Monte Carlo Radiation Transport Modeling Overview (MCNP5/6)

Lecture 7

Special Topics:
Device Modeling

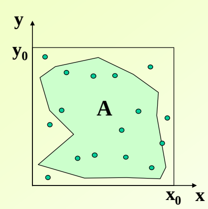
Outline

- Principles of Monte Carlo modeling
- Radiation transport modeling with MCNP5/6
- Utilizing Visual Editor (VisEd) application
- Hands-on examples: energy deposition in a water phantom

Monte Carlo technique: Introduction

- Need to solve a complex mathematical problem, describing physical system
- Two types of computational algorithms: stochastic and deterministic
- With Monte Carlo find physical parameters using statistical sampling
- With deterministic approach solve equations using numerical methods

Monte Carlo technique: Example



Area A~*N*

Find the area of an irregularly-shaped object:

- Define an enveloping rectangle with sides x_0, y_0 and area $A_0 = x_0 * y_0$
- Generate N_0 **random** points with coordinates $(x, y) < (x_0, y_0)$ and count N_{inside} - points falling inside the object
- $A = A_0 * (N_{inside}/N_0)$
- N_0 defines the accuracy

Monte Carlo method

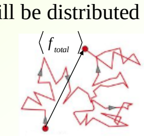
- The MC method is a stochastic method for numerical integration
- According to the Central Limit Theorem, for N random contributions f_i, the integral $f = \sum_{i=1}^{N} f_i$ will obey the Gaussian distribution

$$p(\langle f \rangle) = \frac{\exp[-(\langle f \rangle - f)^2 / 2\sigma^2]}{\sqrt{2\pi}\,\sigma}$$

- Where $\langle f \rangle$ is the sum of all f_i averages, and the dispersion σ is the sum of all dispersions

Monte Carlo method

- Example: in Brownian movement the final displacement of a particle is a sum of random elementary displacements
- After a large number of such displacements over time *t* the final displacement will be distributed by Gaussian distribution
- Can calculate the average and dispersion



$$\langle f \rangle = 0, \quad \langle f^2 \rangle = Dt$$

Monte Carlo radiation transport: Components

- A random number generator
- Methods for sampling random quantities from a probability density function (pdf)
  - Pdf of a continuous random variable describes the relative likelihood for this variable to take on a given value
- Bookkeeping (accumulating the results)
- Geometry description
- Physics input: total and differential cross sections
- Several packages are available, MCNP is one of the most versatile

Radiation transport with MCNP5/6

- MCNP is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport
- Specific areas of application include, but are not limited to, radiation protection and dosimetry, radiation shielding, radiography, medical physics, nuclear criticality safety, detector design and analysis, nuclear oil well logging, accelerator target design, fission and fusion reactor design, decontamination and decommissioning

Radiation transport with MCNP5/6

- The code treats an arbitrary 3D configuration of materials in geometric cells bounded by 1st- and 2nd-degree surfaces and 4th-degree elliptical tori
- Versatile and easy to use source definitions: general source, criticality source, and surface source
- A rich collection of variance reduction techniques; a flexible tally structure
- An extensive collection of cross-section data

Radiation transport with MCNP5/6

- For *photons*, the code accounts for incoherent and coherent scattering, the possibility of fluorescent emission after photoelectric absorption, absorption in pair production with local emission of annihilation radiation, and bremsstrahlung.
- A continuous-slowing-down model is used for *electron* transport that includes positrons, k x-rays, and bremsstrahlung (does not include external or self-induced fields)
- Magnetic field is added to MCNP6

Radiation transport with MCNP5/6

- Has capabilities of both geometry and output tally plotting, but is standard only under UNIX through X-windows
  - Can be configured for Windows as well, but most use VisEd
- MCNP can be configured in a multiprocessing mode on a cluster of workstations with PVM or MPI software

MCNP help/references

- Concise (45 pages – compare to ~800 pages User Manual for MCNP6, or III-volumes help for MCNP5) MCNP Primer is available at http://www.mne.ksu.edu/~jks/MCNPprmr.pdf
- Medical Physics Primer is a good alternative (Chapter 2 MCNP Quickstart), followed by 5 detailed examples
- MCNP5/6 User Manuals are useful as references, but not your first MCNP reading material

Radiation transport

- Start a particle (p, e, n) - a ‘history’ - with energy and position randomly assigned from the problem source range specification
- Transport the particle based on pre-defined set of interactions and their cross-sections, generating secondary particles, depositing energy, etc. until it leaves the problem or deposits all its energy through interactions
- Find coordinate, direction and energy of every particle after every interaction in the problem

Structure of MCNP input file

- Message Card
- – Blank Line
- File Title
- Cell Cards
- – Blank Line
- Surface Cards
- – Blank Line
- Data Cards
- – Blank Line

optional

Input deck

Structure of MCNP input file

- Card entry begins in first 5 columns
- Free field format
- Input line is max of 80 columns
- Upper or lower case can be used (no special characters, e.g., tab!!)
- Continuation: 5 blanks or & on previous card
- Comments: C in column 1 or $ anywhere after data

Structure of MCNP input file

- Typically use horizontal format
- Vertical format is sometimes convenient:
  - # on first card of block in columns 1-5
  - Card names put side by side, example of source spectrum entry:

```
# si1    sp1
  L      d
  1.117  1
  1.333  1
```

MCNP input file special syntax

- nR means repeat preceding entry n times
  - 2 4R is same as 2 2 2 2 2
- nI means insert n linearly interpolated values between entries
  - 1.5 3I 3.0 is same as 1.5 2.0 2.5 3.0
- xM multiplies the previous entry by x
  - 1 1 2M 2M 2M is same as 1 1 2 4 8
- nJ used to jump over entries with default values
  - DD1 0.1 1000 is same as DD1 J 1000

Principles of modeling with MCNP: geometry

- Geometry is specified by cells bounded by surfaces
- Each cell contains a material of a certain composition ID and density
- Cells are physical bodies of homogeneous material, i.e. constant cross section
- Cells can and sometimes have to be subdivided for variance reduction or defined for tallies (f4 type)
- Problem should always have “outside”

Geometry: surface cards

- Standard Surfaces designated by mnemonics
- Planes, cylinders and cones are infinite in extent (macrobodies)
- Surface sense:
  - **Above plane: + or positive sense**
  - **Below plane: - or negative sense**
  - **Inside cylinder or sphere: -**
  - **Outside cylinder or sphere: +**
- All dimensions are expressed in centimeters

Geometry: surface cards

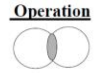
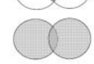
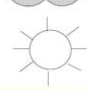
Mnemonic	Type	Description	Equation	Card Entires
P	Plane	General	$Ax + By + Cz - D = 0$	ABCD
PX		Normal to X-axis	$x - D = 0$	D
PY		Normal to Y-axis	$y - D = 0$	D
PZ		Normal to Z-axis	$z - D = 0$	D
SO	Sphere	Centered at Origin	$x^2 + y^2 + z^2 - R^2 = 0$	R
S		General	$(x-\bar{x})^2 + (y-\bar{y})^2 + (z-\bar{z})^2 - R^2 = 0$	$\bar{x}\ \bar{y}\ \bar{z}\ R$
SX		Centered on X-axis	$(x-\bar{x})^2 + y^2 + z^2 - R^2 = 0$	$\bar{x}\ R$
SY		Centered on Y-axis	$x^2 + (y-\bar{y})^2 + z^2 - R^2 = 0$	$\bar{y}\ R$
SZ		Centered on Z-axis	$y^2 + y^2 + (z-\bar{z})^2 - R^2 = 0$	$\bar{z}\ R$
C/X	Cylinder	Parallel to X-axis	$(y-\bar{y})^2 + (z-\bar{z})^2 - R^2 = 0$	$\bar{y}\ \bar{z}\ R$
C/Y		Parallel to Y-axis	$(x-\bar{x})^2 + (z-\bar{z})^2 - R^2 = 0$	$\bar{x}\ \bar{z}\ R$
C/Z		Parallel to Z-axis	$(x-\bar{x})^2 + (y-\bar{y})^2 - R^2 = 0$	$\bar{x}\ \bar{y}\ R$
CX		On X-axis	$y^2 + z^2 - R^2 = 0$	R
CY		On Y-axis	$x^2 + z^2 - R^2 = 0$	R
CZ		On Z-axis	$x^2 + y^2 - R^2 = 0$	R

Geometry: cells

- Cells are the basic geometry unit
- Volumes of space bounded by surfaces
- Sign (+ or -) defines the surface "sense" or side on which the cell space is located
- Boolean operators used to enclose the space
- All space needs to be defined; each region must be uniquely defined
- At least one cell must describe the problem exterior

Geometry: cells

- The surfaces are combined using three operators:

Name	Operation	Designator
Intersection		"blank" space between surface numbers
Union		colon (:) between surface numbers
Complement		# points outside of cell or surface

Geometry: cells

- Need to include importance on cell card or as a data block in order for transport to occur imp:n,p=1 on cell card
- imp:n 1 1 . . . 1 0 as a data block
- Need to have exterior cell with importance equal to 0 to terminate transport or defined the boundaries of the phase space

Data cards

- Source Definition
  - sdef
  - mode
  - nps
- Tally Definition
- Variance Reduction
- Material Specification
- Print and PRDMP

Order can be switched

Data cards: Materials

- Provides unique identification for each cross-section table ZZZAAA.nnX
  - ZZZ - atomic number
  - AAA - atomic weight
  - nn - evaluation identifier
  - X - class of data (continuous, photon, etc.)
- Examples: 92235.60C, 82000.02P

Mn ZAID1 fraction1 ZAID2 fraction2 …
  - fraction: positive = atom fraction of ZAID1
  - negative = weight fraction of ZAID1

Tallies

- MCNP5 provides several standard tallies for photons, neutrons, and electrons
- All tallies are normalized per starting source particles
- To use several tallies of a given type, add multiples of 10 to the tally number. For example, F2, F12, F22, F32, . . . are all type F2 tallies

Tallies

Tally Type		Fn: Units	*Fn: Units
F1:	Surface Current	#	MeV
F2:	Surface Fluence	#/cm²	MeV/cm²
F4:	Cell Fluence	#/cm²	MeV/cm²
F5:	Detector Fluence	#/cm²	MeV/cm²
F6:	Energy Deposition	MeV/gm	*jerks/gm
F7:	Fission Energy Deposition	MeV/gm	*jerks/gm
F8:	Pulse Height	pulses	MeV

* 1 jerk = 10^9 Joule   1 Btu = 1055.1 J

Tally modifiers greatly increase the amount of data obtainable from tallies. For example, can obtain spectral or directional distributions with En and Cn cards.

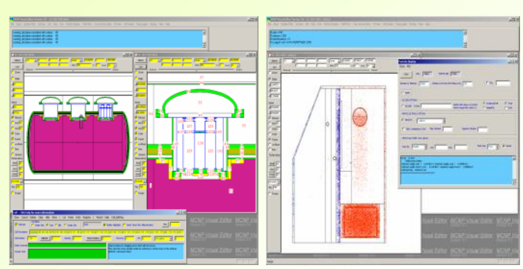
Visual Editor for MCNP

- Graphical User Interface for MCNP
- Display Geometries from input files with 2D views
- Create geometries: add surfaces, cells
  - Universes, fills, lattices
- Some support for data cards: materials, transformations, importances

Visual Editor for MCNP

- Plot particle tracks
  - Source generation points
  - Sites of collisions, surface crossing
- 3D plots–Normal, Radiograph, Transparent, dynamic
- Tally plots
- Cross Section plots

Visual Editor for MCNP



MCNP simulations of medical accelerator head

- Modeled full accelerator head assembly in order to adequately represent beam properties (photon energy spectrum, PDD, etc.)
- Added phantom and detector system to simulations
- Obtained dose distribution in the detector plane, monitoring number of particles crossing the plane
- Optimized the detector system configuration

MCNP simulation: parameter set

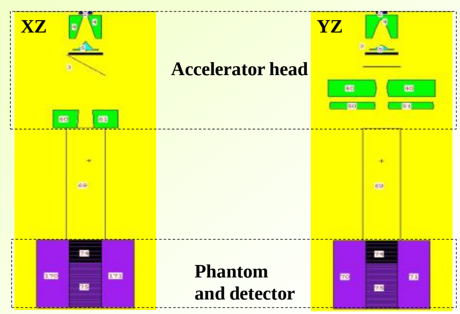
- Photon beams 6 MV and 10 MV
- High energy photons make negligible contribution to dose in CdTe due to its small thickness
- Important parameter – electron cut-off energy, has to be below 0.1 MeV
- Converter thickness optimization
- For image acquisition need to run ~10^8 histories to get error below 5%

Simulated accelerator head and water phantom

View of the Elekta linac upper head for 6 MeV X-ray beams and the water phantom

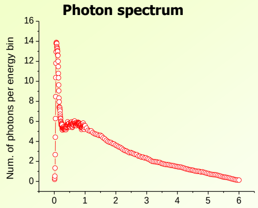
B. Juste, M.E. Mota, R. Miró, et al., CD-ROM, American Nuclear Society, LaGrange Park, IL (2007)

Simulated accelerator head and water phantom

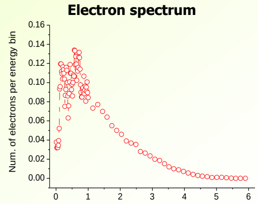


Beam properties: Spectra exiting water phantom

Photon spectrum

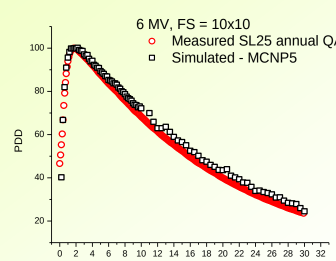


Electron spectrum



- 6 MV photon beam hardens after 20 cm thick water phantom
- Negligible electron contribution (additional air gap > 10 cm before detector)

Beam properties: PDD

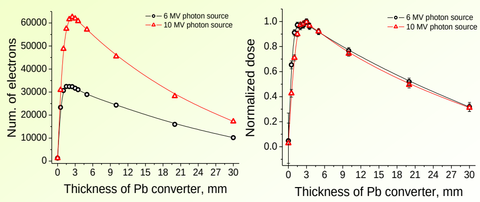


Need to adjust simulated beam properties to fully match measured PDD

Converter layer thickness optimization

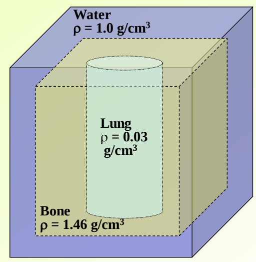
Number of electrons entering CdTe layer after converter

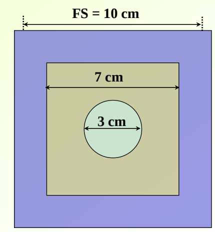
Dose deposited in CdTe layer



Dose in CdTe follows the number of electrons generated in converter layer

Imaging non-uniform phantom

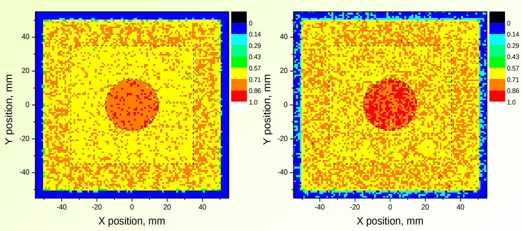




Cross-sectional view

CdTe detector image simulation: normalized dose, FS 10x10 cm

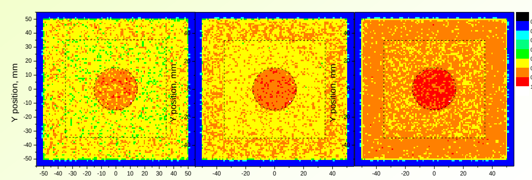
2 mm Pb converter on top **2 mm air on top**



CdTe thickness 500 μm, $4.2x10^7$ histories, Ecut=0.1 MeV, error ~6-7%
Converter image has better contrast, lower error

Image development with 2 mm Pb converter

1.7×10^7 histories mid error ~ 8 % **4.2×10^7 histories mid error ~ 5-6 %** **6.4×10^7 histories mid error ~ 4 %**



Summary

- MCNP is a powerful and versatile Radiation transport Monte Carlo package
- Arbitrary 3D geometry specification
- Multiple applications
- Export controlled software

References

- I. Kawrakow, The Monte Carlo Simulation of Radiation Transport, available at https://www.aapm.org/meetings/06ss/documents/kawrakow_MonteCarlo_color.pdf
- 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)
- H.G. Hughes, "Features of MCNP6 Relevant to Medical Radiation Physics", presentation at RPSD-2012, Nara, Japan, LA-UR-12-24401] (2012)
- http://www.mcnpvised.com/
- Additional references are provided within slides