Monte Carlo code overview and comparison

pCT workshop

November 22, 2016

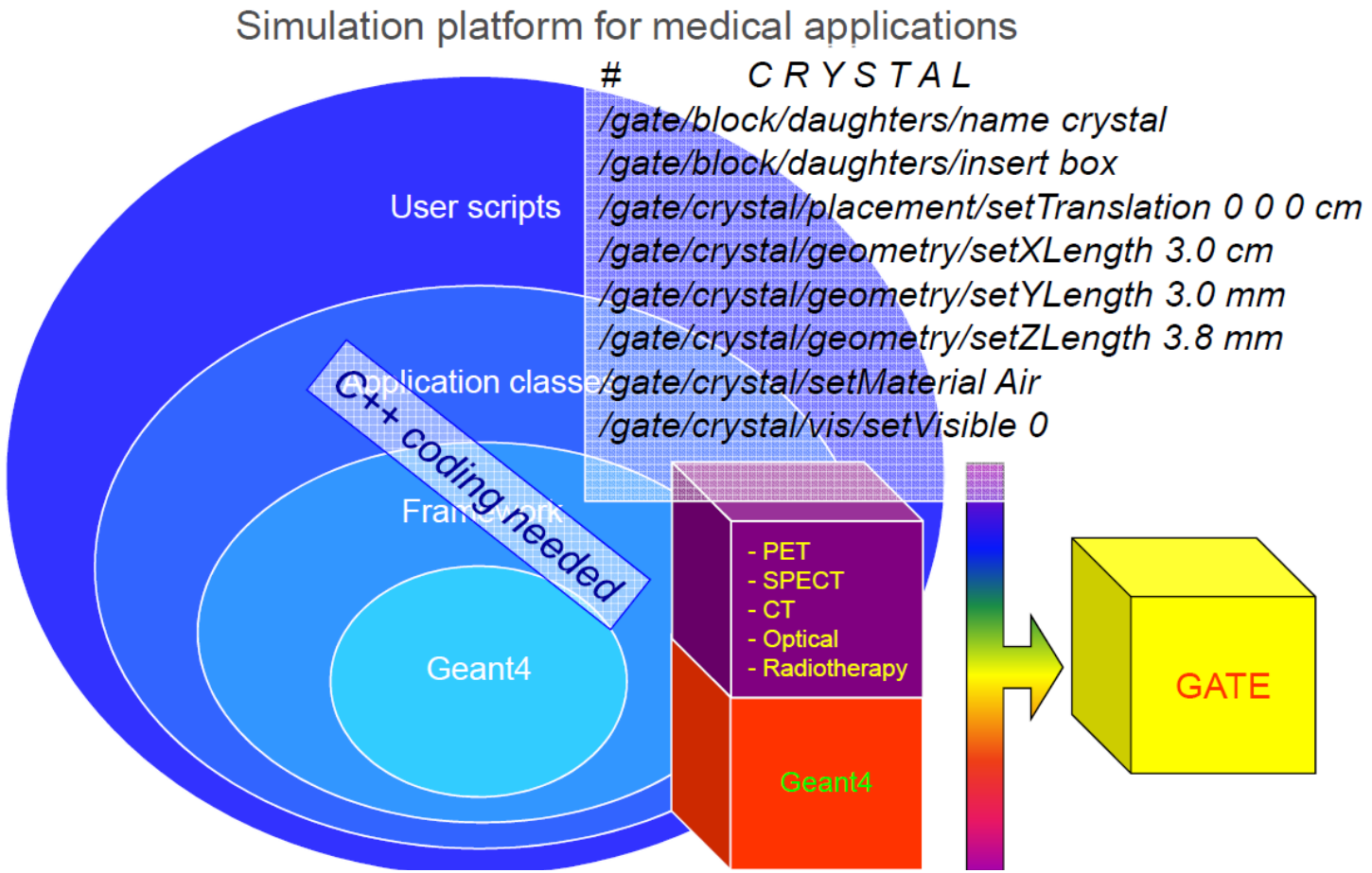
Department of Physics and Technology, Bergen, Norway

Monte Carlo code overview

- GATE 7.2 (OpenGATE Collaboration)
  - Open source
  - www.opengatecollaboration.org
- MCNP6.1 (Los Alamos National Laboratory, USA)
  - Quasi-open source
  - Distributed by RSICC, ORNL
- FLUKA 2011.2c-5 (FLUKA collaboration)
  - Open source
  - www.fluka.org

GATE 7.2

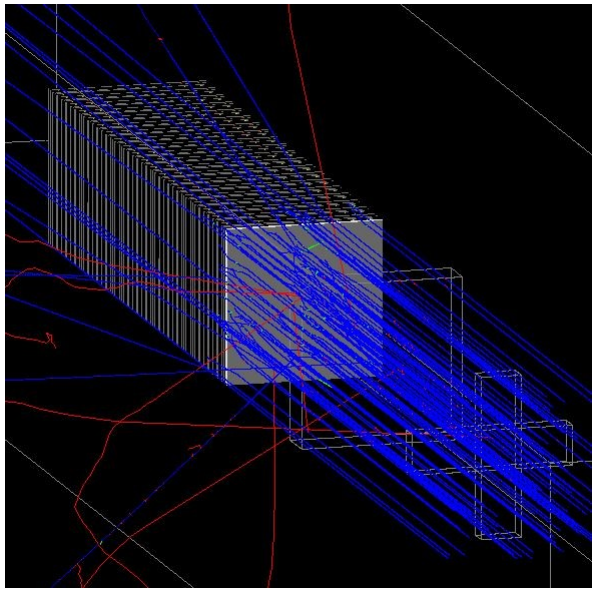
- Scanner geometry
- Phantom geometry
- Set up the physics proc.
- Initialization
- Detector model
- Source(s)
- Data output format
- Start acq.

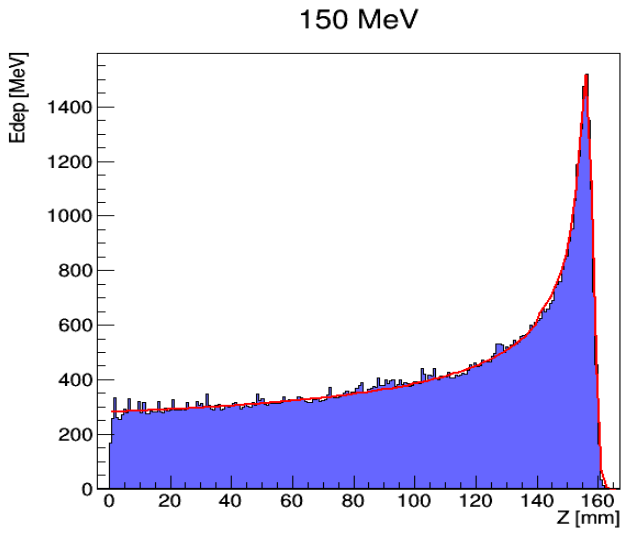


GATE 7.2

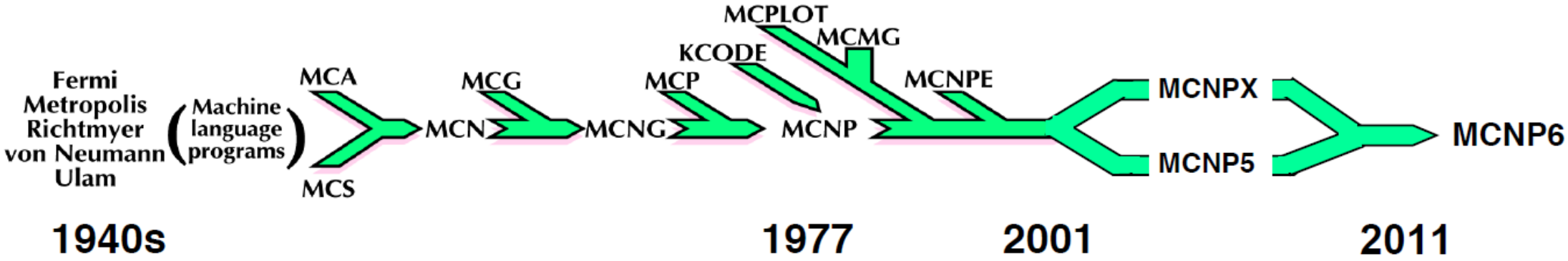
- GEANT4 made easy!
  - Less steep learning curves
- Leptons, baryons, mesons
- Generic ions
- Full analysis possible in ROOT
- Supports parallel computation
  - CPU (Multi-thread & Multi-CPU)
  - GPU

```
/gate/geometry/setMaterialDatabase ../GateMaterials.db

/gate/world/geometry/setXLength 1000. cm
/gate/world/geometry/setYLength 1000. cm
/gate/world/geometry/setZLength 300. cm

/gate/world/daughters/name scanner
/gate/world/daughters/insert box
/gate/scanner/geometry/setXLength 900. cm
/gate/scanner/geometry/setYLength 900. cm
/gate/scanner/geometry/setZLength 250. cm
/gate/scanner/setMaterial Air
/gate/scanner/vis/forceWireframe

/gate/scanner/daughters/name waterbox
/gate/scanner/daughters/insert box
/gate/waterbox/geometry/setXLength 800. cm
/gate/waterbox/geometry/setYLength 800. cm
/gate/waterbox/geometry/setZLength 100. cm
/gate/waterbox/placement/setTranslation 0. 0. 50. cm
/gate/waterbox/setMaterial Water
/gate/waterbox/vis/forceWireframe

/gate/waterbox/attachCrystalSD

#===============#
# Physics       #
#===============#

/gate/geometry/setIonisationPotential Water 75 eV
/gate/physics/addPhysicsList QGSP_BIC_EMY
/gate/physics/SetMaxStepSizeInRegion scanner 0.1 mm
/gate/physics/ActivateStepLimiter proton

/gate/run/initialize

#======================#
# ADD PROTON BEAM      #
#======================#

/gate/source/addSource uniformBeam gps
/gate/source/uniformBeam/gps/particle proton
/gate/source/uniformBeam/gps/ene/type Gauss
/gate/source/uniformBeam/gps/ene/mono {energy} MeV
/gate/source/uniformBeam/gps/ene/sigma {sigma} MeV
/gate/source/uniformBeam/gps/type Plane
/gate/source/uniformBeam/gps/shape Square
/gate/source/uniformBeam/gps/direction 0 0 1
/gate/source/uniformBeam/gps/halfx 25. mm
/gate/source/uniformBeam/gps/halfy 25. mm
/gate/source/uniformBeam/gps/centre 0. 0. -15. cm # -20 cm for scintillator

/gate/output/root/enable
#/gate/output/root/setFileName ../../focalCode/Data/WaterBox/tungsten_{ener
/gate/output/root/setFileName GATE

/gate/random/setEngineName MersenneTwister
/gate/random/setEngineSeed auto
/gate/application/setTotalNumberOfPrimaries {npart}
/gate/application/start
exit
```





MCNP6.1



- MCNP5 – neutrons, photons, electrons
- MCNPX – neutrons, photons, electrons + 33 other particle types
- MCNP6 – merged code + more, released 2012
- Features of interest for radiotherapy applications
  - Full particle tracking options
  - Radiography scoring
  - 3D unstructured mesh

MCNP6.1

- Input scripts of varying complexity
- Define
  - Cells
  - Surfaces or macrobodies
  - Physics
  - Materials
  - Source(s)
  - Built-in or user defined scoring
- Does not support parallel processing for protons and heavy ions

Title Line ... (required)

Cell Cards ...

blank line separator

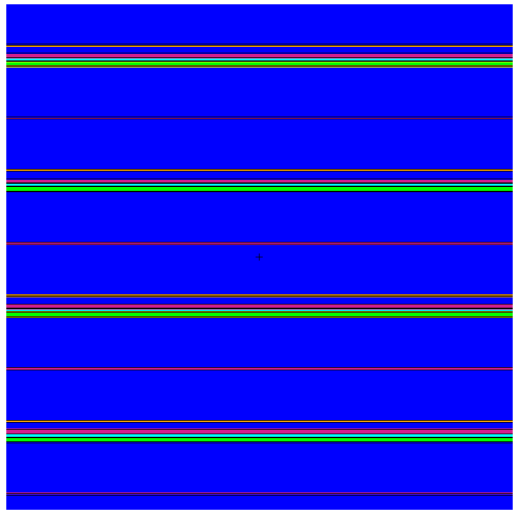
Surface Cards ...

blank line separator

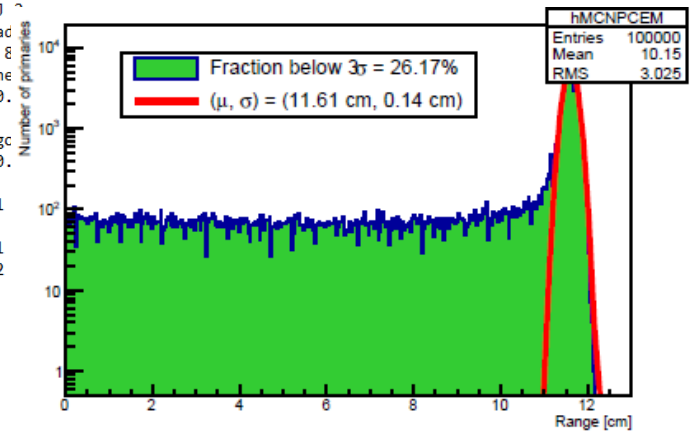
Data Cards ...

blank line terminator (optional)

... any following lines are ignored - useful for notes or saving options



```
     190MeV proton-beam in water
1    0 100              imp:h=0
c
c    Incident upon a water or polystyrene phantom.
c
82   1 -1.0  -5  6 -86 imp:h=1
94   0 -100 #82       imp:h=1

5    cz  50.0
6    pz   0.0
86   pz  40.0
100  so 200.0

mode    h
c       mode    h / z k | n a d t s # p
c       n = neutron
c       p = photon
c       e = electron
c       / = positive and negative pions Mass=139.57MeV lifetime=2.6033e-8
c       z = neutral pions Mass=134.98MeV lifetime=8.4e-17
c       k = positive and negative kaons Mass=493.68MeV lifetime=1.2386e-8
c       h = proton and antiproton Mass = 938.27MeV
c       | = muons
c       a = alphas
c       s = helium3
c       d = deuteron
c       t = triton
sdef    erg=190 x=d1 y=d2 z=-1.0 vec=0 0 1 dir=1 par=h
si1     -3.5  3.5
sp1      0    1
si2     -3.5  3.5
sp2      0    1
c       EMAX EAN TABL  J  ISTRG  J  RECL  J  J  J  MCS  INT  ELS  EFAC
phys:h  195  0    0    j    0    j  0    j  j  j  0    0    0    0.98
ptrac  FILE=ASC MAX=10000000 WRITE=ALL EVENT=TER TYPE=h NPS=1,100000
c      PROBLEM CUTOFFS
cut:h j 0
c cut:e  j 0.01
c cut:p  j 0.01
c       New model 26f
c       LCA     9j 0
c       INCL4 from Ben for proper neutron production
c       LCA     8J
c       Water degrad
m1      1001.24h 2 8
c       (Polystyrene
m2      1001.24h -0.
mx2:h   1001
c       Air w/o Argo
m4      7014.24h -0.
c       Tungsten
m3      74184.24h 1
c       Aluminum
m5      13027.24h 1
prdmp   1e5 1e4 1 2
rand seed=584113
nps     1e5
```

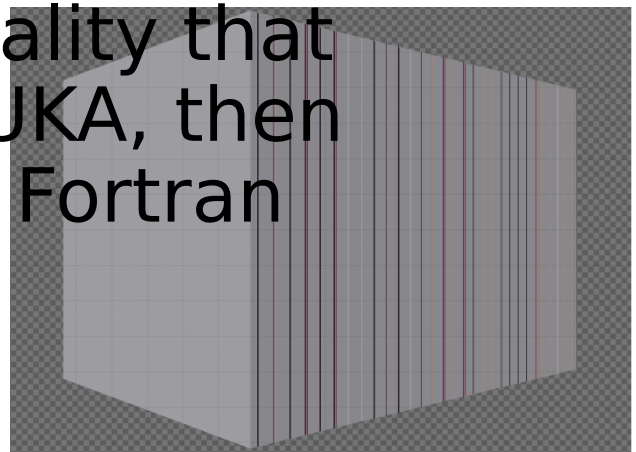


FLUKA 2011.2c-5

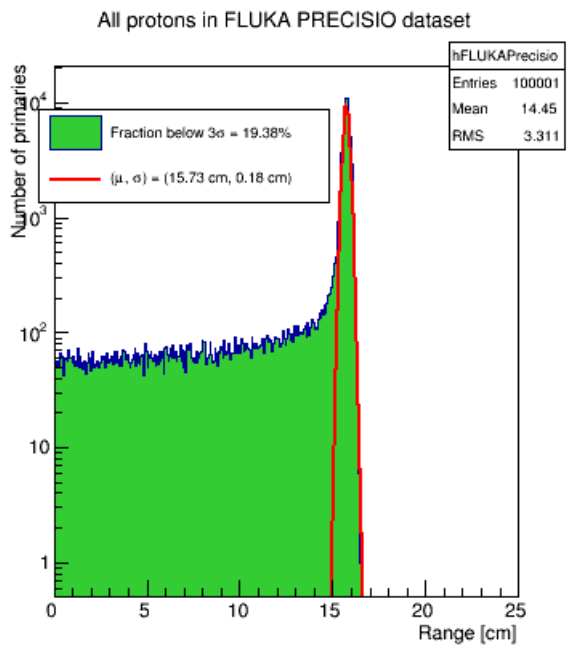
- Multipurpose interaction and transport MC code
- Developed and maintained by INFN and CERN
- > 5000 users
- Applications
  - Neutrino physics, cosmic ray physics, accelerator design etc…
  - Dosimetry, hadrontherapy
- 60 different particles + heavy ions
- Can be used freely for scientific and academic purposes
- Flair – Advanced FLUKA interface

FLUKA 2011.2c-5

- Input scripts (use Flair for FLUKA !!!)
- Define
  - Defaults
  - Beam
  - Geometry
  - Material assignment
  - Scoring
- If you need functionality that is not covered in FLUKA, then you need to code in Fortran 77 and re-link !
  - User routines

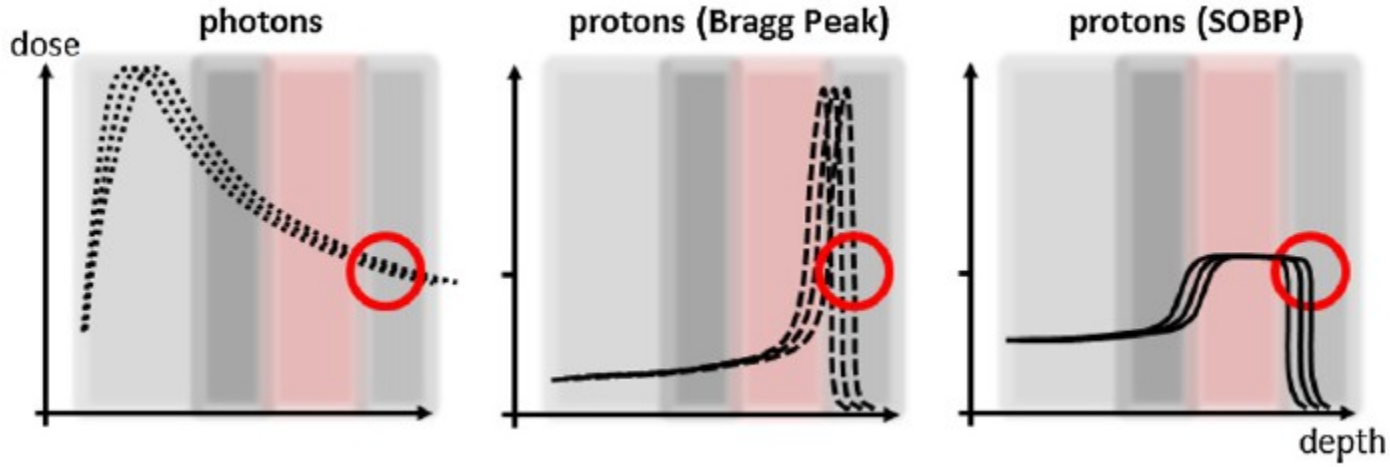


```
TITLE

* Set the defaults for precision simulations
DEFAULTS                                                              PRECISIO
* Define the beam characteristics
BEAM           -0.05                            7.0       7.0         PROTON
* Define the beam position
BEAMPOS                                 -0.1
GEOBEGIN                                                              COMBNAME
    0    0
* Black body
SPH blkbody    0.0 0.0 0.0 1000.0
* Void sphere
SPH void       0.0 0.0 0.0 500.0
* Cylindrical target
RPP target     -20.0 20. -20. 20. 0.0 40.0
END
* Black hole
BLKBODY      5 +blkbody -void
* Void around
VOID         5 +void -target
* Target
TARGET       5 +target
END
GEOEND
* 276 Water liquid H2O
* Chemical Formula:  H -- O -- H
MATERIAL                                 1.0                          WATER
COMPOUND         2.0  HYDROGEN
MAT-PROP                                   7
MATERIAL                                .00120
COMPOUND   -0.000124     CARBON -0.755
COMPOUND   -0.012827      ARGON
* ..+....1....+....2....+....3....+..
ASSIGNMA    BLCKHOLE    BLKBODY
ASSIGNMA      VACUUM       VOID
ASSIGNMA       WATER     TARGET
USERDUMP        100.        30.
*USRBIN          10.   BEAMPART
*USRBIN         -20.       -20.
*USRBIN           0.0  BEAMPART
*USRBIN         -20.       -20.
*USRBIN           0.0     ENERGY
*USRBIN         -20.       -20.
*USRBIN           0.0     ENERGY
*USRBIN         -20.       -20.
* Set the random number seed
RANDOMIZ         1.0
* Set the number of primary histories
START            1E4
STOP
```



MC code comparison

- MC simulations are the gold standard in radiotherapy physics!
- Beamline and nozzle design
- Dosimetry (improvement of pencil beam algorithms)
- Secondary neutron doses
- Shielding design



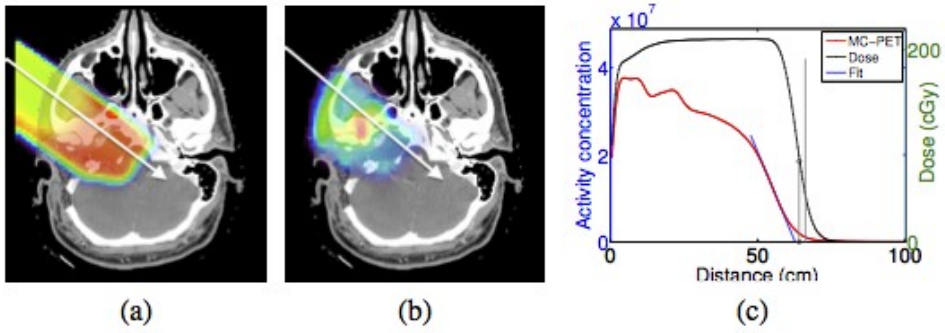
- Knopf and Lomax, 2013

etector and detection system design and develop

Prompt gamma-ray, PET & Bremsstrahlung imaging

Proton CT !

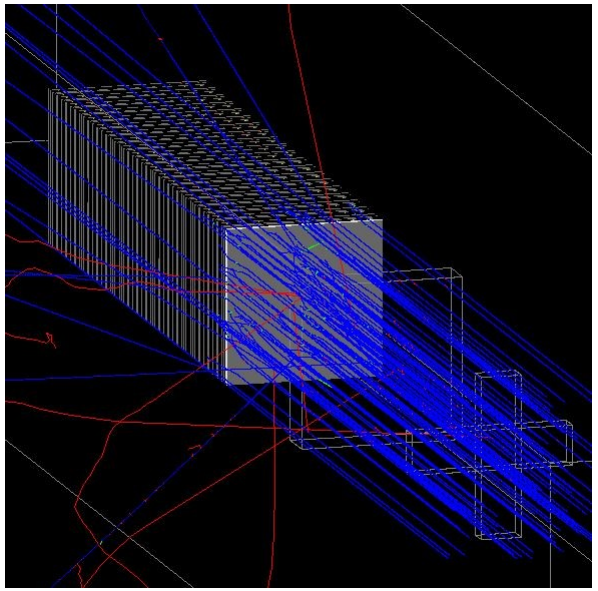
- Look-up tables for converting range to energy and vice versa
- Optimal absorber material / thickness
- Synthetic data for image reconstruction etc...

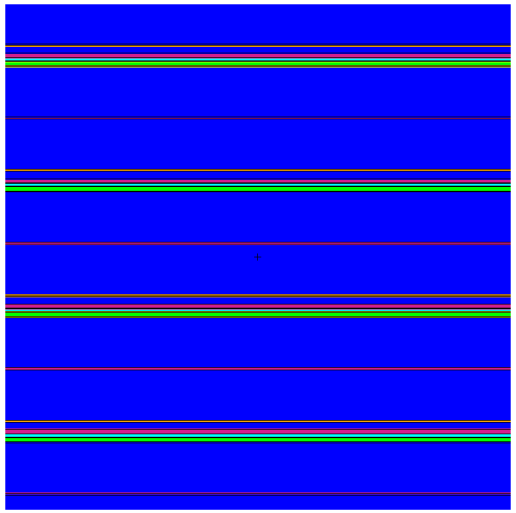


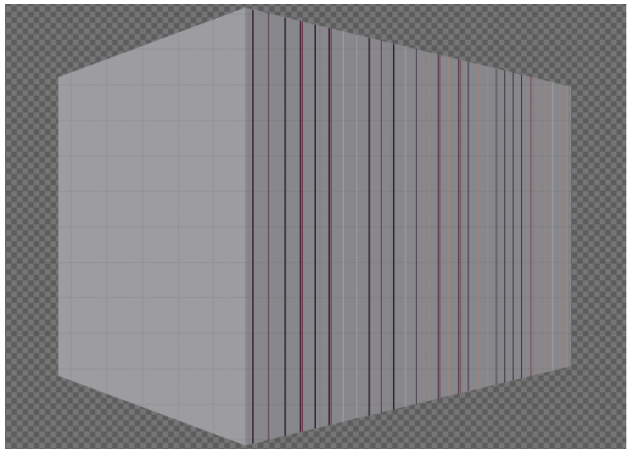
- Courtesy of Gordon Center for Medical Imag

MC code comparison

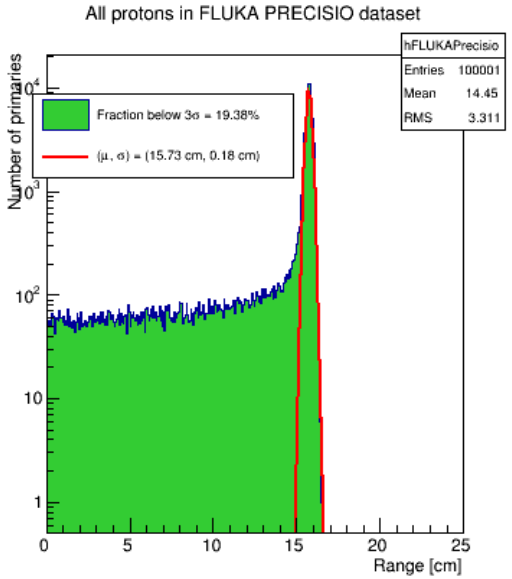
- Range and longitudinal / lateral straggling in relevant materials using FLUKA, MCNP6 and GATE?
- Simple geometries / homogeneous blocks of water and Al
- Detector geometry (10 x 10 cm^2 , 4.3 mm Al absorbers, 120 µm Si-chips)
- Monoenergetic protons
- Beam size, 7 x 7 cm^2
- MCNP6
  - No tabular sampling, only nuclear models
  - Proton cut-off energy 1 keV
  - Vavilov model for charged particle straggling
  - Nuclear elastic scattering is turned on
- FLUKA
  - Default physics models (PRECISIO)
  - Particle transport threshold set at 100 keV
  - All secondaries are simulated
- GATE
  - Physics List – QGSP_BIC_EMY (Hadronic models, ion cascade, em models)
  - Maximum step size 0.1 mm
  - Production cut-off 0.01 mm, max-step

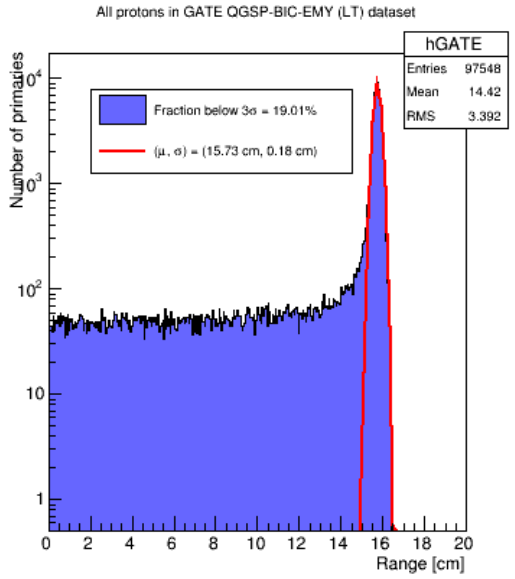


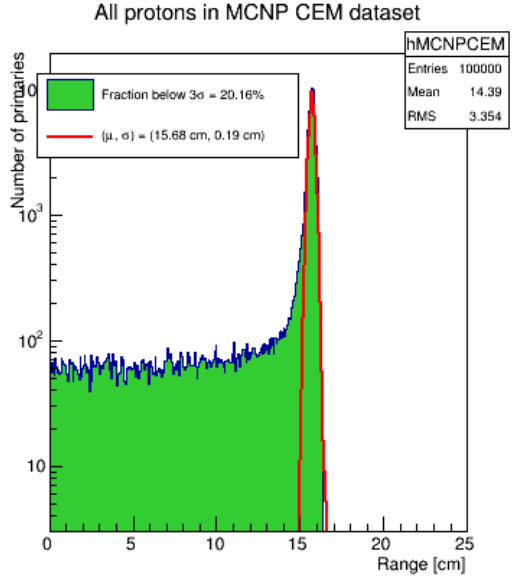




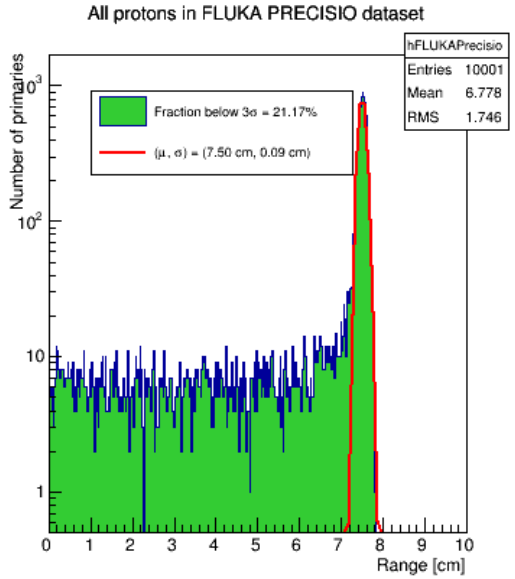
MC code comparison

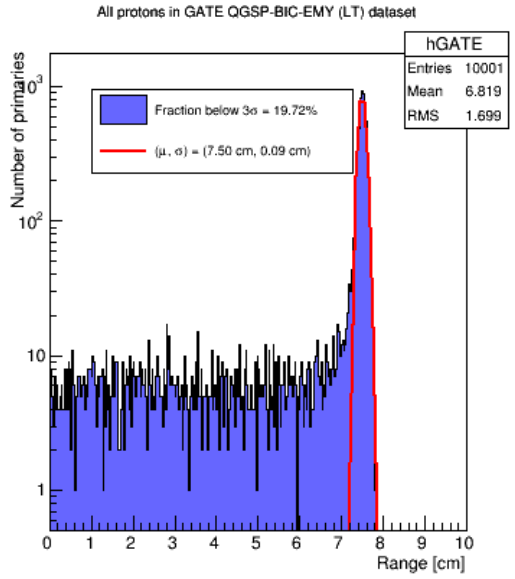


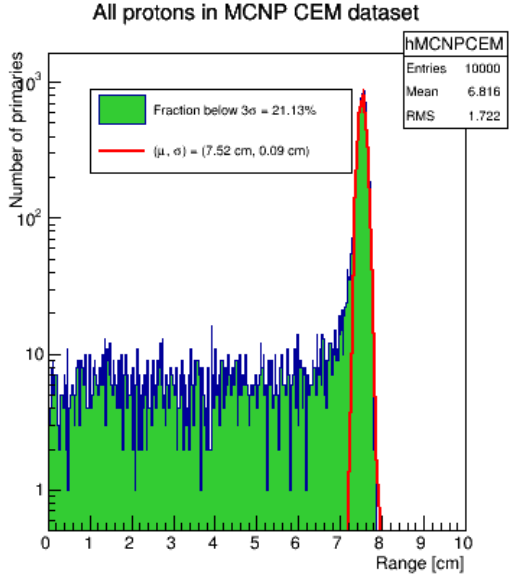




- 100k protons in water
- Monoenergetic, 150 Me

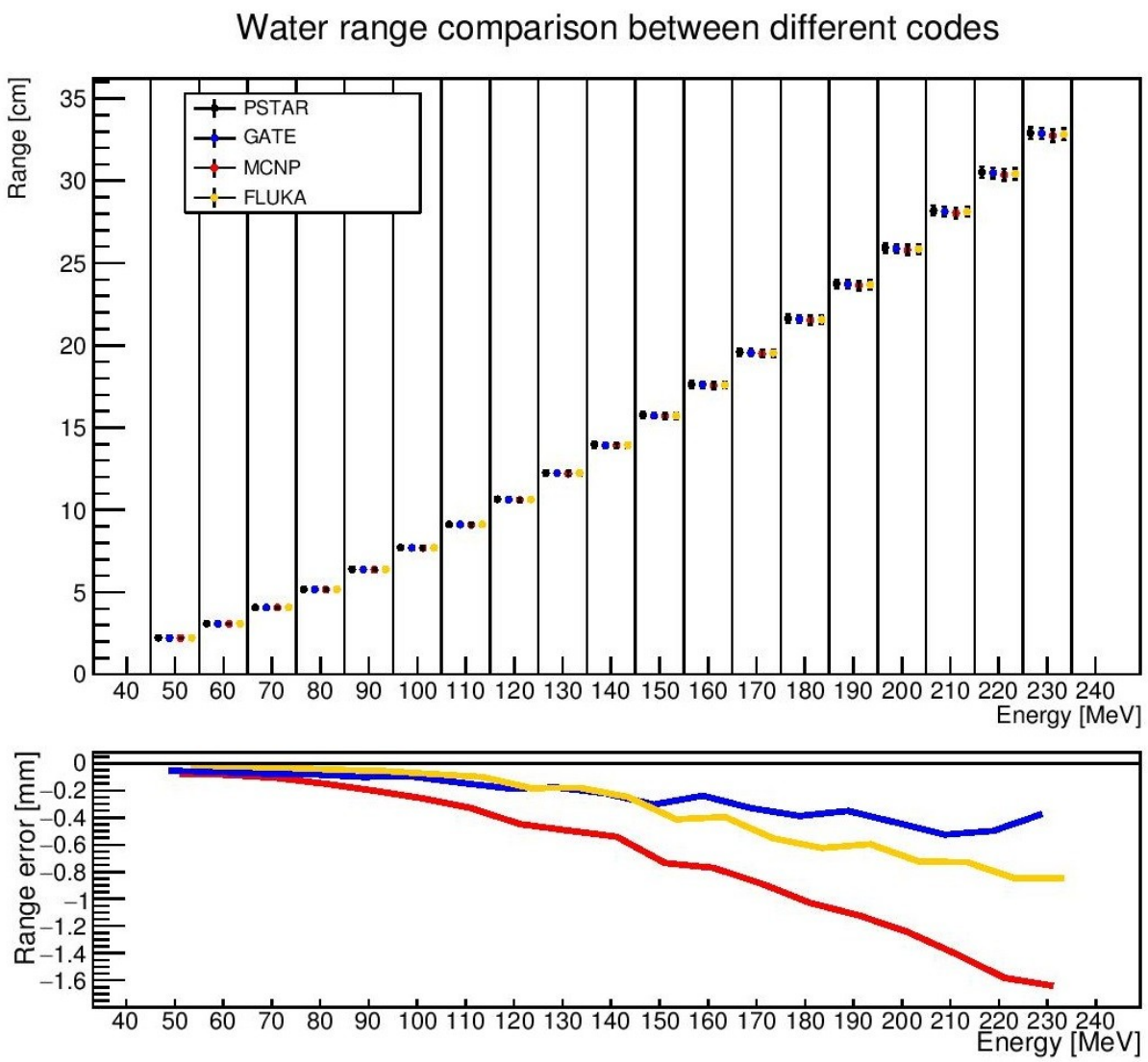


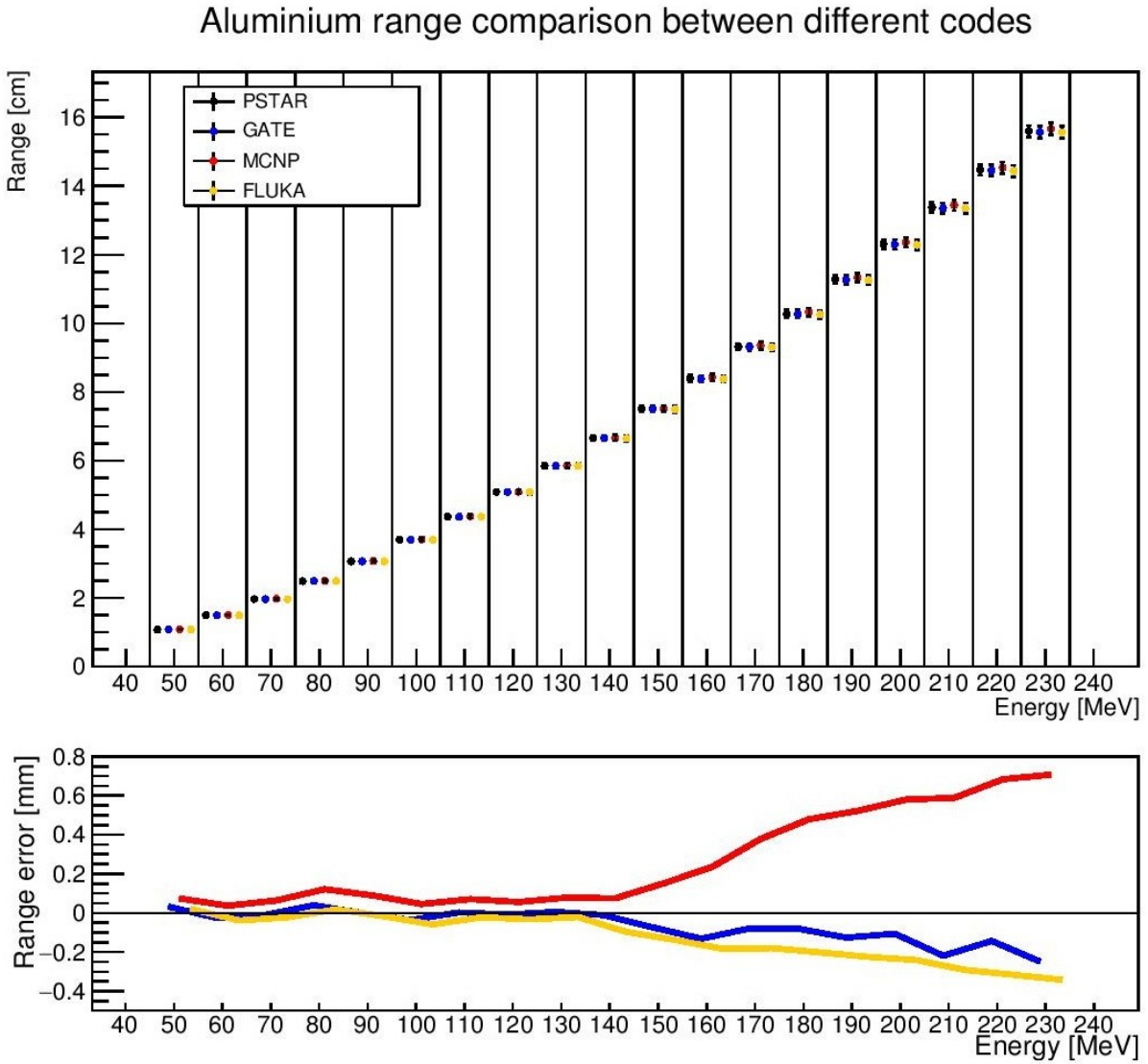




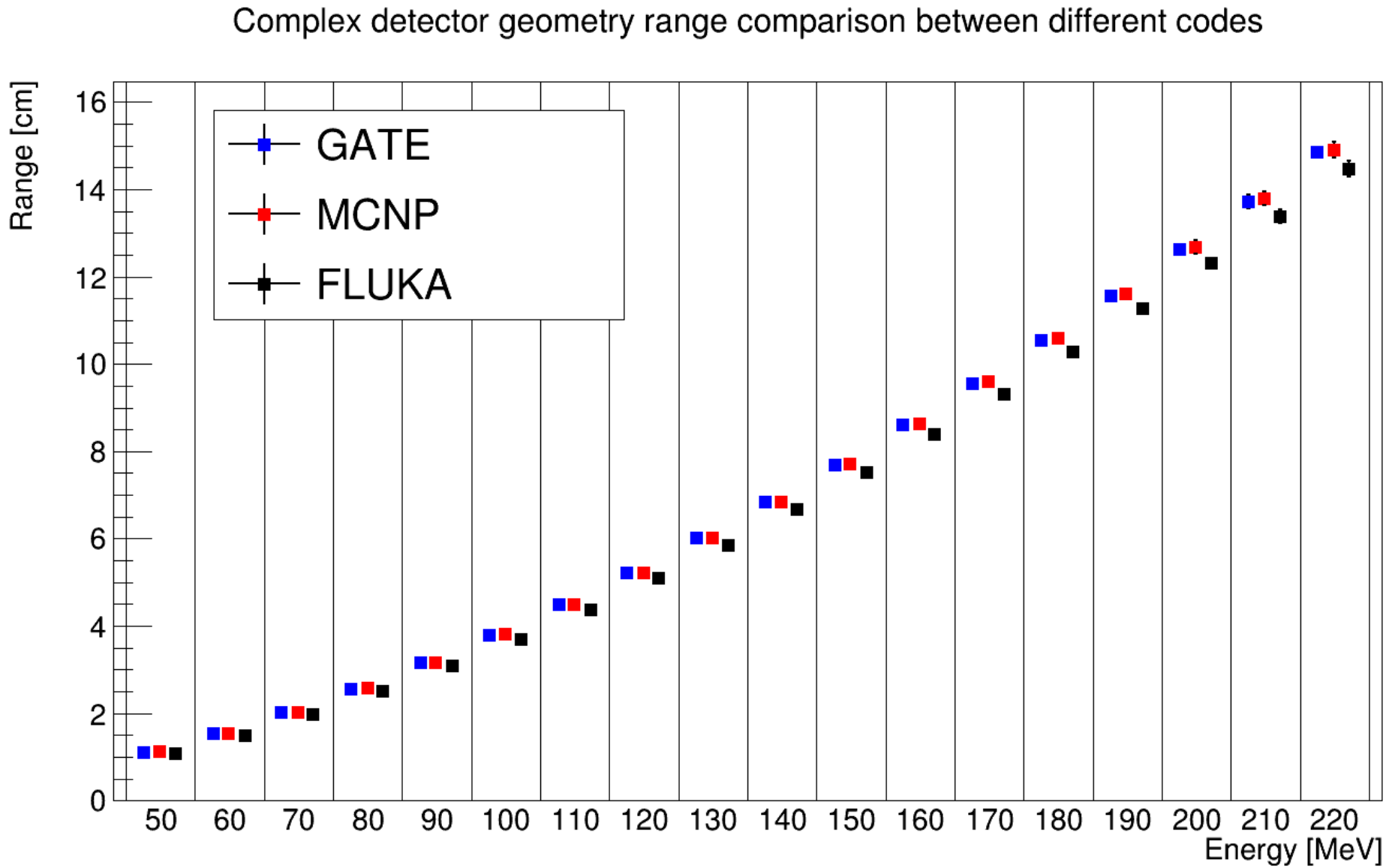
- 10k protons in Al
- Monoenergetic, 150 Me

MC code comparison





MC code comparison



MC code comparison

- MC calculated mean proton ranges in homogeneous materials agree to within ± 1σ, i.e. to within expected range straggling (all codes)
- The largest difference does not exceed 0.7% of the nominal range.
- Differences most likely due to use of different I-values in MCNP – to be investigated further
- GATE and MCNP agree to within ± 1σ in the detector geometry. FLUKA does not
- Major conclusion be very careful and tune your parameters when doing cross-checks with different codes !!!