LA-UR-

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LA-UR-05-2755

Using MCNP5 for Medical Physics Applications

Tim Goorley, X-5 Dick Olsher, HSR-4 Los Alamos National Laboratory



Schedule: 1 pm - 4:30 pm

1.	What can MCNP do?	TG – 15 min
2.	Overview of new MCNP5 features	TG – 30 min
3.	Geometries and Modeling	TG – 30 min
4.	Break	15 min
5.	Sources	DO – 45 min
6.	Tallies	DO – 45 min
7.	Misc (n scattering, VR, Benchmark)	TG – 30 min
0	Additional Defense and	

8. Additional References



Abstract

MCNP is a general-purpose <u>Monte</u> <u>Carlo</u> <u>N-Particle</u> code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport. MCNP5 has a wide range of abilities which make it useful for medical physics calculations. These abilities span its geometry representation, physics models, and source, tally and variance reduction capabilities. This workshop will demonstrate how MCNP5 can be used to calculate dose, simulate a radiograph, or even use CT data to create a voxel model of a human or phantom. A general review of MCNP5 source and tally capabilities, as well as new and future capabilities will also be included.



- Mesh Tallies
- Radiography Tallies
- Photon Doppler Broadening
- More Detectors & Tallies
- >2.1 Billion Histories & RAND #
- Lattice Tally Enhancements
- Mesh Tally Improvements (RSICC_1.40)
- Electron Improvements (RSICC_1.40)
- Stochastic Geometry (RSICC_1.40)
- Large Lattice Improvements
- FUTURE WORK for MCNP5 Teaser

- 1st Release
- 1st Release
- 1st Release
- 2nd Release
- 3rd Release
- 3rd Release



Mesh Tallies

- Original release in MCNP5_RSICC_1.14
- Geometry independent 3-D tally grid used to calculate volume averaged fluxes for each voxel in that grid.
- Cylindrical or rectangular mesh.
- Can be used with DE DF and FM cards to calculate volume averaged doses and reaction rates.
- Can be used with TR cards (transformation).
- Particles must track through mesh to tally.



Mesh Tallies

 Built-in MCNP5 plotter now plots mesh tally grid superimposed over geometry





Mesh Tally – Card Format

FMESHn:p create a mesh track-length tally where n is the tally number. Can be used with DEn, DFn, and FMn cards.

Caution: It is easy to create huge mesh tallies that can overflow computer memory.

Keywords GEOM{xyz} ORIGIN{0,0,0} AXS{0,0,1} VEC{1,0,0} IMESH IINTS{1} JMESH JINTS{1} KMESH KINTS{1} EMESH EINTS{1} FACTOR{1.} OUT(col} TR

GEOM = mesh geometry: Cartesian ("xyz" or "rec") or cylindrical ("rzt" or "cyl") ORIGIN = x,y,z coordinates in MCNP cell geometry superimposed mesh origin AXS = direction vector of the cylindrical mesh axis VEC = direction vector, along with AXS that defines the plane for angle theta=0 IMESH = coarse mesh locations in x (rectangular) or r (cylindrical) direction IINTS = number of fine meshes within corresponding coarse meshes JMESH = coarse mesh locations in y (rectangular) or z (cylindrical) direction JINTS = number of fine meshes within corresponding coarse meshes KMESH = coarse mesh locations in z (rectangular) or theta (cylindrical) direction KINTS = number of fine meshes within corresponding coarse meshes EMESH = values of coarse meshes in energy EINTS = number of fine meshes within corresponding coarse energy meshes FACTOR = multiplicative factor for each mesh TR = transformation number to be applied to the tally mesh HINT: MCNP5 Manual Index – FMESH Card, Mesh Tally,

WARNING: MESH refers to weight windows mesh, used for variance reduction, not tally mesh.



Radiography Tallies

- Introduced in MCNP5_RSICC_1.14. Allows the user to generate images from neutral particles as one would expect from an x-ray or pinhole projections.
- FIR Flux image radiograph
- FIP Flux image pinhole
- FIC Flux image cylinder
- Distinguish between scattered and unscattered flux
- Uses point detector methods.



Radiography Tallies

Radiograph of Anthropomorphic MCAT phantom





Lambeth, Melissa. "Development of a computerized anthropomorphic phantom for determination of organ dose from diagnostic radiology." Thesis, B.S., Massachusetts Institute of Technology, Dept. of Nuclear Engineering, 1997.

Picture from Sabrina

Picture generated with results from MCNP calculation.

Simulated Radiograph

1 M pixels



Radiography Tally – Card Format

- General card format for FIR tally:
 - FIRn:p X1 Y1 Z1 R0 X2 Y2 Z2 F1 F2 F3
- NOTRN: Run only direct contribution to all point detector tallies
- TALNP: Eliminate tally prints with many bins from OUTP file
- NPS: 2nd entry controls the direct contribution for FIR tallies
- FSn and Cn cards control number of pixels in image plane
- Example for simulation of medical radiograph: fir5:p 0 0 15. 0 0 0 -1000. 0 1e20 0 fs5 -55.0 999i 50.0 c5 -30.0 999i 30.0

notrn

talnp

HINT: MCNP5 Manual Index – Radiography Tallies, Pinhole, Flux Image Radiographs HINT: Use with NOTRN card for faster calculations if scattered contributions are not needed.



Photon Doppler Broadening

- Released in MCNP5_RSICC_1.14
- Incoherent Compton event, includes electron binding energy.
- Causes reduction of the photon's total scattering xs in the foreward direction.
- Causes broadening of photons energy spectrum.
- Important $E_p < 1$ MeV.
- Bug fix in MCNP5_RSICC_1.40 release





Doppler - Card Format

- By default, this option is on.
- Photon Doppler broadening will be used if appropriate data (xs library - #000.04p) is available. If xs library not available, comment is issued: "#000.0#p lacks Compton profile data for photon energy broadening"
- To turn off, set 4th entry of phys:p to 1.



More Detectors & Tallies

- With release of MCNP5_RSICC_1.20
- Maximum # of detectors increased from 20 to 100.
- Maximum # of tallies increased from 100 to 1000.
- Limit for a specific tally type still 100



>2.1 Billion Histories

- With MCNP5_RSICC_1.30, more than 2.1 billion histories can be run (<1E20)
- Done by explicitly declaring ~30 variables as 8 byte integers.
- Supported Cards: NPS, PRDMP, RAND, PTRAC, MPLOT
- Large PTRAC files also supported (250+ Gigabytes)
- Larger random # stride (not default): RAND card
 - Prevent re-use of random numbers

- Old Period : ~10¹⁴ New Period: ~10¹⁹ HINT: MCNP5 Manual Index - NPS card, other card entries.

WARNING: # of histories does not correlate to simulated source strength!



Lattice Tally Speed Enhancement

- With release of MCNP5_RSICC_1.30, if certain conditions are meet, then runtimes can be significantly reduced (5-500 times shorter, depending on problem).
- Stringent Conditions: F4, DE DF, 1st level lattice.
- MCNP will attempt to determine if these conditions have been meet or not, and will attempt to use the enhancement if appropriate. Messages either way. Fast and slow runs will track.
- Card: SPDTL



SPDTL – Card Format

- In data card section: spdtl <force or off>
- "spdtl force" will cause the lattice tally enhancements to be used if at all appropriate.
- "spdtl off" will enforce the older (slower) tally routines.
- MCNP5 will automatically check for nearly all conflicts and respond.
- Documentation LA-UR-04-3400 provided with MCNP5 distribution



MCNP5 Mesh Tally Plotting

•Built-in plotter now plots mesh tally results on top of geometry outline

~Summer 2005

Proton Storage Ring at LANSCE accelerator

Dose rate calculation for cable penetrations

Images from MCNP5 plotter









MCNP5 Mesh Tally Plotting

Use SF (Surface Flag) and CF (Cell Flag) cards as for a regular tally, except: ~Summer 2005

- Only one tally (the flagged tally) is produced
- Negative cell or surface values interpreted as "anti-flag". Scores only those particles that do not cross the surface or leave the cell





MCNP5 Mesh Tally Plotting

~Summer 2005

By using a very fine mesh, particle tracks from individual histories can be plotted. 2000 x 1100 x 1 mesh





Diagnostics

Applications

Group (X-5)

Los Alamos

Health Physics

Measurements

(HSR-4)



Radiographs of VIPMan model,1x1x1 mm voxels (above),2x2x2 mm voxels (right)Images from MCNP5 plotter

http://www.rpi.edu/dept/radsafe/public_html/home.htm



~Summer 2005

Electron Improvements

- Positron Source
- For condensed-history electron transport, tables of Landau parameters were precomputed for a fixed stepsize
- This could introduce errors for geometry with spacings less than the assumed Landau step-size
- Computing the Landau parameters on-the-fly for the current step-size & geometric distance eliminates these problems



Hughes M&C 2005 Conference Paper



Stochastic Geometry

- On-the-fly random translations of embedded universes in lattice
- Developed for pebble bed reactors.
- Potential for medical physics applications?
 - Alveoli
 - Sinuses
 - Bone marrow

Fuel kernel displaced randomly within lattice element each time that particle enters

Monte Carlo 2005 Plenary talk by Forrest Brown, Wed am "Monte Carlo Methods & MCNP Code Development"

~Summer 2005



Image of the stochastic geometry of fuel kernels from MCNP5 plotter



Large Lattice Improvements

- Increase limit on number of voxels from ~20 Million to ~200+ Million.
- Reduce startup times from hours or days to a few hours.
- Windows OS limit of 2 Gigabytes of Memory per program. (Use 64 bit chip & OS)



Goorley, Tu 10:50 am, "Issues Related to the use of MCNP code for an Extremely Large Voxel Model VIP-MAN"



FUTURE WORK for MCNP5 Teaser

- Proton transport
 - Continuous-energy physics up to 50 GeV
 - Direct tracking through magnetic fields
 - COSY-map tracking through magnetic fields
- Many additional particle types
- ENDF/B-VII (Data Team)
- Improved electron transport
- Automated variance reduction, using deterministic adjoint
- Continuously varying tallies

Monte Carlo 2005 Plenary talk by Forrest Brown, Wed am **"Monte Carlo Methods & MCNP Code Development"**



Diagnostics Applications Group (X-5) Health Physics Measurements (HSR-4)



Geometries & Modeling





	2	
-	Los Alamos	
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Diagnostics Health Physics Applications Measurements Group (X-5) (HSR-4)

Geometries and Modeling

- Analytical Phantoms

 MIRD Phantoms
- Voxel Phantoms

 CT based Geometries
- Phantom Database
 - Set of MIRD and CT based Phantoms
 Distributed with MCNP5_RSICC_1.40



Images of Snyder Head Phantom from MCNP5 plotter.



Analytical Models

- Conversion of equations into input deck, usually by hand. (sometimes tedious)
- MCNP Cells correspond to specific organs
 - Easy to tally
 - Easy to define materials (ICRU 46)
- Calculate (flux/dose/reaction rate) distribution within organ with mesh tally or other user-defined surfaces
- Usually requires little memory

Geometries & Modeling



Analytical Models

Geometry plots from

Observe differences

MCNP5 plotter



in organs and materials.



Yanch - MIT



- Obtain CT image data
 - Can be patient specific
 - CTs preserve distances and volumes (better than MRI)
 - Can take CT of experimental phantom to compare calculations to experiments
 - Possible use of CT contrast agent



- Image manipulation
 - Remove artifacts from CT(dental fillings, for example)
- Align multiple data set with fiducial markers

Images from NIH Image, Data from Beth Israel Deaconess Medical Center









- Image conversion from DICOM or other medical format into MCNP input.
 - Reduction in # of voxels and increase voxel size.
 - Homogenization of small voxels into large voxels.
 - Threshold Hounsfield # (12 bit) to correspond to materials (air, tissue, bone – or more complex)
 - Manually define certain regions (outline tumor and fill it with different material, for example).
- Uses the MCNP lattice feature
 - Each different material corresponds to different filling universes and at a lower level, different cells. If possible, different organs have different materials.
 - Example on following page.

Memory Test of large lattices in MCNP5. 1K * 1	1K * 20 = 20,000,000 = 20M voxels.			
1000 0 -11 10 -21 20 -31 30				
lat=1 fill= 0: 999 0: 999 0: 19	fill=i1:i2 j1:j2 k1:k2, change k1,k2			
56 50 19999998r	\$ 56 Xr, change X equal to (# voxels - 1)			
u=100 \$	3 lattice cell is universe 100			
56 156 -1.29300E-03 -70 u= 56	\$ Cell which fills each lattice voxel			
50 150 -1.29300E-03 -70 u= 50	\$ Cell which fills each lattice voxel			
1001 0 10 -12 20 -22 30 -32 fill=100 \$ "Window" Cell, looking into lattice				
1002 0 (-10: 12:-20: 22:-30: 32) -1000	\$ Outside window cell, inside bounding sphere			
1003 0 1000 \$	Exterior of problem, particles die here			
c BLANK LINE				
10 px -10.500000				
11 px -10.479000 \$ size to generate 1,000 lattice locations across x dimension				
12 px 10.500000				
20 py -10.500000				
21 py -10.479000 \$ size to generate 1,000 lattice locations across y dimension				
22 py 10.500000				
30 pz -12.500000				
31 pz -11.250000 \$ size to generate 20 lattice locations across z dimension				
32 pz 12.500000				
c Lattice entries = $1K * 1K * 20 = 20,000,000 = 20M$ voxels.				
1000 so 10.0E+01				
70 so 5.0E+01				
c BLANK LINE				
mode n p				
imp:n 1 3r 0				
imp:p 1 3r 0				
m156 7014 -0.77780 8016 -0.22220 \$ Air				
m150 1001 2 8016 1 \$Water				





- Tally in regions of interest
 - Tally over entire lattice (use of lattice speed tally capability possible)
 - Tally over cells (i.e. organs) of interest.
 - Use Mesh Tally to overlay geometry.
- Possibly use post-processor to visualize isodose contours.

Image from clinical trials using NCTPlan (Harvard-MIT & CNEA)





- Can easily consume Gigabytes of memory
- Large input decks, difficult to modify
- Limit in MCNP5_RSICC_1.30 to ~20 million voxels (lattice locations)
- Many users have created their own patches to speed up large voxel model calculations. (ORANGE, Speed Tally Patch)
 - Monte Carlo 2005 Talk Tues 4:45 Fast Monte Carlo Dose Calculations For All Particles: ORANGE By Steven Van Der Marck
- Users are welcome to submit their patches for review and potential inclusion into MCNP.

Geometries & Modeling

Conversion Programs

- Currently available to the public: ۲
 - NCTPlan: Neutron Capture Therapy Plan. By Harvard-MIT & CNEA, Argentina (free – wskiger@mit.edu)*
 - Scan2MCNP: by White Rock Science (commercial website)
- Not ready for public release (but soon)
 - MiMMC: MultiModal Monte Carlo Treatment Planning System. By Harvard/Beth Israel Deaconess Medical Center.
 - MCNPTV: MCNP Therapy Verification. By Mark Wyatt (University of TN)
 - JCDS: JAERI Computational Dosimetry System.*
 - ImageJ & OEDIPE, by IRNS, France (irns.org)
- Not for public release?
 - In-house versions at Ohio State, RPI.
 - THORPlan: By TsingHua University in Taiwan.
 - * Indicates use in human clinical trial irradiations.








Zubal Phantom

- Voxel Phantom of Head
- 85 x 109 x 120 voxels
- 2.2 x 2.2 x 1.4 mm³
- 25 Brain structure tallies
- 15 materials
- Jeff Evans, Ohio State



Image from MCNP5 plotter



VIP Man

- Whole Body Phantom
- Based on NIH VIP-Man Project
- 6, 100, 300 Million Voxel Models
- 1 or 4 mm³
- Available from Prof. Xu of RPI – not in MP database



http://www.rpi.edu/dept/radsafe/public_html/home.htm

Image from MCNP5 plotter



Voxel Model Talks at Monte Carlo 2005

papers available on conference CDROM

- Mon, 1:15 GSF Male And Female Adult Voxel Models Representing ICRP Reference Man By Keith Eckerman
- Mon, 1:45 Effective Dose Ratios For The Tomographic Max And Fax Phantoms By Richard Kramer
- Mon, 2:05 Reference Korean Human Models: Past, Present and Future By Choonsik Lee
- Mon, 2:25 The UF Family of Pediatric Tomographic Models By Wesley Bolch and Choonik Lee
- Mon, 2:45 Development And Anatomical Details Of Japanese Adult Male/ Female Voxel Models By Tomoaki Nagaoka
- Mon 3:25 Dose Calculation Using Japanese Voxel Phantoms For Diverse Exposures By Kimiaki Saito
- Mon 3:45 Stylized Versus Tomographic Models: An Experience On Anatomical Modeling At RPI By X. George Xu
- Mon 4:05 Use Of MCNP With Voxel-Based Image Data For Internal Dosimetry Applications By Michael Stabin
- Mon 4:45 Application Of Voxel Phantoms For Internal Dosimetry At IRSN Using A Dedicated Computational Tool By Isabelle Aubineay-Laniece
- Tues 10:45 Issues Related To The Use Of MCNP Code For An Extremely Large Voxel Model VIP-MAN By Tim Goorley
- Tue 2:40 Conversion Of Combinatorial Geometry To Voxel Based Geometry In Moritz By Kenneth Van Riper



MP Geometry Database

- A database of Medical Physics phantom input decks distributed with MCNP5.
- Analytical
 - Snyder Head, ORNL MIRD, MIT MIRD
- Voxel
 - Snyder Head, Water Cubes, Zubal Head
- Contributions Welcome!



Sources



Source Term Definition

- Powerful feature: allows specification of spatial extension, energy, direction, and particle type.
- Source extension need not coincide with the outline of an existing cell
- A large variety of sources may be defined by the user
 - point source
 - area source
 - volume source
 - multiple sources
- Biasing of one or more aspects of the source term is possible.

For example, some directions or energies may be sampled more frequently (but with reduced weight) to improve transport efficiency.



Source Term Definition

The SDEF card (together with si and sp cards) allows complete specification of the source term.

Syntax: sde	ef variable ₁	variable ₂	variable ₃	
si card:	information about t (bins, discrete valu	he variable es. distributio	on numbers)	
sp card:	probability of choosing a particular value (provide actual probability or use build-in function			

- starting particle type & weight
- source spatial extension & location
- energy spectrum
- starting angular distribution (isotropic is default for point

& volume sources)

Default: 14 MeV isotropic point source at position 0,0,0 with weight 1



Source Term Definition

(1)	explicit value:	erg = 2	monoenergetic source with energy	
			equal to 2 MeV	
(2)	distribution:	erg = d1	distribution "d1" is to be described by	
			si1 and sp1 cards	
(3)	function of another variable:			
	sdef	pos = d1	erg fpos d2	



Diagnostics Health Physics Applications Measurements Group (X-5) (HSR-4)

The source variable "par" is used to designate starting particle type:

- Par = 1 Neutron (default)
- Par = 2 Photon
- Par = 3 Electron

Note: Only one particle type may be started. However, one may start neutrons and electrons and tally for secondary photons.



SDEF Card:

Source Spatial Extension & Location

(1) **Point Source**

$$pos = x y z$$

(2) Line Source (uniform distribution)





(3) Rectangular Area Source (uniform spatial distribution)



sdef	x = d1		y = d2	z = 10
si1	h	0	10	
sp1	d	0	1	
si2	h	0	10	
sp2	d	0	1	



(4) Disc on a Plane Surface (uniform spatial distribution)



sdefsur = 5pos = x y zrad = d1si1h0rsp1-211

uniform sampling in circle with radius = r

Probability of picking radius:
$$P(r) = cr$$



(5) Spherical surface: Source on surface of a sphere

(uniform spatial distribution)





(6) Box Source (uniform volume distribution)







SDEF Card:

Diagnostics Health Physics

Measurements

(HSR-4)

Applications

Los Alamos

Source Spatial Extension & Location

(7) Cylindrical Source (uniform volume distribution)





(8) Cylindrical Shell Source (uniform spatial distribution)





(9) Spherical Volume Source (uniform volume source)



Probability of picking radius: $P(r) = cr^2$



(10) Spherical Shell Source









Note: Entries on the sp1 card do not need to be normalized. You could simply enter the respective photon emission rates, assuming P_1 , P_2 , and P_3 are photon sources.



SDEF Card: Multiple Rectangular Volume Sources

Box #1 = 10-cm cube	sdef	erg=0.662 z=fx=d7	x=d1	y=fx=d4
Box #2 = 5-cm x 5-cm x 10-cm	si1	s 2 3		
Å –	sp1	4 1		
\uparrow	si2	-10 0		
	sp2	0 1		
1	si3	05		
	sp3	0 1		
	ds4	s 5 6		
	si5	0 10		
Ý	sp5	0 1		
	si6	-5 0		
X 2	sp6	0 1		
	ds7	s 8 9		
	si8	0 10		
	sp8	0 1		
	si9	-10 0		
	sp9	0 1		



Arbitrary Volume Source



Specify a volume source (cartesian, spherical, or cylindrical) that completely contains a particular cell of arbitrary shape.

sdef pos = x y z rad = d1 cel = 6si1 $h \ 0 \ r$ defines spherical volume source

If the sampled point is found to be inside cell #6, it is accepted. Otherwise, it is rejected and another point is sampled.



Use source variable ERG

(1) Monoenergetic Sources

erg = 10 energy equals 10 MeV

(2) Discrete Spectrum

erg = d1 si1 L 0.5 1.0 2.0 c discrete energies of 0.5, 1.0, and 2.0 MeV sp1 d 0.25 0.25 0.5



(3) Histogram Distribution

erg = d1

si1 h 0.01 0.02 0.05 0.1 0.5

Histogram Distribution:

0.001 - 0.01 (or from Ec to 0.01) (1 keV = photon

0.01 - 0.02 energy cutoff)

0.02 - 0.05

0.05 - 0.1

0.1 - 0.5

Entries on the si card define the top of each bin in increasing order.

Two possible sp1 cards:

sp1 d 0 0.2 0.2 0.3 0.3 sp1 c 0 0.2 0.4 0.7 1.0 ↑ cumulative



(3) Histogram Distribution (cont.)

Can also use vertical format for data entry:



useful for pasting in energy spectra.



- (4) Built-in Function
 - erg d1
 - sp1 -2 a

This invokes one of the built-in functions for energy

(See Table 3.3, P. 3-50)

-2 a: Maxwell fission spectrum where a is the temperature in MeV.

The Cf-252 neutron fission spectrum can be described in the energy range from 100 keV to 10 MeV by such a spectrum with a temperature of 1.42 MeV (ISO 8529).

SDEF Card: Direction Specification

- (1) For point and volume sources, the default is an isotropic distribution.
- (2) The variable dir is used to specify direction and refers to μ , the cosine of the angle between a particle's line of flight and a reference vector VEC.
- (3) For a surface source, the default is a cosine distribution. However, it is possible to specify an isotropic distribution.

Consider a disc source on surface m:



sdefsur = mpos = x y zrad = d1si1h0rsp1-211

Health Physics

Measurements

(HSR-4)

Diagnostics

Default: $p(dir) = 2 \cdot \cos\theta$

Los Alamos **SDEF Card:** Direction Specification

To modify direction to isotropic:

(a) First define a reference vector (vec) for direction. All particle lines of flight will be referenced relative to vec. This is a unit vector with x, y, and z components:



Example 1: vec = 0 0 1 is a unit vector pointing along the positive z axis

Health Physics

Measurements (HSR-4)

Diagnostics

Applications

- Example 2: vec = 0.707 0.707 0 is a unit vector in x-y plane at 45-deg. from x and y axis
- Example 3: vec = 0.707 0.707 0.5 is a unit vector 60-deg. from z axis and 45-deg. from x and y axes

 $vec = cos\theta_x cos\theta_v cos\theta_z$

SDEF Card: Direction Specification

(b) Specify direction as a distribution (dir = d2) relative to vec:



 θ = polar angle

0 = azimuthal angle - sampleduniformly between 0 and 2π

Diagnostics

Applications

Los Alamos

Health Physics

Measurements

(HSR-4)

 $\mu = \cos\theta$ (range is from -1 to 1)

si2 h -1 0 1 sp2 d 0 0.5 0.5 \$ equal probability for each cosine cone

This specifies an isotropic directional distribution

SDEF Card: Direction Specification

In general, polar angle space can be specified using direction cosine cones:



si1 -1 cos
$$\theta$$
 1
sp1 0 $\frac{1 + \cos \theta}{2}$ $\frac{1 - \cos \theta}{2}$

The sp card specifies an isotropic distribution.

• Los Alamos Applications Measurements **SDEF Card:** Direction Specification

Health Physics

(HSR-4)

Diagnostics

Discrete Directions are Possible:

sdef sur = m pos = x y z rad = d1 vec = 0 0 1 dir = 1

This gives a monodirectional parallel beam along the + Z axis.

pos = x y z dir = 1 vec = 0 0 1sdef

mono-directional point source.



Tallies

- Calculating dose w/ different tallies
- Flux to Kerma factors (DE DF cards)
- Calculating reaction rates



MCNP Tallies

- Standard Fluence Tallies are:
 - F2 Fluence averaged across a surface (#/cm²)
 - F4 Fluence averaged across a cell (#/cm²)
 - *F2 Energy Fluence (MeV/cm²)
 - *F4 Energy Fluence (MeV/cm²)
- Easy to use: syntax f4:p 8 ← tally cell no.
 ↑
 particle type
- f14, f24, f34, ... are all type F4 tallies f12, f22, f32, ... are all type F2 tallies
- Multiple tallies are allowed
 Several tally types may be mixed in the input deck



Diagnostics Health Physics Applications Measurements Group (X-5) (HSR-4)

MCNP Tallies

- By virtue of the nature of the simulation, MCNP builds up a picture of the radiation field:
 - Position
 - direction
 - energy
 - weight
- MCNP is ideally suited to determine current or fluence quantities.
- Fluence (particles/cm²) is of paramount importance, because it can be converted into absorbed dose or dose equivalent if the differential distribution in energy is known.





Fluence Quantities

Fluence at a Point:



dL = sum of track lengths of all the particles traversing volume element dv

Track length definition is extended to surfaces and volumes in MCNP

Type F2 Tally: Surface (Planar) Fluence

Health Physics

Diagnostics



For each track:

Tally score =
$$\frac{W}{A|\cos\theta|} = \frac{W}{A|\mu|}$$

F2 = $\frac{1}{N} \sum \frac{W}{A|\mu|}$

For $|\mu| < 0.1$, MCNP sets $|\mu| = 0.05$

Los Alamos Group (X-5) (HSR-4) Type F4 Tally: Average Fluence in a Cell

MCNP uses track length (T_1) estimator for fluence averaged over a cell volume: $\phi = \sum \frac{T_L}{V}$



For each track: tally score

Health Physics

Applications Measurements

Diagnostics

$$4 = \frac{1}{N} \sum \frac{W T_L}{V}$$

where N = number of source particles

NOTE: Cell collisions are not necessary. A particle may cross the cell more than once during its history.


Type F2 & Type F4 Tally Relationship

In the limit, as the cell thickness (δ) goes to zero:



Diagnostics Los Alamos **Applications Measurements** Group (X-5) Point Detector Tally (Type F5)

Health Physics

(HSR-4)

A deterministic estimator of fluence at a point ۲

units: cm⁻²

Input card: •

f5:n x y z R_0

n = particle type

x y z = coordinates of tally point

 R_0 = radius of sphere of exclusion located around tally point

A necessity in situations where the analog random walk is inefficient ۲



- Silo restricts dose rate at point D to skyshine and groundshine
- We wish to calculate dose rate in a small volume element, V, around D
- F4 tally fails because V is poorly sampled by random walk



At every collision site, we will calculate the probability of a particle scattering toward and penetrating to point D. Three factors affect this probability:

- distance between collision and detector
- probability of scattering toward D, rather than in original direction
- material absorption between the collision site and D

We then multiply the track weight by this probability and place the result at point D as a score.

Point Detector Tally (Type f5)

Diagnostics Health Physics

Applications Measurements

Los Alamos

MCNP calculates the point detector contribution using the following equation:



where:

 $\mu = \cos\theta$

- $\lambda = \sum_{i} \mu_{i} x_{i}$ = total number of mean free paths (mfp) integrated over the trajectory from the source or collision point to the detector
- R = distance to detector from collision site or source creation event
- $p(\mu) =$ value of probability density function at μ , the cosine of the angle between the particle trajectory and the direction to the detector

For a point isotropic source in a void:



The contribution to a point detector for each source creation event

Point Detector Tally (Type f5)

Sphere of Exclusion

• For point detectors located in scattering media, collisions are possible very near the detector:

As $R \rightarrow 0$, $\phi \rightarrow$ infinity, variance \rightarrow infinity

The sphere of exclusion eliminates the 1/R² singularity of the point detector



For collisions within the sphere $(R < R_0)$, the detector contribution becomes a volume average:

Health Physics

Measurements

(HSR-4)

Diagnostics

Applications

$$\varphi = \frac{W p(\mu) (1 - e^{-\Sigma_t R_0})}{2/3 \pi R_0^3 \Sigma_t} ,$$

where Σ_t = total macroscopic cross section

Point Detector Tally (Type f5)

Diagnostics Health Physics Applications Measurements Group (X-5) (HSR-4)

<u>Caveats</u>

- Avoid use inside heavily scattering medium or very near a scattering surface. Use F2 or F4 type tallies instead
- It is permissible to locate a point detector in a lightly scattering medium such as air. But use an exclusion sphere with $R_0 \ge 50$ cm.
- Pay special attention to tally convergence:

Error may decrease $< \frac{1}{\sqrt{N}}$

– False convergence



- Early in transport, detector contributions are from source (uncollided flux) and collisions in 1st mfp. All of these scores are small and tightly bunched. Error appears to converge nicely.
- As more histories are followed, some photons reach deep in the shield and contribute very large scores. The variance jumps as does the standard error.
- The key is to adequately sample collisions deep in the shield.

Tally Normalization

Diagnostics Health Physics Applications Measurements

(HSR-4)

- All MCNP tallies (except in criticality problems) are normalized to one starting source particle.
- The user is responsible for scaling the tally to the desired source strength.
- Tally normalization is tied to how the source strength is defined:

- If the source strength for a given problem is specified in terms of photons/sec, normalize by multiplying the tally result by the actual photon emission rate - irrespective of whether the source is a point, area, or volume source.

- If, however, the source strength is specified as C particles per unit area or per unit volume, then the normalization must include the actual area of volume of the source.



Tally Normalization

<u>Example</u>: a tally for a volume source of 100 cm³ with an actual source strength of C photons/sec per cm³, would be normalized as follows:

(Tally result)(100 cm³)(C)

This is so, because the MCNP source strength is 1/V and the actual source strength is C photons/sec per cm^3.

<u>Source</u> <u>Type</u>	MCNP Source Strength	Desired Normalization	Normalization Factor
Point	1 particle	S particles/sec	S
Area	<u>1 particle</u> A	S particles/sec • cm ²	(A) (S)
Volume	<u>1 particle</u> V	S particles/sec • cm ³	(V) (S)

- A = source area in cm^2
- $V = source volume in cm^3$



Tally Modifier Cards

En $E_1 \ E_2 \ \dots \ E_k$ MeVTn $T_1 \ T_2 \ \dots \ T_k$ (shakes, 1 shake = 10^{-8} seconds)Cn $C_1 \ C_2 \ \dots \ C_k$ (-1 to 1)

n = tally number

 E_i , T_i , C_i = upper bound of the ith energy, time, or cosine bin in increasing magnitude.

A response function may be folded in with tally by specifying appropriate DE and DF cards.

 E_i = energy points (MeV)

 F_i = corresponding value of the dose function

A = LOG or LIN energy interpolation method (LOG is default)

B = LOG or LIN dose interpolation method (LOG is default)

FM Card (Tally Multiplier): $C \cdot \int \phi(E) R_m(E) dE$

FMn $(C_1 \ m_1 \ R_1) \ (C_2 \ m_2 \ R_2) \dots T$

- n = tally number
- C_i = multiplicative constant
- m_i = material number identified on an Mn card
- R_i = a combination of ENDF reaction numbers (a space = multiply and a colon = add)

Common R Values for Photons

- -1 incoherent scattering cross section
- -2 coherent scattering cross section
- -3 photoelectric cross section
- -4 pair production cross section
- -5 total cross section
- -6 photon heating number

Common R Values for Neutrons

Health Physics

Measurements

Diagnostics

- 1 = total cross section
- -2 = absorption
- -4 = heating (MeV/collision)
- -6 = fission cross section
- -8 = fission Q (MeV/fission)



Determination of Dose

- MCNP normally calculates absorbed dose on the basis of the KERMA approximation: Kinetic energy transferred to charged particles is assumed to be locally deposited.
- Conditions under which the KERMA approximation is valid:
 - Low-energy photons (secondary electrons have very short range)
 - Charged Particle Equilibrium (CPE) or at least transient CPE exists: range of primary radiation is >> than that of secondaries
 - Radiative losses in medium are negligible
- Under condition of CPE:

Absorbed Dose = KERMA Exposure in Roentgens = $\frac{\text{Dose (air)}}{0.876}$



Determination of Dose

Charged - Particle Equilibrium (CPE)

In practical situations, the conditions for CPE or transient CPE are not fulfilled in the following cases:

- In the vicinity of an interface between two different materials especially near an air - material boundary.
- Near the edges of a beam or in regions very close to a radiation source.
- Large change in photon spectrum with depth of penetration.
- High-energy photon beam incident on high-Z target.



- MCNP assumes that kinetic energy of electron-positron pair = E 1.022
- Actual KE = E 1.022 E_x where E_x = energy of bremsstrahlung photons radiated away.

Diagnostics Health Physics Applications Measurements Los Alamos (HSR-4)

Dose Calculation

Three basic approaches:

- Track Length Heating Method: F4/FM4 or type F6 Tallies (Kerma approximation) for a specified cell.
- (2) *F8 Tally: rigorous dosimetry for situations where Kerma approximation does not hold (only for photons and electrons).
- (3) Fold in Fluence to Dose Conversion Function using DE/DF cards.
 Valid for irradiation geometry implicit in conversion function – typically whole body irradiation.

Track Length Heating Method

Diagnostics Health Physics Applications Measurements

(HSR-4)

Group (X-5)

- H(E) = Average MeV per collision
- For photons: kinetic energy transferred to secondary electrons
- H(E) is part of cross section tables
- <u>Step 1:</u> Calculate collisions / gram in tally cell

$$\left(\frac{\text{atoms}}{\text{gram}} \right) \left(\sigma_{t} \text{ barns} \right) \left(\phi \text{ cm}^{-2} \right) \left(\begin{array}{c} 1 \text{ x } 10^{-24} \frac{\text{cm}^{2}}{\text{barn}} \right)$$

• <u>Step 2:</u> Calculate MeV/gram in tally cell

$$\left(\frac{\text{collisions}}{\text{gram}}\right) \quad \left(\begin{array}{c} H \frac{\text{MeV}}{\text{Collision}} \end{array} \right)$$

 <u>Step 3:</u> Convert to absorbed dose in rads Multiply Step 2 by: 1.602x10⁻⁸ rad/MeV/g



Track Length Heating Method

• Average dose per source photon: $D (rads) = \frac{C}{N} \sum_{i=1}^{N} \phi \sigma_t H$ where, $C = (1.6 \times 10^{-8}) (1 \times 10^{-24}) \left(\frac{N_a \eta}{M}\right)$

$$N_a = Avogadro's Constant = 6.022 \times 10^{23} \text{ mol}^{-1}$$

- η = number of atoms per molecule
- M = molar mass of material in grams
- ϕ = fluence score
- σ_t = total atomic cross section for energy of scoring track in barns
- H = Heating Number (MeV / Collision) at energy of scoring track



Health Physics

Measurements (HSR-4)

- The Tally Multiplier Card (FM) allows us to fold in the required cross section and heating number to obtain absorbed dose
- This method works in conjunction with F2, F4, and F5 fluence tallies.



Dose Calculations: Heating Tally (F6)



- Basic tally units are MeV/g. The energy deposition is for the material filling the tally cell.
- Works identically to f4/fm4 dose calculations. The code generates the proper tally multiplier card. The tally cell must be filled with material.
- The constant (1.602e-8) on the fm6 card converts MeV/g to rads.

Fluence to Dose Conversion Functions Fluence to Dose Conversion Functions

Health Physics

Measurements

(HSR-4)

• Use DE/DF cards to fold in an appropriate conversion function

Example:

С	ICRP 51, Table 11: Fluence to Air Dose Conversion		
С	Function, radcm ²		
de5	0.01 0.015 0.02 0.03 0.04 0.05 0.06 0.08 0.1 0.15 0.2		
	0.3 0.4 0.5 0.6 0.8 1 1.5 2 3 4 5 6 8 10		
df5	7.43e-10 3.12e-10 1.68e-10 0.721e-10 0.429e-10		
	0.323e-10 0.289e-10 0.307e-10 0.371e-10 0.599e-10		
	0.856e-10 1.38e-10 1.89e-10 2.38e-10 2.84e-10		
	3.69e-10 4.47e-10 6.12e-10 7.5e-10 9.87e-10		
	12e-10 13.9e-10 15.8e-10 19.5e-10 23.1e-10		

• Each fluence score is multiplied by a value of the conversion function corresponding to the energy of the scoring track:

 $(s cm^{-2}) (y rad cm^{2}) = sy rad$

where s = score

y = value of the conversion function

• This method may be used with any of the fluence tallies:



Fluence to Effective Dose Conversion Functions

- Typically based on Monte Carlo simulations using anthropomorphic phantoms
- Valid for a specific irradiation geometry: AP, PA, LAT, ROT, ISO
- Published ICRP functions are based on expanded and aligned field: do not apply for partial body irradiation
- Factors for partial body irradiation require calculations from first principles using anthropomorphic phantoms:
 - Voxelized human phantom
 - MIRD phantom: commercial version by White Rock Science



The *F8 Tally

Whenever CPE does not hold, absorbed dose may be calculated from first principles using the *F8 tally:





*F8 Tally: Mode Card Selection

• mode p e

Most rigorous: Both photons and electrons are transported.

Use when electron transport is important

- small tally cells
- high photon energies
- mode p

Only photons are transported. Electron energy is locally deposited. TTB is used by the code to generate secondary bremsstrahlung. Much faster than coupled electron - photon transport.



*F8 Type Tally: Physics

Negative Energy Score

 An artifact of the condensed-history electron transport model used by MCNP



- E₃ is the energy of the delta ray produced during the first substep in the tally cell
- The energy of the primary electron is not correlated with the energy of the delta ray
- If $E_3 > (\Delta_1 + \Delta_2 + \Delta_3)$ the energy balance is negative
- Only an issue in thin detector cells where a fraction of the delta rays produced during electron transport may escape



Misc

- $S(\alpha,\beta)$ neutron scattering treatment
- Simple Variance Reduction
- Benchmarking Studies
 - Computing Radiation Dosimetry CRD 2002, Sacavem, Portugal June 22-23 2002 (published by OECD)
 - QUADOS (EU intercomparison) Bologna, Italy July 14-16 2003 http://www.nea.fr/download/quados/quados.html

• What MCNP5 cannot do

- High-Energy Particles (muons, pions, etc..)
- Coincident Counting (lacks code and data)
- Photon Polarization
- Proton Transport (available with release of MCNP6)
- MCNP Help
- Obtaining MCNP



Neutron Scattering Treatment

• Accounts for **Fotal Hydrogen XS (barns)** 1 MeV molecular effects on target With $S(\alpha,\beta)$ nucleus velocity data for low energy (few eV) n scattering. 0.025 • Usually low Z, eV varies with 1 eVmolecule 10 - 1210. 100. 0.01 0.11. 10 - 910 - 80.001 Image from Neutron Energy MCNP5 plotter



Neutron Scattering Treatment

• Use can cause significant differences.

Goorley T, et. al. Med. Phys. 29 (2) 2002. pp. 145-156.





Variance Reduction

- Exchange user time for computational time
- Few hours of user time often reduces computational time by 10-1000
- Truncation methods truncates parts of phase space that do not contribute significantly
- Population control use particle splitting and Russian roulette to control # samples in phase sp
- Modified sampling alters statistical sampling of problem to increase # of tally contributions
- Partially deterministic methods circumvent part of the random walk process by using know expected values.



Simple Variance Reduction

- Implicit Capture
 - Reduces weight of particle by probability of capture
 - Automatically on
 - WC1 parameter on PHYS card
 - Population control technique
- Geometry Splitting
 - Cause splitting or Russian Roulette when changing to cell of different importance
 - Change with the IMP card
 - Population control technique.



Simple Variance Reduction

- Point Detectors
 - Covered in Tally section of this workshop
 - F5 tally type
- Source Biasing
 - Sample from a fictitious density function instead of the true density function. This distortion must be corrected for by altering the particle's weight.
 - SB card w/ SI SP cards
- Weight Cutoff
 - Kills particles whose weight falls below a certain limit
 - Automatically on
 - WC1 and WC2 parameters on CUT card



Verification & Validation

- Electron Benchmarks
- Computing Radiation Dosimetry CRD
- QUADOS Code Comparison



Electron Transport

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- Gierga, DP, Adams KJ, Electron/Photon Verification Calculations Using MCNP4B. Los Alamos National Laboratory, LA-13440, 1999.
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- Chibani, O, Li, XA, Monte Carlo calculations in homogeneous media and at interfaces: A comparison between GEPTS, EGSnrc, MCNP and measurements. Medical Phys, May 2002, vol 29 (5), p. 835-47.



QUADOS

- Quality Assurance of Computational Tools for Dosimetry
- Results presented June 14-16, 2004 Italy
- http://www.nea.fr/download/quados/quados.html
- 8 Case Studies, some had 10+ participants
- Used MCNP5 for 6 cases, most good agreement



QUADOS

- Brachytherapy 192 Ir γ , dose distribution in H2O
- Endovascular ${}^{32}P\beta$ -, dose in vessel wall
- Proton Therapy of Eye 50 MeV p, depth dose
- TLD-Albedo Response $n + \gamma$, 4 element TLD
- Phantom Backscatter X ray ISO beams, slab
- Environmental Scatter ²⁵²Cf n, concrete room
- HPGe Detector $-15 \text{ keV} 1 \text{ MeV} \gamma$, pulse height
- Consistency check device -241Am-Be, ³He detector


What MCNP5 Can't Do

- High-Energy Particles (muons, pions, etc.)
 - Will be available with MCNP6
- Proton Generation and Transport
 - Will be available with MCNP6
- Magnetic Field Tracking
 - Will be available with MCNP6
- Coincident Counting
 - lacks code and data
 - Monte Carlo 2005 Talk An Upgraded Multidetector Pulse Height Tally For MCNP By Andriy Berlizov
- Photon Polarization



Obtaining MCNP

- Can be obtained from RSICC (even if outside US)
 - http://www-rsicc.ornl.gov/
 - Two CDROM versions
 - Executables, Source and Full Manual limited release
 - Executables, no source, and Vol I & II of Manual broader release
- All CDROMs Contain
 - MCNP5 executables for Linux, Mac, Windows
 - the latest data (pre ENDF/B-VII)
 - MCNPVisual Editor
 - Test Suite to ensure proper installation and compatibility
 - MCNP5 Manual and other documentation



Help with MCNP

- Read the manual
- User forum: mcng
- X-5 (limited): mcnp@la
- MCNP home page:

mcnp-forum@lanl.gov mcnp@lanl.gov

- http://www-xdiv.lanl.gov/x5/MCNP/index.html
- RSICC e-notebook:
 - http://www-rsicc.ornl.gov/
 - Go to eNotebooks tab

References



Monte Carlo 2005 MCNP Talks

- Mon 10:50 am Ballroom E MCNP5 For Proton Radiography, H. Grady Hughes
- Tues 10:50 am Meeting Room 5 Issues Related To The Use Of MCNP Code For An Extremely Large Voxel Model VIP-MAN, Tim Goorley
- Tues 3:30 Meeting Room 4 Stochastic Geometry & HTGR Modeling with MCNP5, Forrest Brown, WR Martin, W Ji, J Conlin, JC Lee
- Wed 9:00 am Ballroom E Monte Carlo Methods & MCNP5 Code Development, Forrest Brown
- Wed 9:25 am Meeting Room 6 Analysis Of The Fourth Zeus Critical Experiment With MCNP5, Russell Mosteller
- Wed 10:50 am Meeting Room 5 Comparison Of Phantom Models For External Dosimetry Computations, Richard Olsher

References



2005 MCNP Classes

- X-5:
- June 14-17: Introduction to MCNP LANL
- June 27-July 1: Intermediate/Advanced Tokyo
- Aug 23-25: Advanced Variance Reduction LANL
- HSR-4:
- June 6-10: Practical MCNP for the Health Physicist, Medical Physicist, and Radiological Engineer -LANL



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