Geant4 validation on proton stopping power

Tsukasa Aso
Toyama National College of Maritime Technology,
JST CREST
Introduction

• The validation of proton physics models with respect to reference data is a critical issue

• Proton physics is fundamental for space and medical application
  – i.e. Proton radiation therapy demands rigorous comparisons for patient’s safety
    – Position determination < 1 mm
    – Dose determination < 5 %

• Bragg peak distribution must agree between the simulation and the measurement
  – Bragg peak consists of many physics processes such as ionization, multiple scattering, hadronic process etc.
Bragg peak and processes

Proton Bragg peak in Water

- (1) Ionisation energy loss
- (2) (1)+Energy fluctuation
- (3) (2)+Multiple Coulomb Scattering
- (4) (3)+Hadron elastic scattering
- (5) (4)+Hadron inelastic scattering

Observables
- Peak position (Range)
- Width of peak
- Peak to Plateau ratio

Basis of observable quantities
- Stopping power ~ Range
- Excitation energy of material
- Best interaction models
Previous works

- Validation
  - “Comparison of Geant4 Electromagnetic Physics Models Against the NIST Reference Data” had already been published in IEEE TNS 52-4(2005)910-918, K.Amako et al., under the condition without multiple scattering and energy fluctuations

- Our previous work
  - “Verification of the Dose Distributions with Geant4 Simulation for Proton Therapy”, IEEE TNS, 52-4(2005) 896-901
    - The agreement is better than 0.1%, 0.3%, and 0.2% for water, lead, and aluminum, respectively
    - There was a long story to reach these results
    - It must be understood systematically

Using Low energy EM with SRIM2000, transition energy 10 MeV.

Range cut 3 micron.
100 micron sliced geometry

Lines : PSTAR NIST
Red symbols: Simulation

\[ G4\text{v7} \]
This work

- Study of more detail comparison concentrating on proton stopping power for sub-millimeter scale consistency
  - Proton range validation to NIST/ICRU reference value
    - Using Stopping power models
    - Range cut / step limit dependencies
    - Std EM and Low EM differences

- The validation is done in terms of “Proton range”
Electromagnetic physics models in Geant4

- Geant4 electromagnetic processes

- Many choice of stopping power parameterisations for protons

### Standard EM
- Multiple scattering
- Bremsstrahlung
- Ionisation
- Annihilation
- Photoelectric effect
- Compton scattering
- Rayleigh effect
- Gamma conversion
- E+e- pair production
- Synchrotron radiation
- Transition radiation
- Cherenkov
- Refraction
- Reflection
- Absorption
- Scintillation
- Fluorescence
- Auger

### Low Energy EM
- Ionisation energy loss
  \[ \text{dE/dX table} + \text{Energy fluctuation model} \]

### Ionisation
- Bethe-Bloch formula
- Below 2 MeV by default
- NIST for NIST material (G4_Water) [v8.x]
- ICRU49 (ChemicalFormula)
- Bragg rule (ICRU49 element)

### Proton Ionisation
- Stopping power

- Specialized according to
  - the particle type
  - energy range of process

- Many choice of stopping power parameterisations for protons

- Proton Ionisation:
  - Stopping power

- Ziegler1977 (Bragg rule)
- ICRU49 (ChemicalFormula)
- Ziegler1985 (Bragg rule)
- SRIM2000 (Bragg rule)
- Bragg rule (ICRU49 element)

### ICRU composite material
- \( \text{Al}_{20.3}, \text{CO}_{2}, \text{CH}_{4} \)
- \( \text{Al}_{20.3}, \text{CO}_{2}, \text{CH}_{4} \)
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- \( \text{Al}_{20.3}, \text{CO}_{2}, \text{CH}_{4} \)
Range study(1) : Validation of stopping power

- 100 microns sliced water phantom
- 200 MeV proton
- CSDA range
  - Only Ionisation process
    - Multiple scattering, Hadronic interaction (Elastic/Inelastic) are turned off
    - Range cut is set to 3 micron
  - Count number of protons in each layer

\[ dz = 100 \text{ micron} \]
Comparison of STD EM with Low EM

G4v7

200 MeV proton

Proton survival probability

w/ MeanExcitationEnergy = 75 eV (ICRU)
e-,e+,gamma = 3 um
RED G4hIonisation
BLK G4hLowEnergyIonisation
w/o ChemicalFormula("H_2O")
NuclearStoppingOff
i.e. Bragg rule is applied

Depth in water (mm)

ICRU 259.6 mm

200 MeV proton

Under specified circumstances:

- Low energy EM process gives consistent range with NIST PSTAR prediction
- Standard EM process gives shorter range than NIST PSTAR prediction

Discussion will be back later, but let’s adopt Low EM for study
Comparison of stopping power functions

G4v7
200 MeV proton in Water

Low EM:
- Bragg rule
- ICRU param.?

ICRU49 259.6 mm

G4hLowEnergyIonisation
- BLK: Bragg rule
- NuclearStoppingOff

BLU: ICRU H_2O parameterization
- NuclearStoppingOff

GRN: ICRU H_2O parameterization
- NuclearStoppingOn

diff. ~ 500 micron

Low energy EM process + ICRU Bragg rule

Low energy EM process + ICRU parameterization function for water
Proton Range in water - Ionization Loss Table -

At low energy region,
- RED: Bragg rule
- GRN: ICRU49 param. function

Energy loss in Bethe-Bloch formula is factored to ensure a smooth transition to the low energy model.

Energy loss with ICRU49 parameterisation tends to be overestimated than Bragg rule’s calculation at the kinetic energy range from 100s MeV to 1 MeV.
Correction Factor: ParamB

The collection factor to the Bethe-Bloch formula is called as "ParamB" in low energy EM.

\[
e_{\text{loss}}^* = (1 + \text{paramB} \times \text{kinetic\_energy} / \text{Transition\_energy})
\]

Smooth connectivity of stopping power parameterization is desirable for precise range calculation.

SRIM2000 with 10 MeV cutoff was used in our previous study.
Range cut and step size dependence

- **Range cut** may be set by users according to expected simulation accuracy.
  - (Step limit can be set by users, but normally it is limited by geometry.)
  - The assurance of simulated result should be kept consistent within the accuracy.
- We observed a systematic variation of simulated range compared to the expected value from the production cut.
  - *The range of 200 MeV proton becomes about 3 mm longer than NIST prediction by applying a looser production cut.*

![Graph showing survived proton probability vs. depth in water](image)

**Production Cut**

- 500um
- 100um
- 50um
- 10um
- 5um
- 3um
- 1um

We have to apply very tiny production cut in order to get reasonable result?
Range study(2): Range cut and Step limit optimization

- **Bulk Water (no geometrical slices)**
- **190 MeV proton**
- **Range cut dependence:** 0.015, 0.050, 0.1, 0.5, 1 mm
- **Step limit dependence:** 0.01, 0.015, 0.020, 0.040, 0.050, 0.100, 0.500, 1.0 mm

190 MeV proton
Proton Range in bulk water

Only 10um Step Limit reproduces NIST range. The range is independent to the production cut in this case.
Proton Range in bulk water

Simulated Range changes with the step limit size. Range becomes longest when step limit is around 100um.
Energy fluctuation: ElectronicLossFluctuation()

if( EnlossFlucFlag && 0.0 < eloss && finalT > MinKineticEnergy) {
    // now the electron loss with fluctuation
    eloss = ElectronicLossFluctuation(particle, couple, eloss, step);
    if(eloss < 0.0) eloss = 0.0;
    finalT = kineticEnergy - eloss - nloss;
}

Eloss by dE/dX Table

<table>
<thead>
<tr>
<th>Eloss dE/dX = 0.00417 MeV / 10um</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eloss dE/dX = 0.0417 MeV / 100um</td>
</tr>
<tr>
<td>Eloss dE/dX = 0.21 MeV / 500um</td>
</tr>
</tbody>
</table>

These values are typical for 225MeV proton

Mean value of these distributions are:
-7.163 (keV)/500um
-1.244(keV)/100um
-0.01013(keV)/10um

RangeCut=10mm

(Fluctuated Eloss) - ( Eloss by dE/dX ) [keV]
Range with or without Energy fluctuation

- G4hLowEnergyhIonisation
- 225 MeV proton in Water
- Range cut = 10 mm

Without energy fluctuation, LowEM hIoni. reproduces NIST range at the step size below 5 mm. Energy fluctuation obviously distorts energy deposition with the underestimation.
Low EM or Std EM

200 MeV proton

$\text{w/ MeanExcitationEnergy} = 75\text{eV (ICRU)}$

$\text{e-,e+,gamma} = 3\text{um}$

RED G4hIonisation
BLK G4hLowEnergyIonisation

w/o ChemicalFormula("H}_2\text{O")
NuclearStoppingOff
i.e. Bragg rule is applied

ICRU49 259.6mm

Low energy EM process gives consistent range with NIST PSTAR prediction

Standard EM process gives shorter range than NIST PSTAR prediction
Range with or without energy fluctuation

Std EM uses G4UniversalFluctuation
LowE EM uses G4hLowEnergyIonisation::ElectronicFluctuation()
Both calculation based on “Energy loss in thin layers in GEANT4”, NIM A362(1995)416-422. But the implementation is slightly different.

0.1keV-100TeV  120bin
=>0.1keV-1GeV 36000bins
Summary

• Source of problem and desired improvements
  – Importing stopping power function
    • Interconnectivity to the Bethe-Bloch formula
      – ~10% difference causes ~500um shift of range in water
        😱 Should Geant4 be capable to import user’s stopping power function? or Need to ensure non-stress way for interpolation
    – Energy fluctuation model
      • Calculation model does not stable at around 100 micron step size
        – Underestimation of energy loss makes the range longer
        😱 Need to fix the unstable behavior
      – dE/dX table resolution might be needed
        • The fine binning
          – It changes expected range about 1 mm
            🙄 Table binning should be adjustable for the application
Accuracy versus Execution time?

- **Geometry:** Sliced in 100um thickness
- **225MeV proton**
- **ProductionCut=1mm, StepLimit=Default**
  - Range 322.2mm
  - CPU 915.89s/10000ev
- **ProductionCut=1mm, StepLimit=10um**
  - Range 317.487mm
  - CPU 5609s/10000ev
- **ProductionCut=3um, StepLimit=Default**
  - Range 317.787mm
  - CPU 9921s/10000eV
Step Limits を 10μm にすると、ProductionCut 15μm と同じ意味になる。
Proton range in water

Range in Si

- Std NIST w/o Fluc
- Std NIST w/ Fluc

Step Limit (mm)

Range (mm)