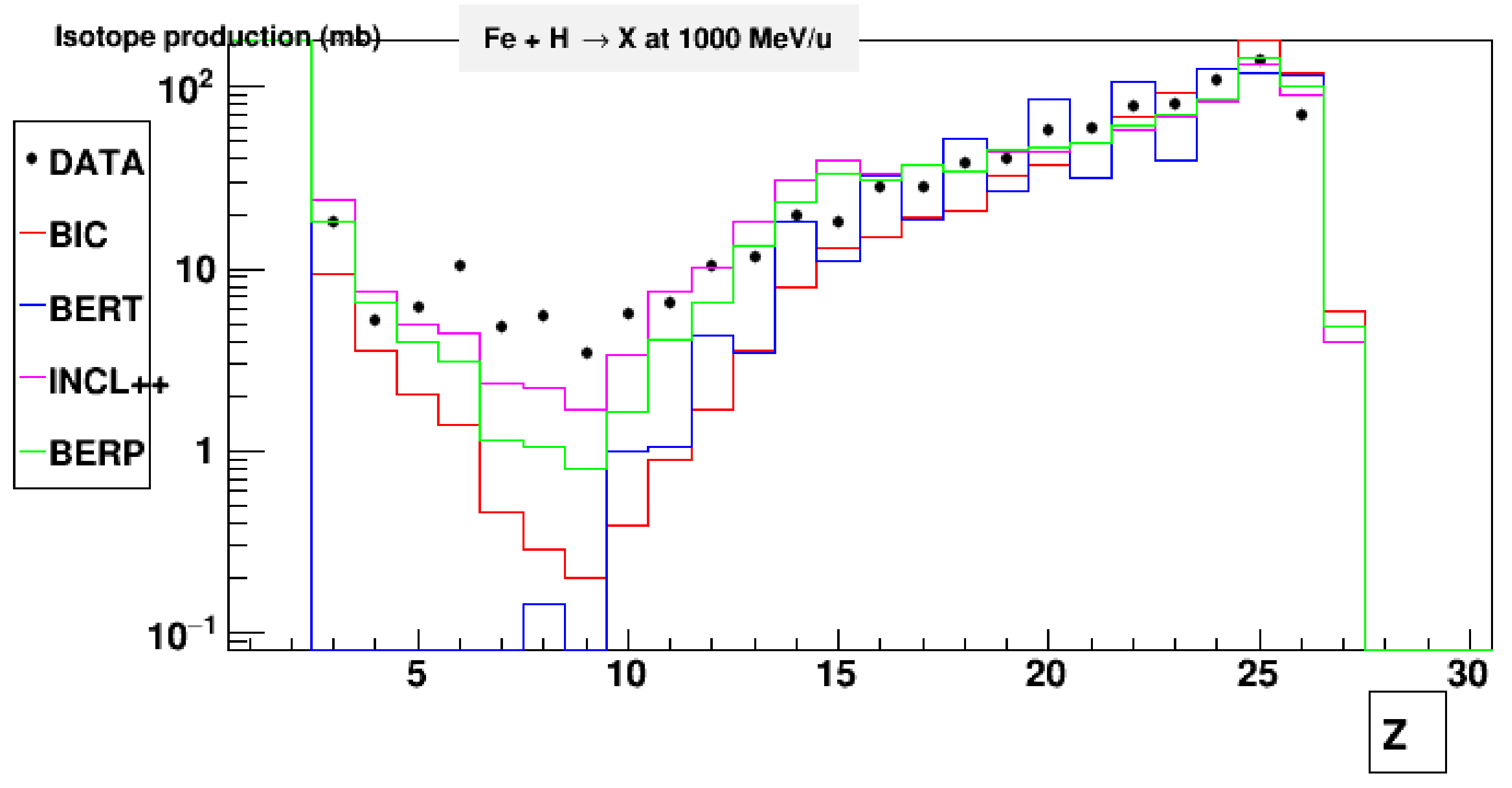
- Old G4FermiBreakUp model was based on hard-coded data
  - *A pool of 112 states, Z < 9, A < 17*
  - *Precomputed probabilities of decay of each state from this pool into 2-, 3-, 4-body final state from this pool*
- New G4FermiBreakUpVI model fully based on data of G4GAMMALEVELDATA
  - *A pool of 260 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
  - *An extra set of 80 unphysical fragments not known from data*
    - Including very exotic intermediate states like H_8 or He_2
  - *Only binary decay chains are considered*
    - A standard Coulomb barrier computation is used
  - *Probability of the first decay is computed on fly because initial excitation of the primary fragment is not fixed*
  - *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, which has no Fermi decay channel*
- The model for 10.5 is slightly slower than the old one but is more correct physically

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
  - $Ld = \alpha \bullet A \bullet (1 + \beta / A^{1/3})$
  - 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 new default Ld = 0.075*A

Isotope production by 1 GeV protons in Fe target

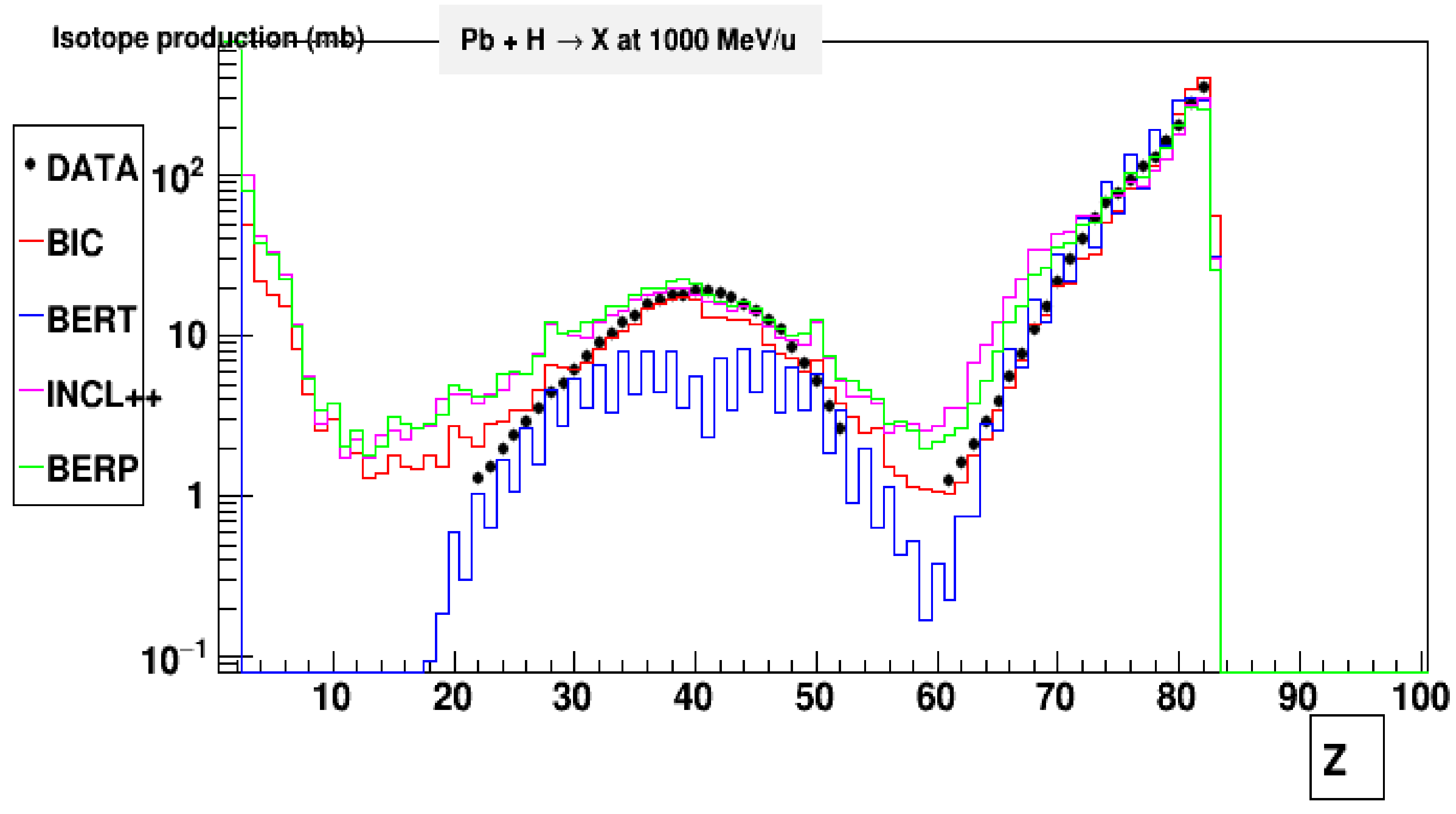
C.Villagrasa et al., AIP Conference Proceeding 769 (2005) 842



- 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 and plans

- General re-design and migration to the updated data structure on nuclear levels was completed in general for Geant4 10.4
  - *For Geant4 10.5 number of problems and bug reports are fixed and data sets are updated*
  - *Cross sections for neutrons, protons and ions are updated for 10.5*
  - *Radioactive decay may work with HEP Physics Lists*
  - *We recommend use recent Geant4 10.5p01 for nuclear physics applications*
- From Geant4 benchmarks one can conclude:
  - *The Binary cascade is the most accurate in general below 1 GeV/u*
  - *At higher energies the Bertini cascade and INCL++ become competitive*
    - INCL++ demonstrate the best performance for some benchmark data
- Our plans for 2019:
  - *Tuning of pre-compound/de-excitation parameters*
  - *Improving computations of probabilities of nuclear decay channels*
  - *Addition of gamma transitions to the Fermi Break-up reaction list*
  - *Complete migration of GEM model to the new design*