Pre-Compound and de-excitation models upgrade for 9.4beta

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Outline

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Problems of Geant4 9.3

- Significant upgrade of pre-Compound and de-excitation models have been carried out in 2009 and included into 9.3
- Problems:
  - Number of numerical problems in FTF based Physics Lists
  - Not precise results for light ion production
  - Deviation of 4-momentum balance in the Binary Cascade
  - Fermi Break-Up, Multi-Fragmentation Model (MFM) and GEM by default were disabled
  - Factor 4 over-production of photons
  - Wrong energies of photons
  - No Doppler broading in photon spectra

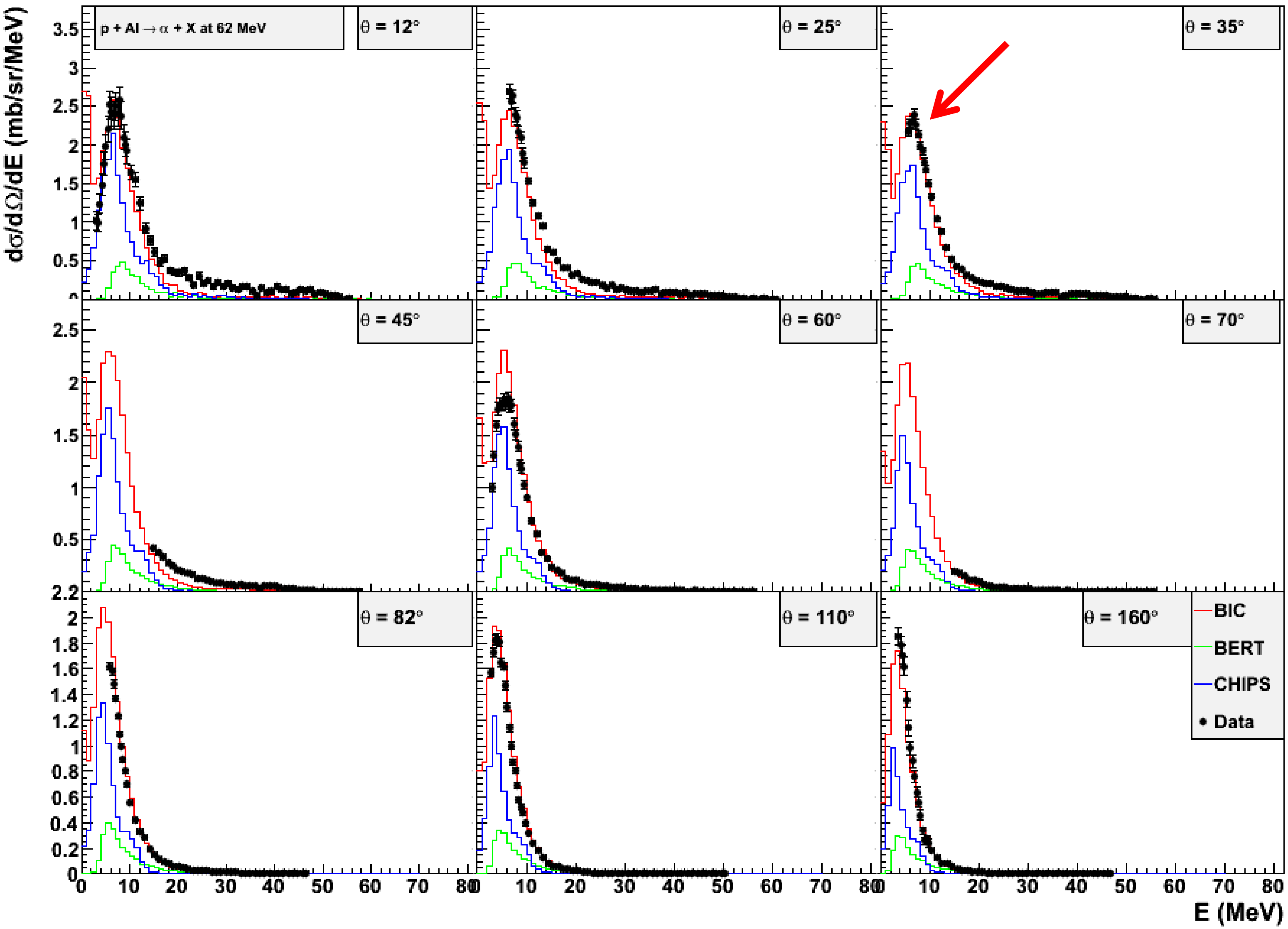
Development History and Strategy for 2010

- Fixed numerical problems in pre-Compound with FTF
- Activated MFM, Fermi Break-Up, GEM
    - Fixed new problems when this models are active
- Decreased number of photons emission
- Improved parameterisations of pre-Compound and de-excitation models
- Significant slow down of simulation have been observed
- Cleanup of the few utility classes was required in order to clean logic and improve CPU performance
    - Hundreds of other classes unchanged
- After each iteration test30, iaea and partially test35 were run

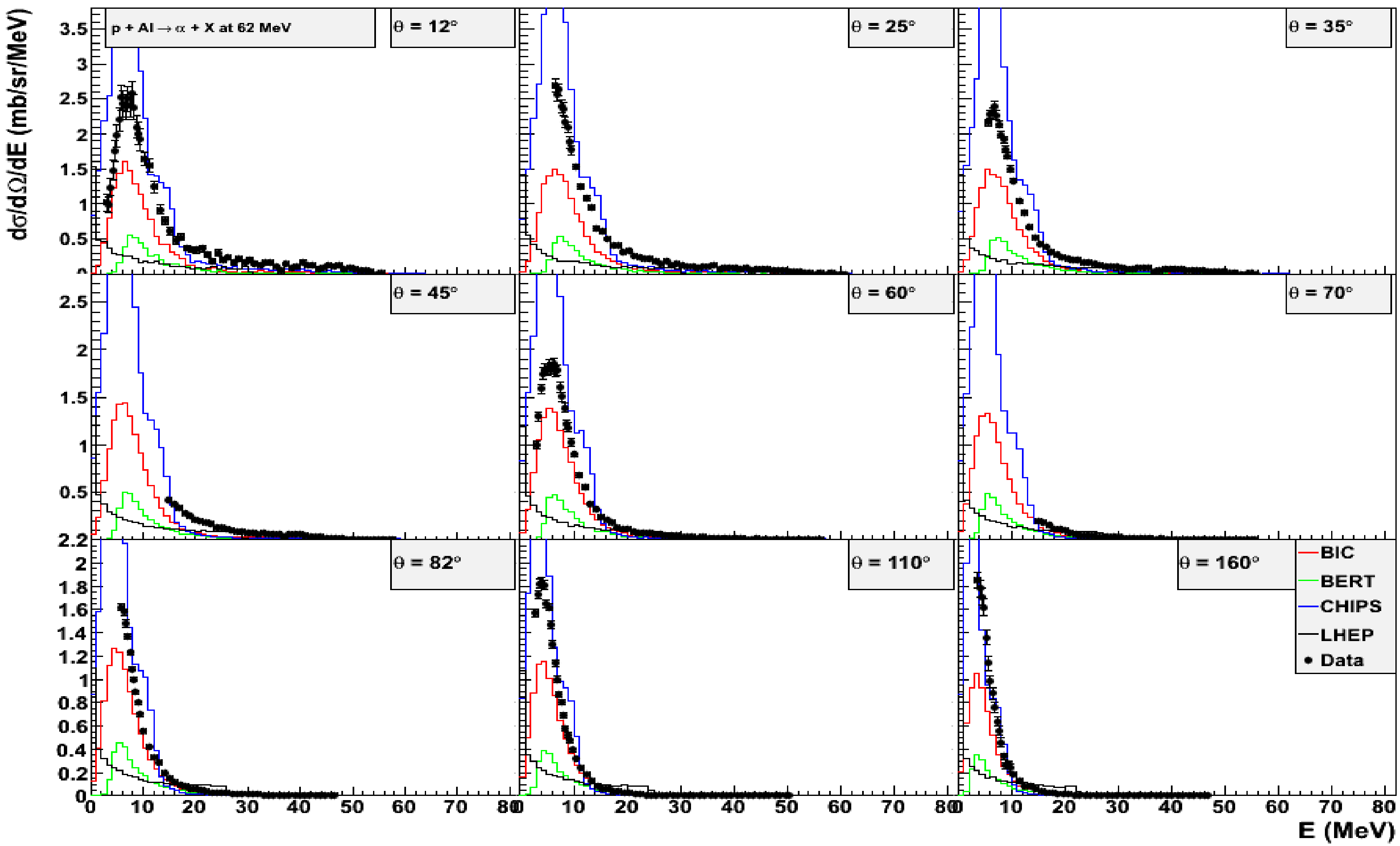
Pre-Compound Model (JMQ + VI + AI)

- Bug for proton interaction identified in Al target at low energies; J.M. Quesada has fixed parameterization of inverse probabilities for protons and light ions in pre-compound and de-excitation models
- Fixed usage of Coulomb barrier
- Fixed numerical problems in case of high initial excitation to avoid FPE Exceptions

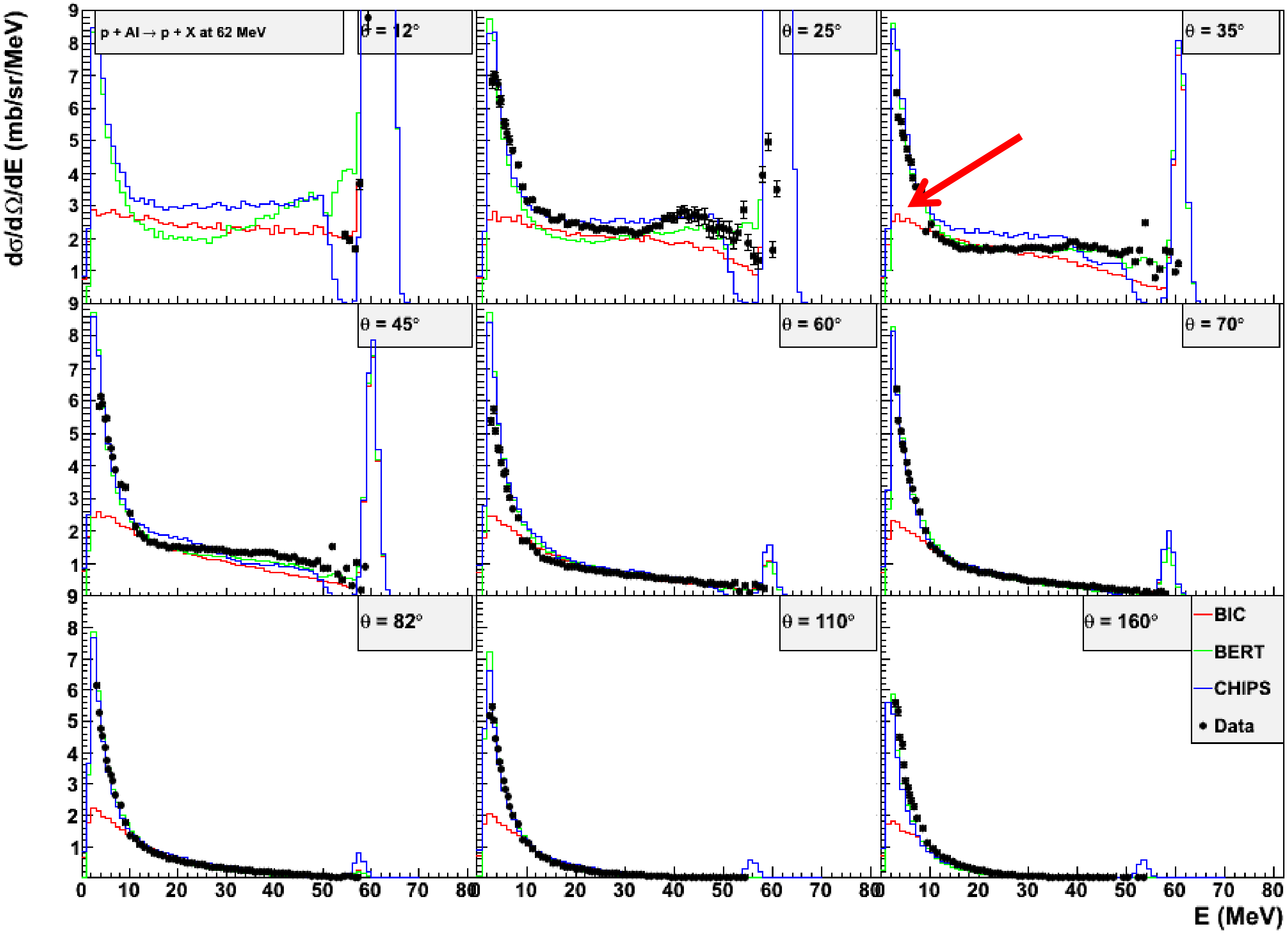
Al (p,xa) 61.5 MeV, 9.3p01



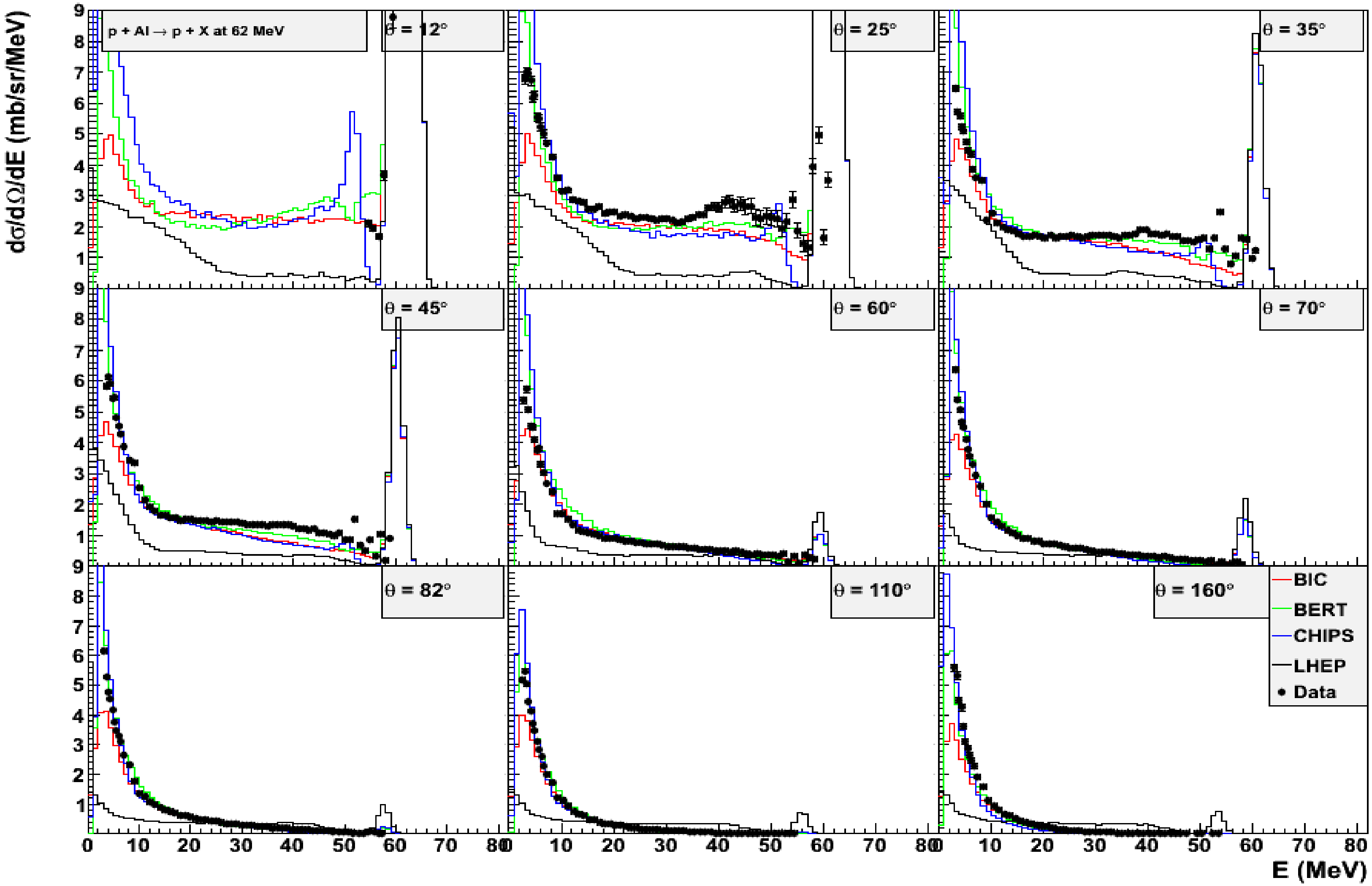
Al (p,xa) 61.5 MeV, 9.3ref04d



Al (p,xp) 61.5 MeV, patch01



Al (p,xp) 61.5 MeV, 9.3ref04d



G4Fragment (VI)

- Addition of access method to integer Z and A
    - Constructor used integer Z and A by access was via double
- Refinement of inline methods
- Refinement computation of the ground state mass and excitation energy
- Ground state mass as a member of the class
- Cleanup constructors and exceptions

G4ExcitationHandler (JMQ + VI)

- Use integer Z and A
- Use only 2 loops and 2 intermediate list of G4Fragments
  - Evaporation and photon-evaporation
  - Before there were more loops and vectors
- For the primary G4Fragment try out the MFM if excitation is above the threshold
  - Disabled for 9.4beta
- For any fragment try out Fermi Break-Up if Z and A below threshold values (9, 17)
- Removed condition A > 4 for the evaporation loop
- G4Fragment coincided as stable if
  - excitation energy below 1 keV (before was 0.1 eV)
  - it has non-zero natural abundance (new condition)

Fermi Break-Up Model (JMQ)

- The pool of fragments now is coherent with G4PHOTONEVAPORATIONDATA
- Fragments with A<5 can be decaied
- Kappa parameters is set to 6 (was 1)
- Condition of stability more loose:
  - excitation energy below 1 keV (was 0.1eV)

Multi-Fragmentation Model (VI)

- Should be applied for highly excited nuclei
- There was exceptions in FTF_BIC and QGS_BIC reported by Alberto Ribon
- Exception happens in the numerical algorithm to resolve transcendental equation for nuclear temperature – is fixed
- Unfortunately, there are still problems:
  - CPU profile demonstrate that MFM dominates
  - 4-momentum balance is violated
- By default MFM is disabled for 9.4beta

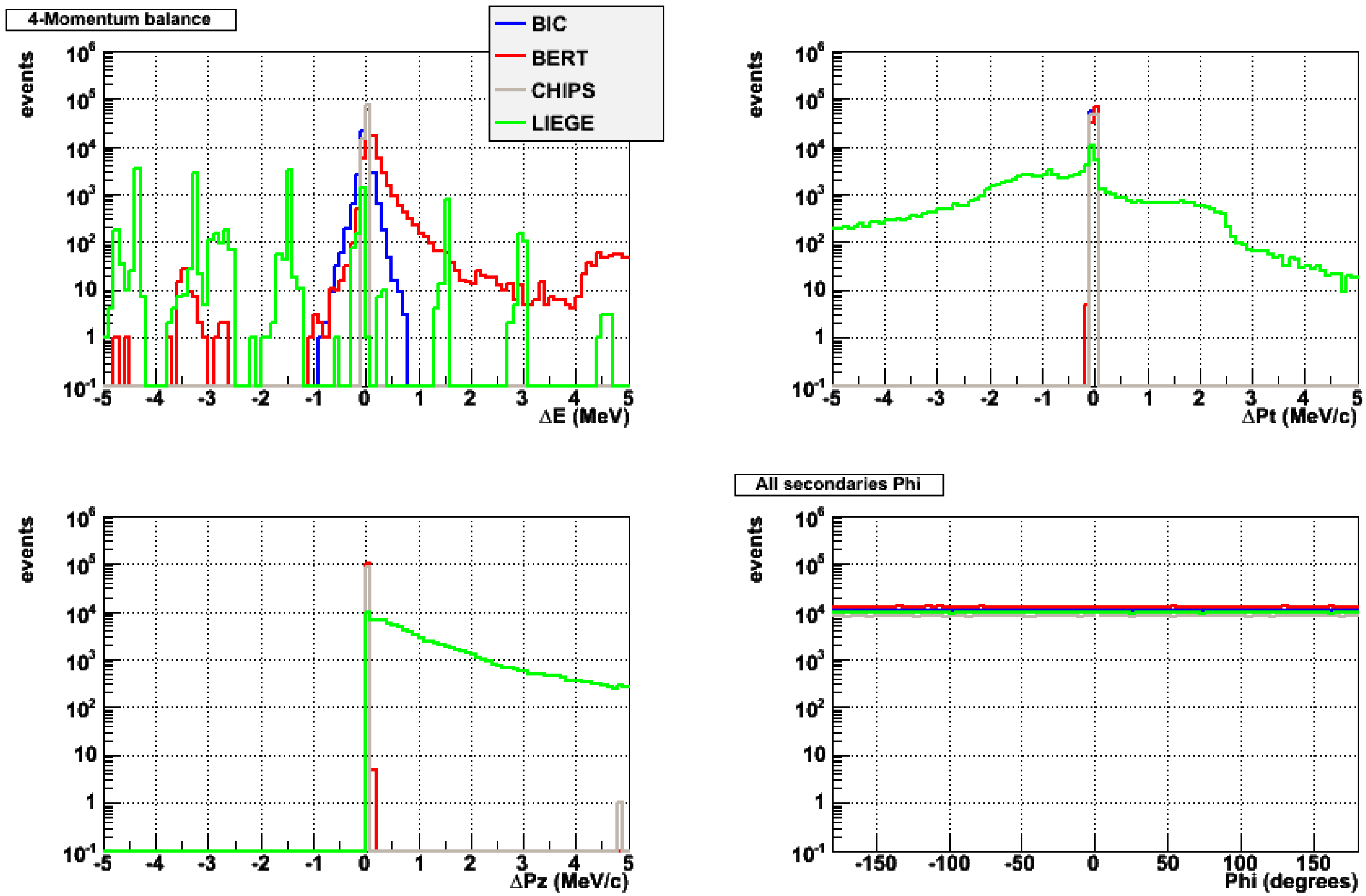
G4Evaporation (VI)

- Constructor rewritten
  - Array of probabilities is created at initialisation
  - Order of channels changed – photon evaporation is first, fission – second, after all other channels in same order as before
- Main method completely rewritten
  - Integer Z and A
  - Minimized "new" and "delete" of intermediate objects
- New class G4UnstableFragmentBreakUp is called to decay exotic residual fragments (2n, 2p, ….)
  - A channel with maximum energy deposition is selected
  - No sampling of probabilities

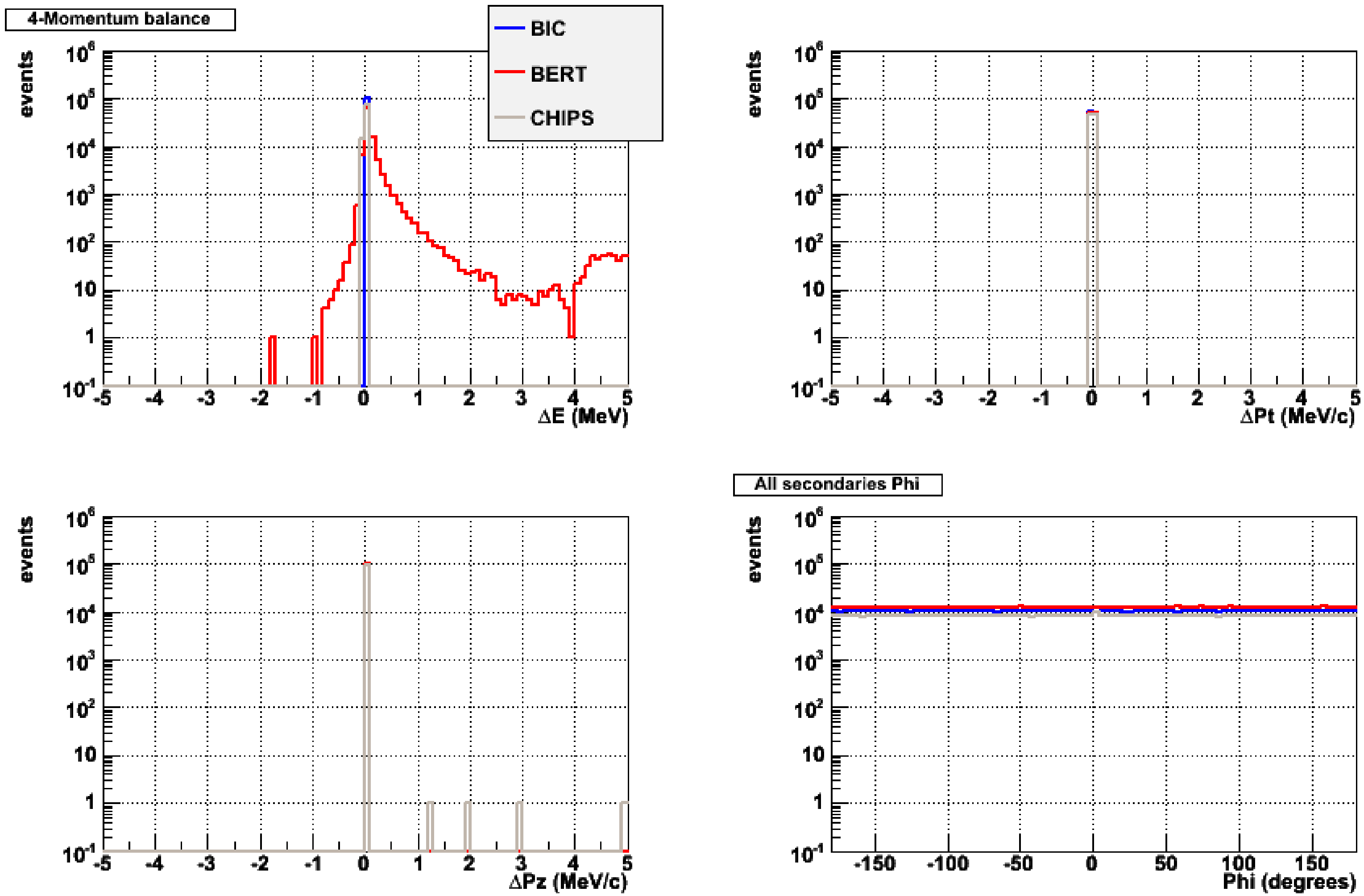
G4PhotonEvaporation (JMQ + VI)

- Messy design with many small classes which were instantiated each other at each call to photon evaporation
- First round of the cleanup was done for the main methods and new methods were introduced for G4PhotonEvaporation
- Kinematics of photon emission in G4VGammaDeexcitation is rewritten
  - 4-momentum balance in the Binary Cascade
- Fixed energy of photons
- Fixed energy of e- and code logic if internal conversion is selected

Al (p,xn) 1.5 GeV, 9.3p01



Al (p,xn) 1.5 GeV, 9.3ref05



CPU performance for simple geometry

20 GeV P off Pb target

Physics List	9.3p01	9.3ref05
LHEP	183	174
QGSP_BERT	239	219
QGSP_BERT_EMV	111	115
QGSP_BERT_EMX	189	184
QGSP_FTFP_BERT	265	245
FTFP_BERT	248	230
CHIPS	646	594
QBBC	335	232
QBCC_XGGSN	315	230

Comments:

- Multiple scattering still dominating factor
- "ApplyCuts" option is important
- QGSP_BERT speed-up due to Bertini clean up?
- QBBC become as fast as QGSP_BERT
  - mainly due to disabling of MFM
- Fermi Break-Up and GEM are enabled

What can be done to improve CPU performance of pre-Compound/de-excitation after 9.4beta?

- Profiler results for test30 shows that CPU is mainly spend by utility classes of the Binary Cascade, likely due to frequent computation of exp and log
  - Current CPU profile:
  - http://vnivanch.web.cern.ch/vnivanch/verification/verification/hadronic/test30/geant4-09-03-ref-04prof/pn_pb_113/pb_113_prof.txt
    - There is an opportunity to speedup (in particular, using cache)
- In summary pre-Compound classes are second
    - Cleanup may be transparent
- Photon emission probability computation
    - There concerns to physics
- Base GEM method to compute probability is visible
- Fermi Break-Up not seen anymore