Monte Carlo Radiation Transport Modeling: capabilities and examples

Lecture 8

Special Topics:
Device Modeling

Outline

- Overview of radiation transport packages (other than MCNP), with capabilities and examples
- New features in MCNP6
- Hands-on examples
  - Use of VisEd
  - Make simple changes to Example files

Introduction

- Modern Monte Carlo modeling approach was developed in late 1940's by Stanislav Ulam working on nuclear weapons projects at LANL
- Coincided with development of the first electronic computer ENIAC (Electronic Numerical Integrator And Computer)
- Several general-purpose and specialized radiation transport packages are available
- Most are free for the academic use

Some radiation transport packages

- The list is non-exhaustive
  - ETRAN (Berger, Seltzer; NIST 1978)
  - EGS4 (Nelson, Hirayama, Rogers; SLAC 1985) www.slac.stanford.edu/egs
  - EGS5 (Hirayama et al; KEK-SLAC 2005) rcwww.kek.jp/research/egs/egs5.html
  - ⚹ EGSnrc (Kawrakow and Rogers; NRCC 2000) www.irs.inms.nrc.ca/inms/irs/irs.html
  - ⚹ Penelope (Salvat et al; U. Barcelona 1999) www.nea.fr/lists/penelope.htm

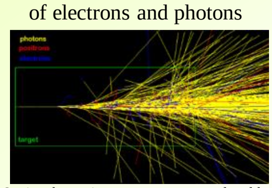
Some radiation transport packages

- The list is non-exhaustive
  - ⚹ Fluka (Ferrari et al; CERN-INFN 2005) www.fluka.org
  - Geant3 (Brun et al; CERN 1986) www.cern.ch
  - ⚹ Geant4 (Apostolakis et al; CERN++ 1999) geant4.web.cern.ch/geant4
  - MARS (James and Mokhov; FNAL) www-ap.fnal.gov/MARS
  - ⚹ MCNPX/MCNP5 (LANL 1990) mcnpx.lanl.gov

List by Michel Maire (Lapp/Annecy), Introduction to Monte Carlo radiation transport codes, 2016

Electron-Gamma Shower (EGS)

- The Electron-Gamma Shower (EGS) computer code system is a general purpose package for the Monte Carlo simulation of the coupled transport of electrons and photons



- Features an arbitrary geometry
- For particles with energies from a few keV up to several TeV

Massive shower in a tungsten target produced by a single 10GeV incident electron; image from http://rcwww.kek.jp/research/egs/egs4_source.html

Electron-Gamma Shower (EGS)

- The EGS4 code can be downloaded and used by any interested party for non-commercial purposes
- Disclaimer: the code is copyrighted by Stanford University and the Canadian government, either explicitly or implicitly
- National Research Council (NRC) contributes to the development and application of the Monte Carlo method in the modelling of radiation transport since the early 1980s

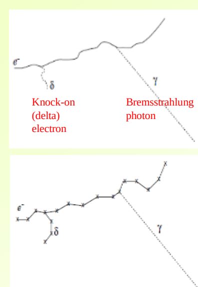
EGSnrc/BEAMnrc/DOSEXYZnrc

- EGSnrc is an extended version of the EGS4 code system developed jointly by NRC and the Stanford Linear Accelerator Center (SLAC) in the 1980s
- Includes a C++ geometry library for defining the geometry of complex simulation environments and particle sources (e.g., medical linacs)
  - The BEAMnrc/DOSXYZnrc component is an improved version of the original BEAM package developed by NRC and the Univ. of Wisconsin-Madison in the 1990s (DWO Rogers et al. BEAM: A Monte Carlo code to simulate radiotherapy treatment units. Med.Phys. 22, 1995).

BEAMnrc/DOSEXYZnrc

- Full set of photon interactions
- Electron transport is handled with condensed history approach, user can choose the step size
- Variance reduction techniques are available
- Tracking particle's history is available
- Result: a phase space file (psf) at a scoring plane; can be further processed with DOSEXYZ or other psf processing utility

Condensed history algorithm



- A complete electron history, where elastic scattering events that are below threshold energies for large energy-loss processes (shown here are the setting in motion of a knock-on electron, and creation of bremsstrahlung photon) are replaced with CSDA steps
- The step size depends on the algorithm
- Absorption of the primary and knock-on electrons at their track ends (based on cut-off energy)

BEAMnrc/DOSEXYZnrc

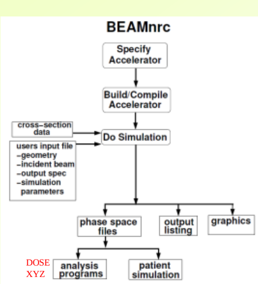
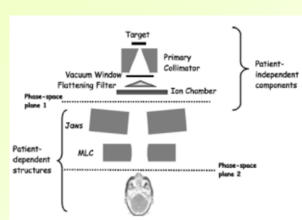


Figure 4: The steps involved in using the BEAMnrc system, from ref [3].

- Widely used for MC simulations of medical linacs
- User interface tailored to building accelerator head with components
- Parallelization capabilities
- Some limitations with respect to geometry

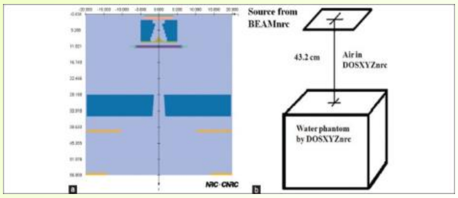
BEAMnrc/DOSEXYZnrc



Chetty *et al.*: AAPM Task Group Report No. 105: Monte Carlo-based treatment planning, Med. Phys. 34, 2007 , pp. 4818-4850

- Illustration of the components of a typical Varian linear accelerator treatment head in photon beam mode
- Phase space planes for simulating patient-dependent and patient-independent structures are also represented

BEAMnrc capabilities



- Modeling of the Siemens ONCOR linear accelerator in 6 MV and 18 MV beams was performed. The results of simulation were validated by measurements in water by ionization chamber and extended dose range (EDR2) film in solid water

K. Jabbari, H. S. Anvar, et al., J Med Signals Sens. 2013, 3(3): 172–179.

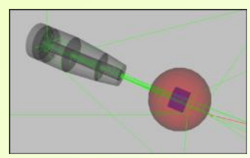
GEANT 4

- Geant 4 (GEometry ANd Tracking) is a toolkit for the simulation of the passage of particles through matter; it is general-purpose by nature
- Its areas of application include high energy, nuclear and accelerator physics, medical and space science
- Wide range of energies and scales: very high energies (Hadron collider) to very low energies (DNA-extension can simulate particle-matter interactions in liquid water and the chemistry initiated by water radiolysis; down to ~eV and nm)

GEANT 4

- The toolkit includes: user interfaces, built-in steering routines, and command interpreters which operate at every level of the simulation
- Geant4 is written in C++ and exploits object-oriented technology; Unix, MAC, Windows are supported (involves C++ compilation even under Windows)
- Pretty steep learning curve (for programming-inclined)
- Its development, maintenance and user support are taken care by the international Geant4 Collaboration (http://www.geant4.org/geant4/)

GEANT 4 examples



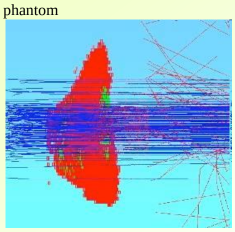
201 sources are replaced with 1 source and rotating phantom

Example from https://twiki.cern.ch/twiki/bin/view/Geant4/AdvancedExamplesGammaknife

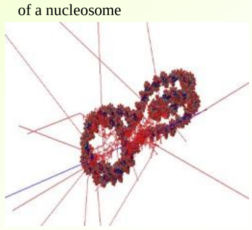
- The GAMMAKNIFE example simulates an advanced device for Stereotactic Radiosurgery (Leksell Gamma-Knife unit)
- ^{60}Co sources (1.25 MeV) arranged in a hemispherical shape, focusing on the isocenter, the collimation system with 4 to 18mm beam diameters
- Spherical water phantom (r=8 cm) simulating the phantom

GEANT4-DNA examples

Single cell irradiation by 3 MeV α-particles in a high resolution Cellular phantom



Direct DNA strand break estimation from a single 100 keV proton irradiation of a nucleosome



M.A. Bernala, M.C. Bordage, et al., Track structure modeling in liquid water: A review of the Geant4-DNA very low energy extension of the Geant4 Monte Carlo simulation toolkit, Physica Medica 31, 2015, pp 861–874.

PENELOPE

- PENELOPE is an acronym for "Penetration and ENErgy LOss of Positrons and Electrons"
- A general-purpose Monte Carlo simulation code developed at the University of Barcelona
- Distributed by the OECD/Nuclear Energy Agency Data Bank (Paris) and the RSICC (Oak Ridge).
- More than 1,000 copies distributed
- List server: http://www.oecd-nea.org/lists/penelope.html

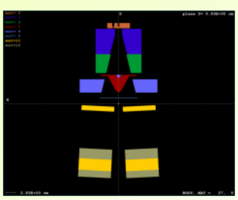
PENELOPE

- Main code features:
  - Realistic, well defined interaction models, energy range from 50 eV to 10^9 eV
  - Fast and accurate random sampling algorithms
  - Efficient tools for tracking particles through complex geometries (constructive quadric geometry)
- Complementary tools:
  - variance reduction
  - transport of electrons and positrons in electromagnetic fields
  - tabulation of macroscopic interaction parameters

PENELOPE

- Written in Fortran, i.e., they can be run on any operating system with a Fortran compiler
- The output is formatted for visualization with the plotting program gnuplot (Windows and Linux)
- Main applications:
  - Radiotherapy and Nuclear Medicine
  - Dosimetry and radiation metrology
  - Electron microscopy (SEM, electron-probe microanalysis)
  - Detector response, x-ray generators, ...

PENELOPE

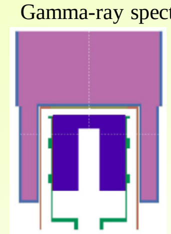


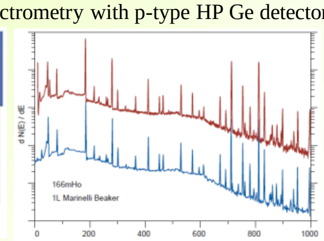
What you see is what is passed to the simulation program

Geometry viewers: 2- and 3-dimensional

PENELOPE examples

Gamma-ray spectrometry with p-type HP Ge detector

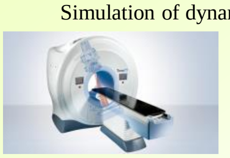




p-type HP Ge detector, Marinelli beaker (García-Toraño, *NIMA*, 2005)
^{166m}Ho (Holmium) is a betta-emitter, decaying to ^{166}Er (Erbium) with the subsequent emission of about 20 strong and well distributed gamma-rays over the energy range 50-1000 keV

PENELOPE examples

Simulation of dynamic jaws tomotherapy



Monte Carlo-based simulation of dynamic jaws tomotherapy, E. Sterpin1, Y. Chen, Q. Chen, W. Lu, T. R. Mackie, and S. Vynckier, Med. Phys. **38**, 5230 (2011)

- MC model called TomoPen, based on PENELOPE code, previously validated for the original TomoTherapy system
- Devised a comprehensive and efficient MC-based model for dynamic jaws-dynamic couch TomoTherapy treatments
- Calculation efficiency was ~8h for one plan

FLUKA

- FLUKA is a multi-purpose Monte Carlo code which can transport a variety of particles over a wide energy range in complex geometries
- The code is a joint project of INFN (National Institute for Nuclear Physics of Italy) and CERN
- Applications in many fields of physics such as high energy experimental physics (up to TeV), engineering shielding, detector and telescope design, cosmic ray studies, dosimetry, medical physics and radiation therapy

FLUKA

- FLUKA evolved from a code specialized in high energy accelerators and shielding, into a multipurpose multi-particle code successfully applied in a very wide range of fields and energies
- Types of particles transported 63 (including elementary particles like muons, (anti)neutrinos, hyperons), plus all kinds of heavy ions
- Particle decays are modeled
- Transport in magnetic fields is well-handled

FLUKA examples

FLUKA Monte Carlo simulation for the Leksell Gamma Knife Perfexion radiosurgery system: Homogeneous media, G. Battistoni, F. Cappucci, et al., Physica Medica, 2013, 29, pp. 656-661.

- Simulations and measurements have been performed in the simplest situation of 192 collimators opened and for a homogeneous water equivalent phantom
- FLUKA model was successfully validated; treatment planning is the next step

New features of MCNP6

- A new feature of the particle transport code MCNP6 is the ability to transport photons and electrons to the new lower limits for energy cutoffs: to 1 eV for photons and 10 eV for electrons
- Numerous tally enhancements
- Explicit tracking of all charged particles in magnetic fields
- Multiple additional specialized features

New features of MCNP6

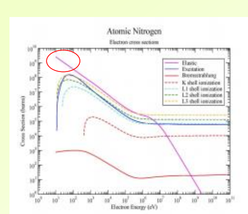
- Three aspects of the new capability:
  - extension of photon transport to lower energies
  - enhancement of the atomic relaxation processes treatment
  - introduction of a single-event electron transport method at lower energies
- All three of these features require new data, based on release 8 of ENDF/B VI (new library eprdata12, meaning Electron-Photon-Relaxation DATA, new format works only in v.6)

Condensed history algorithm

- Electron transport
  - By default MCNP6 continues to transport electrons by the condensed-history algorithms down to 1 keV, and switches to the new single-event method below that energy.
  - User control through optional 15-th entry on the physics card:

phys:e 100. 13j 0.01 $ switch to single-event at 10 keV

New features of MCNP6



ENDF/B VI.8 electron cross sections for atomic nitrogen, showing elastic, excitation, bremsstrahlung, and ionization by individual shells

- Single-event transport switch should never be <1 keV since condensed-history methods may rapidly collapse: at E just above 10 eV the electron can no longer lose energy and only experiences a large number of elastic scatterings
- There is not yet a fatal error for this attempt, but there will be in future versions of the code

Summary

- Several general-purpose and specialized Monte Carlo radiation transport packages are available
- Most are free for the academic use
- Some have very steep learning curve
- The trends are towards:
  - – Conversion to "general-purpose" packages
  - – Expanding low-energy limit

References

- Fundamentals of the Monte Carlo method for neutral and charged particle transport, Alex F Bielajew, 2000
- BEAMnrc Users Manual, D.W.O. Rogers, B. Walters, I. Kawrakow, NRCC Report PIRS-0509(A)revL, 2016
- http://www.geant4.org/
- F. Salvat, J. M. Fernández-Varea, J. Sempau, PENELOPE. A code system for Monte Carlo simulation of electron and photon transport
- http://www.fluka.org/
- H. Grady Hughes, Quick-Start Guide to Low-Energy Photon/Electron Transport in MCNP6, MCNP6 User Notes LA–UR–12–21068, 2013-04-29 (Rev.3)
- Other references are given within slides